



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 07:59 am BST

PDB ID : 1RZI  
Title : Crystal structure of human anti-HIV-1 gp120-reactive antibody 47e fab  
Authors : Huang, C.C.; Venturi, M.; Majeed, S.; Moore, M.J.; Phogat, S.; Zhang, M.-Y.; Dimitrov, D.S.; Hendrickson, W.A.; Robinson, J.; Sodroski, J.; Wyatt, R.; Choe, H.; Farzan, M.; Kwong, P.D.  
Deposited on : 2003-12-24  
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

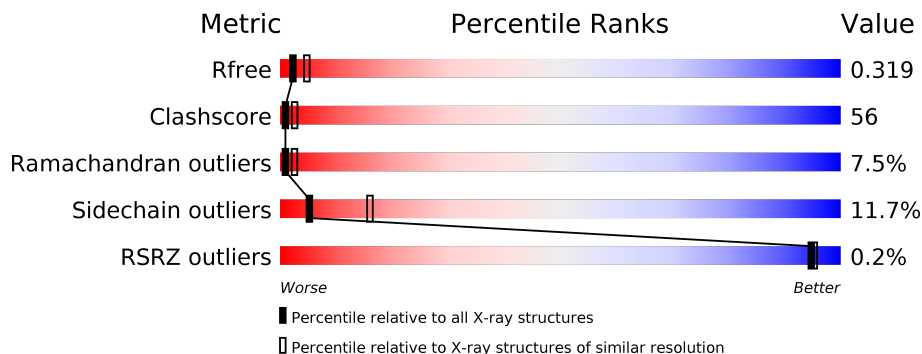
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





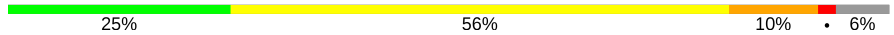
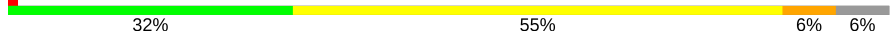
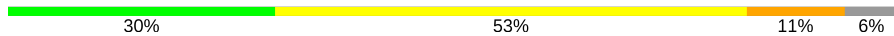
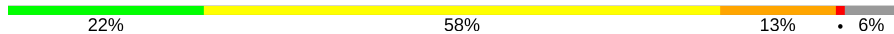
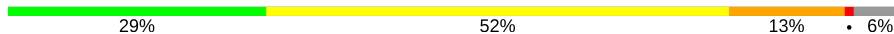
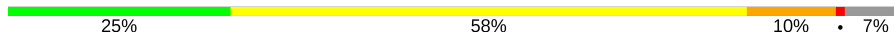
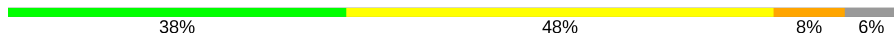
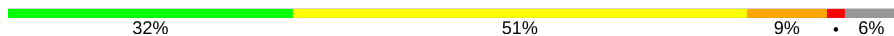
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	212	
1	C	212	
1	E	212	
1	G	212	
1	I	212	
1	K	212	

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Mol	Chain	Length	Quality of chain
1	M	212	
1	O	212	
2	B	230	
2	D	230	
2	F	230	
2	H	230	
2	J	230	
2	L	230	
2	N	230	
2	P	230	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25973 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Fab 47e light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	211	Total 1620	C 1012	N 272	O 331	S 5	0	0	0
1	C	212	Total 1628	C 1016	N 273	O 334	S 5	0	0	0
1	E	211	Total 1620	C 1012	N 272	O 331	S 5	0	0	0
1	G	211	Total 1620	C 1012	N 272	O 331	S 5	0	0	0
1	I	211	Total 1620	C 1012	N 272	O 331	S 5	0	0	0
1	K	211	Total 1620	C 1012	N 272	O 331	S 5	0	0	0
1	M	211	Total 1620	C 1012	N 272	O 331	S 5	0	0	0
1	O	211	Total 1620	C 1012	N 272	O 331	S 5	0	0	0

- Molecule 2 is a protein called Fab 47e heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	216	Total 1576	C 992	N 263	O 314	S 7	0	0	0
2	D	216	Total 1576	C 992	N 263	O 314	S 7	0	0	0
2	F	217	Total 1586	C 998	N 265	O 316	S 7	0	0	0
2	H	216	Total 1576	C 992	N 263	O 314	S 7	0	0	0
2	J	216	Total 1576	C 992	N 263	O 314	S 7	0	0	0
2	L	215	Total 1572	C 990	N 262	O 313	S 7	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	216	Total	C	N	O	S	0	0	0
			1576	992	263	314	7			
2	P	216	Total	C	N	O	S	0	0	0
			1576	992	263	314	7			

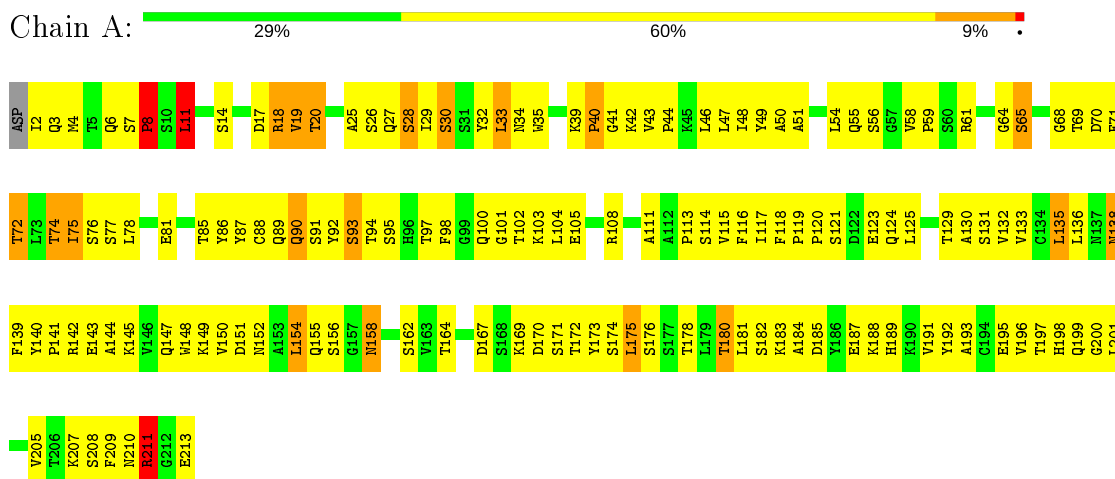
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	34	Total	O	0	0
			34	34		
3	B	29	Total	O	0	0
			29	29		
3	C	25	Total	O	0	0
			25	25		
3	D	27	Total	O	0	0
			27	27		
3	E	26	Total	O	0	0
			26	26		
3	F	18	Total	O	0	0
			18	18		
3	G	23	Total	O	0	0
			23	23		
3	H	31	Total	O	0	0
			31	31		
3	I	21	Total	O	0	0
			21	21		
3	J	17	Total	O	0	0
			17	17		
3	K	21	Total	O	0	0
			21	21		
3	L	20	Total	O	0	0
			20	20		
3	M	23	Total	O	0	0
			23	23		
3	N	31	Total	O	0	0
			31	31		
3	O	22	Total	O	0	0
			22	22		
3	P	23	Total	O	0	0
			23	23		

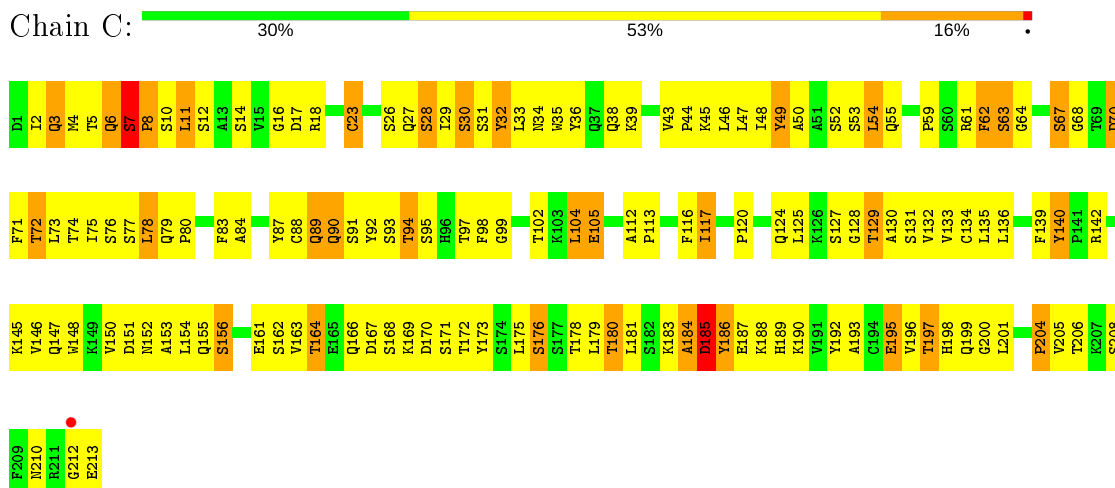
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Fab 47e light chain

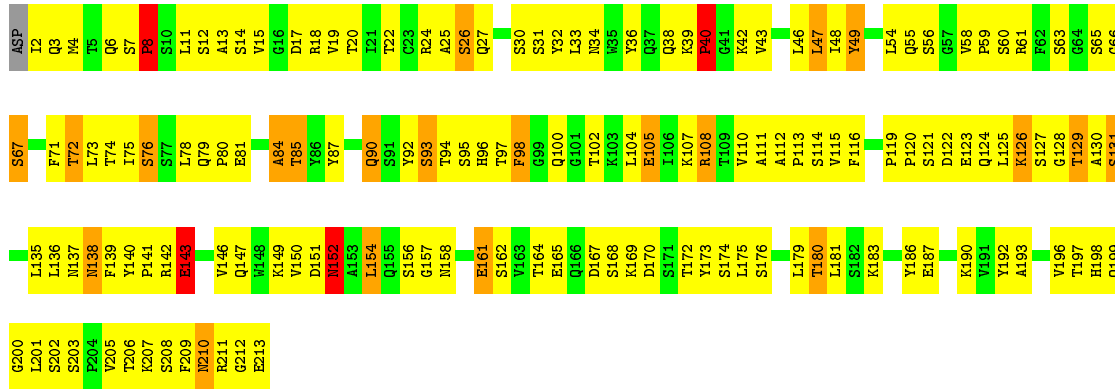


- Molecule 1: Fab 47e light chain

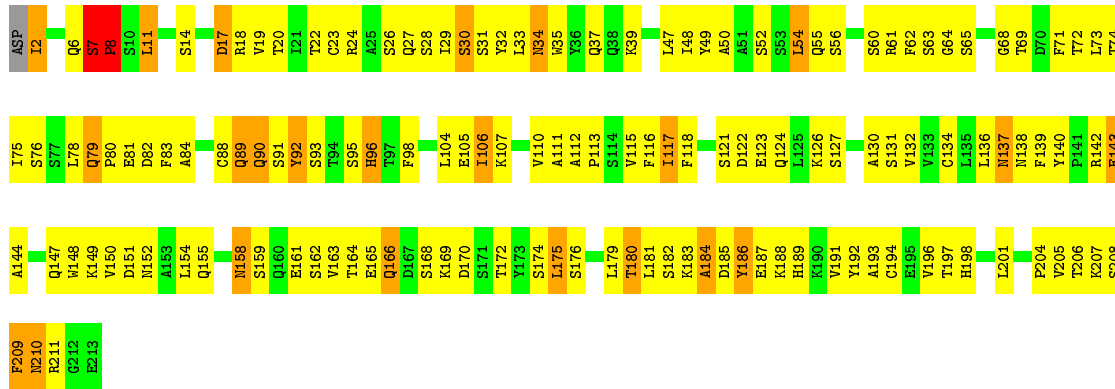


- Molecule 1: Fab 47e light chain

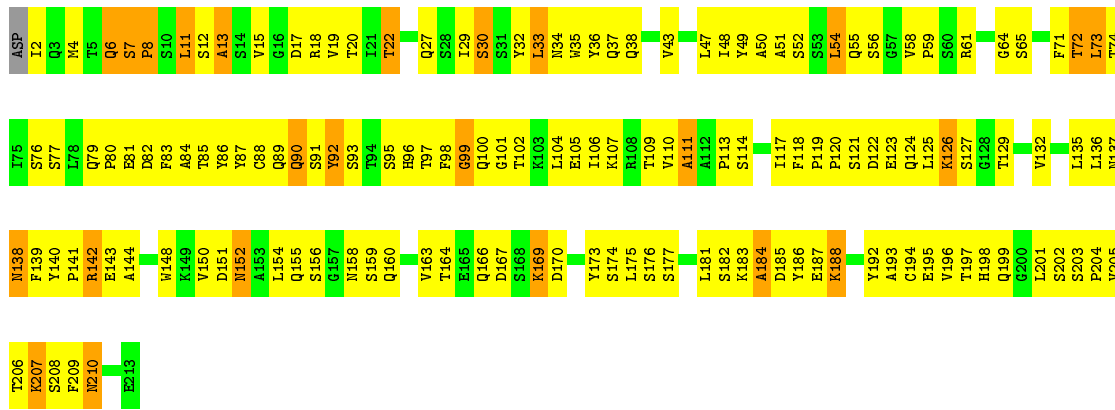




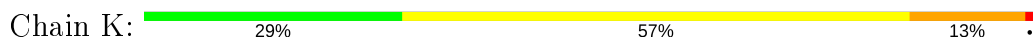
• Molecule 1: Fab 47e light chain

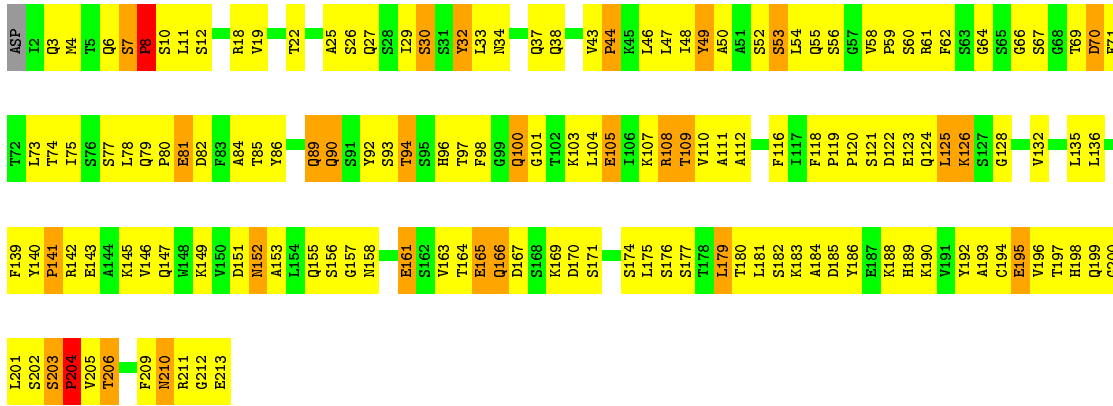


• Molecule 1: Fab 47e light chain



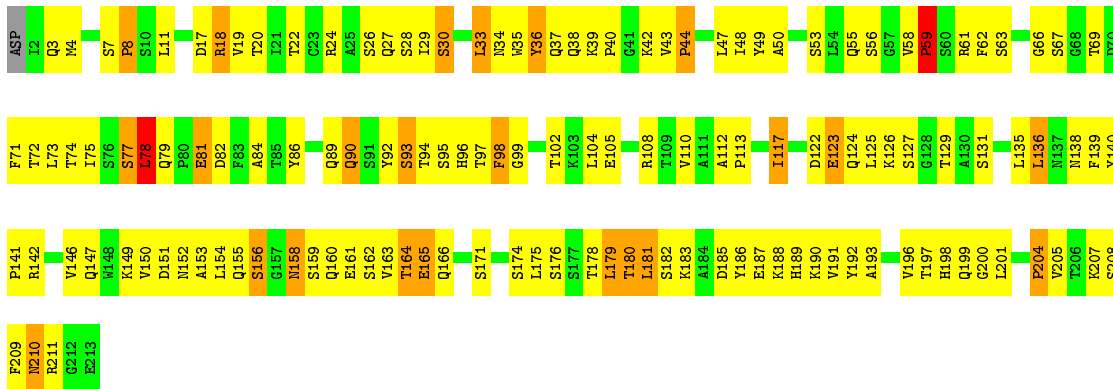
• Molecule 1: Fab 47e light chain





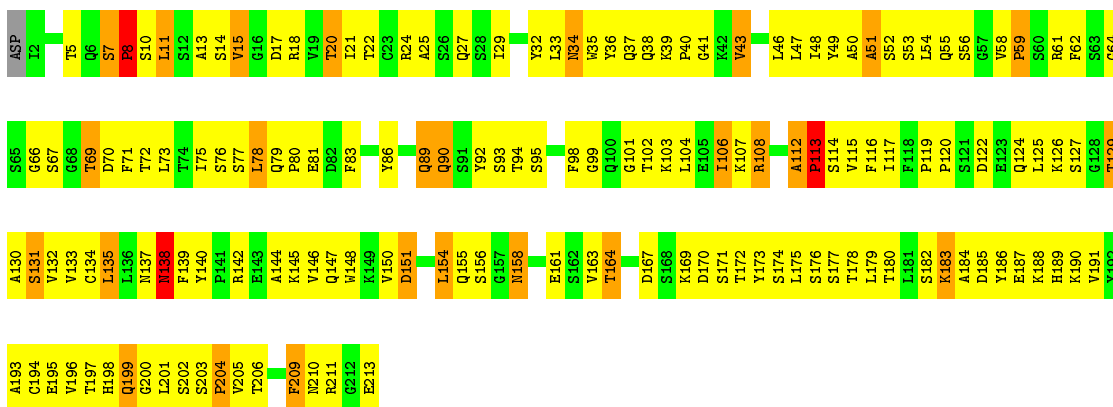
- Molecule 1: Fab 47e light chain

Chain M: 34% 53% 11%



- Molecule 1: Fab 47e light chain

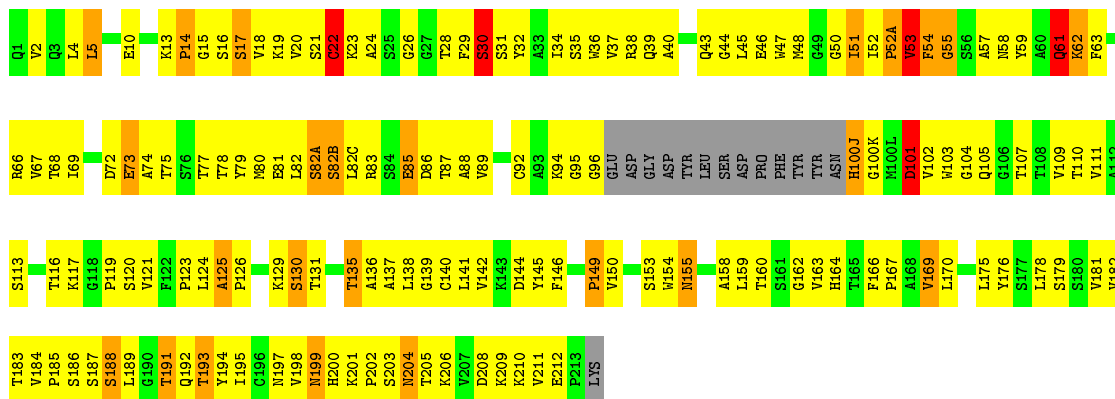
Chain O: 26% 59% 12%



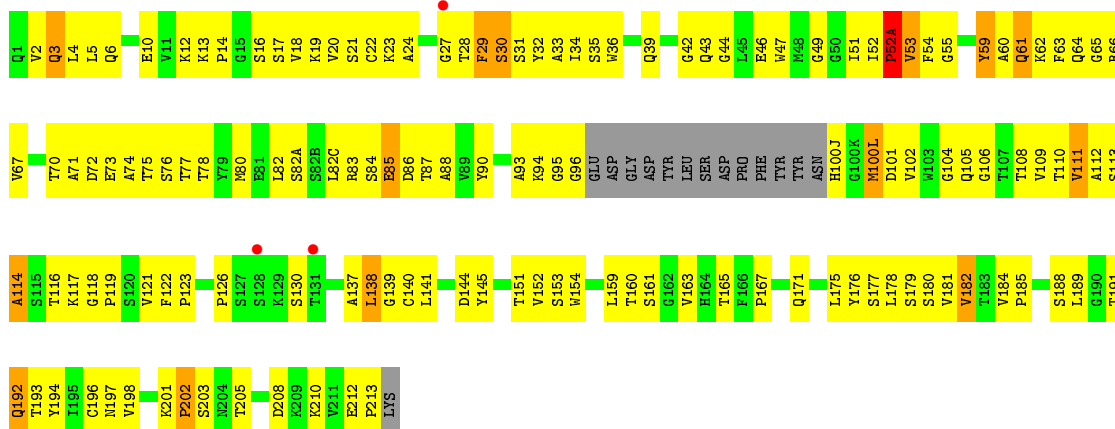
- Molecule 2: Fab 47e heavy chain

Chain B: 25% 56% 10% 6%

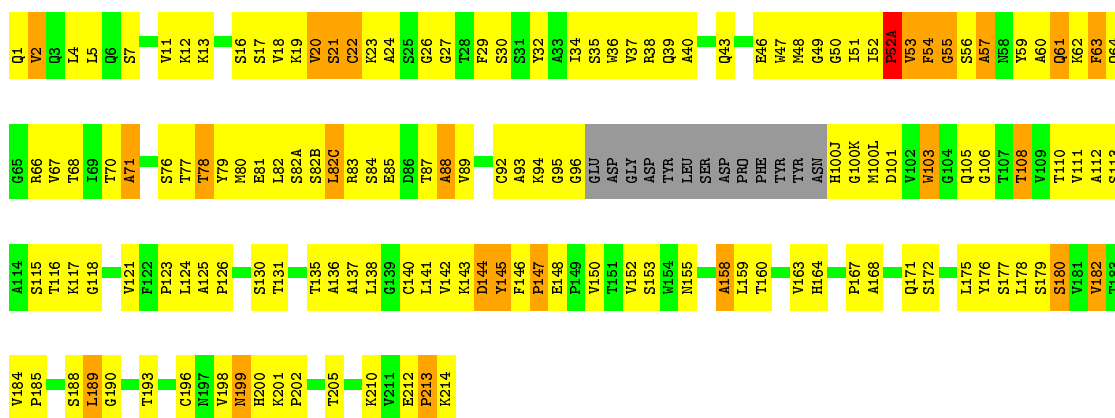




- Molecule 2: Fab 47e heavy chain

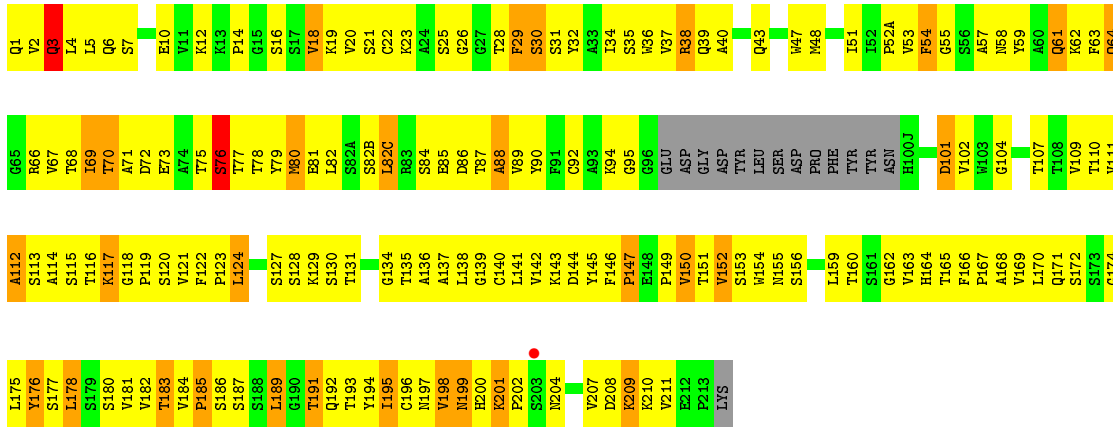


- Molecule 2: Fab 47e heavy chain



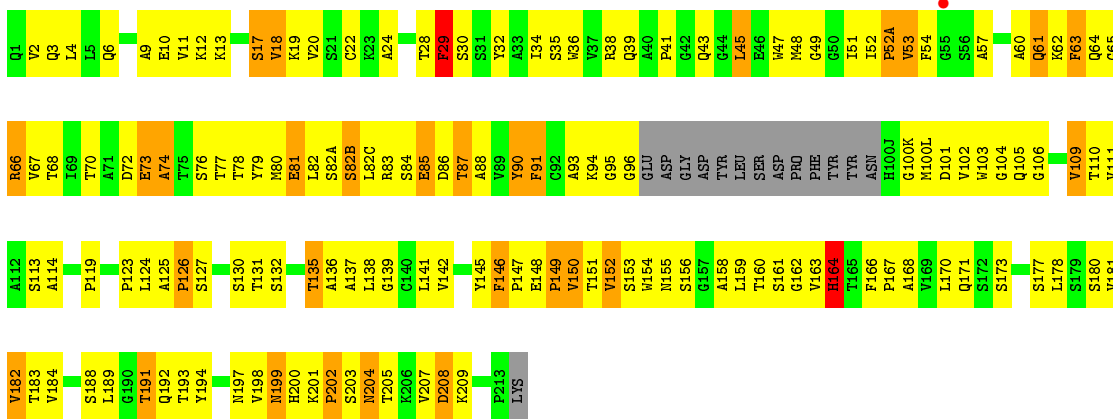
- Molecule 2: Fab 47e heavy chain





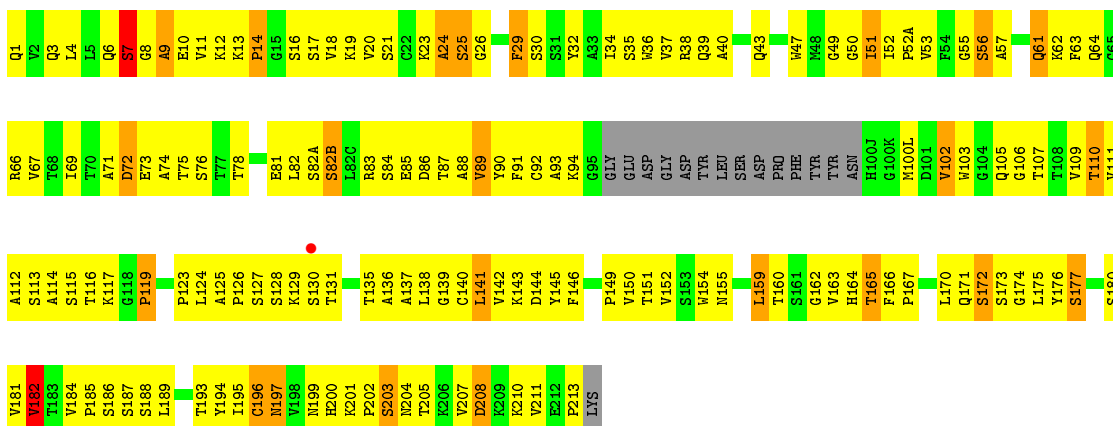
- Molecule 2: Fab 47e heavy chain

Chain J: 29% 52% 13% 6%



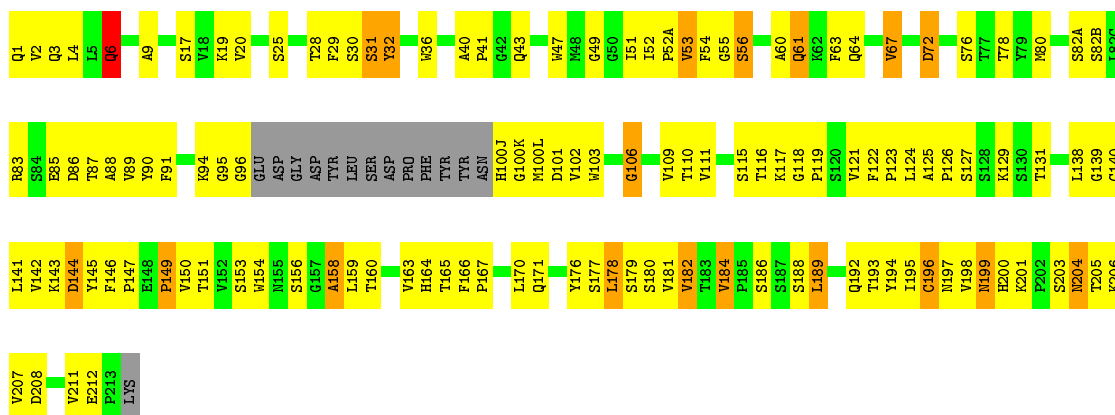
- Molecule 2: Fab 47e heavy chain

Chain L: 25% 58% 10% 7%



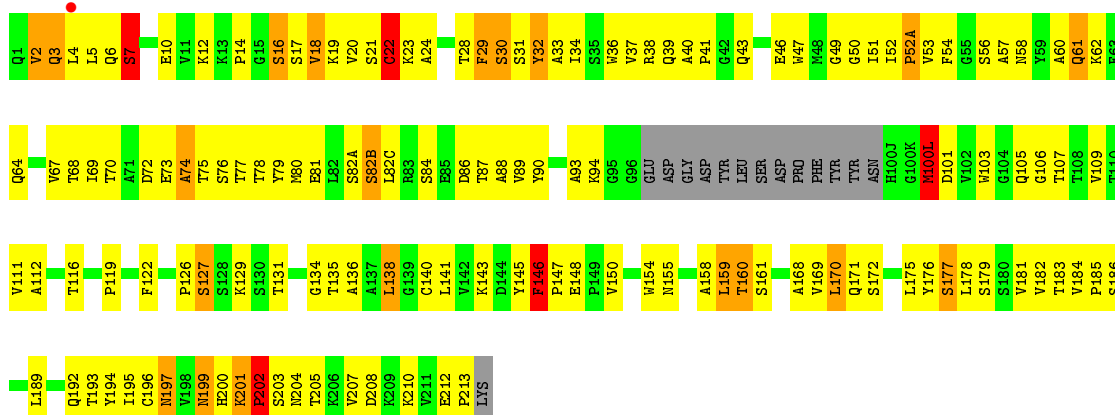
- Molecule 2: Fab 47e heavy chain

Chain N: 38% 48% 8% 6%



- Molecule 2: Fab 47e heavy chain

Chain P: 32% 51% 9% 6%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.43Å 111.64Å 133.31Å 85.48° 90.00° 89.71°	Depositor
Resolution (Å)	20.00 – 2.90 19.88 – 2.70	Depositor EDS
% Data completeness (in resolution range)	81.8 (20.00-2.90) 69.2 (19.88-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.97 (at 2.71Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.233 , 0.321 0.232 , 0.319	Depositor DCC
$R_{free}$ test set	7997 reflections (9.48%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.1	Xtrriage
Anisotropy	0.401	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 35.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	0.299 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	25973	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.02% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.62	1/1654 (0.1%)	1.01	5/2244 (0.2%)
1	C	0.54	2/1662 (0.1%)	0.97	7/2255 (0.3%)
1	E	0.52	1/1654 (0.1%)	0.94	8/2244 (0.4%)
1	G	0.51	1/1654 (0.1%)	0.93	4/2244 (0.2%)
1	I	0.60	3/1654 (0.2%)	0.90	8/2244 (0.4%)
1	K	0.56	2/1654 (0.1%)	0.93	4/2244 (0.2%)
1	M	0.55	0/1654	0.97	3/2244 (0.1%)
1	O	0.58	0/1654	0.99	10/2244 (0.4%)
2	B	0.45	0/1611	0.73	0/2192
2	D	0.47	0/1611	0.72	0/2192
2	F	0.44	0/1621	0.73	0/2203
2	H	0.42	0/1611	0.70	0/2192
2	J	0.44	0/1611	0.70	0/2192
2	L	0.45	0/1607	0.71	0/2187
2	N	0.46	0/1611	0.74	0/2192
2	P	0.46	0/1611	0.72	0/2192
All	All	0.51	10/26134 (0.0%)	0.85	49/35505 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	K	0	1
All	All	0	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	7	SER	C-N	8.01	1.49	1.34
1	K	7	SER	C-N	6.78	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	7	SER	C-N	6.56	1.46	1.34
1	K	10	SER	N-CA	6.17	1.58	1.46
1	I	7	SER	CA-C	5.69	1.67	1.52
1	G	7	SER	C-N	5.60	1.44	1.34
1	C	7	SER	C-O	-5.46	1.12	1.23
1	C	7	SER	N-CA	5.33	1.56	1.46
1	I	7	SER	N-CA	5.09	1.56	1.46
1	E	6	GLN	N-CA	5.06	1.56	1.46

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	7	SER	C-N-CD	-21.67	72.93	120.60
1	G	7	SER	C-N-CD	-19.01	78.78	120.60
1	O	7	SER	C-N-CD	-18.75	79.34	120.60
1	C	7	SER	C-N-CD	-18.65	79.58	120.60
1	K	7	SER	C-N-CD	-18.12	80.74	120.60
1	A	7	SER	C-N-CD	-15.80	85.83	120.60
1	I	7	SER	C-N-CD	-14.51	88.68	120.60
1	G	7	SER	C-N-CA	13.74	179.71	122.00
1	E	7	SER	C-N-CD	-13.52	90.85	120.60
1	K	7	SER	C-N-CA	13.12	177.11	122.00
1	A	7	SER	C-N-CA	12.74	175.50	122.00
1	C	7	SER	C-N-CA	11.85	171.78	122.00
1	M	7	SER	C-N-CA	10.73	167.08	122.00
1	K	8	PRO	CA-N-CD	-10.21	97.21	111.50
1	O	7	SER	C-N-CA	9.73	162.87	122.00
1	A	8	PRO	CA-N-CD	-9.25	98.55	111.50
1	O	8	PRO	C-N-CA	8.63	143.27	121.70
1	O	8	PRO	CA-N-CD	-8.60	99.46	111.50
1	M	8	PRO	CA-N-CD	-7.96	100.36	111.50
1	O	8	PRO	O-C-N	7.92	135.37	122.70
1	O	8	PRO	CA-C-N	-7.92	99.79	117.20
1	C	8	PRO	N-CA-C	7.91	132.67	112.10
1	I	7	SER	C-N-CA	7.86	155.00	122.00
1	G	8	PRO	CA-N-CD	-7.53	100.96	111.50
1	O	7	SER	N-CA-C	-7.48	90.80	111.00
1	C	7	SER	CA-C-N	7.44	137.94	117.10
1	E	7	SER	C-N-CA	7.36	152.90	122.00
1	I	8	PRO	CA-N-CD	-7.31	101.26	111.50
1	G	8	PRO	N-CA-C	7.29	131.06	112.10
1	E	6	GLN	CB-CA-C	-7.21	95.98	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	PRO	N-CD-CG	7.20	113.99	103.20
1	E	7	SER	N-CA-C	7.09	130.14	111.00
1	E	6	GLN	C-N-CA	-7.02	104.15	121.70
1	I	7	SER	N-CA-CB	-6.64	100.54	110.50
1	I	7	SER	N-CA-C	6.52	128.62	111.00
1	I	99	GLY	N-CA-C	-6.45	96.97	113.10
1	E	8	PRO	CA-N-CD	-6.41	102.53	111.50
1	K	8	PRO	C-N-CA	6.03	136.78	121.70
1	I	6	GLN	CA-C-N	5.95	130.29	117.20
1	C	8	PRO	C-N-CA	5.89	136.42	121.70
1	C	7	SER	CA-C-O	-5.82	107.87	120.10
1	O	8	PRO	N-CA-CB	5.77	110.23	103.30
1	O	8	PRO	CB-CA-C	-5.68	97.79	112.00
1	A	7	SER	N-CA-C	-5.59	95.92	111.00
1	O	99	GLY	N-CA-C	-5.58	99.15	113.10
1	C	8	PRO	CA-C-N	-5.45	105.20	117.20
1	I	6	GLN	O-C-N	-5.27	114.26	122.70
1	E	7	SER	CA-C-O	-5.27	109.03	120.10
1	E	7	SER	CA-C-N	5.04	131.22	117.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	140	TYR	Sidechain
1	K	49	TYR	Sidechain

## 5.2 Too-close contacts [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1620	0	1575	198	0
1	C	1628	0	1582	169	0
1	E	1620	0	1575	167	0
1	G	1620	0	1575	202	0
1	I	1620	0	1575	186	0
1	K	1620	0	1575	205	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	M	1620	0	1575	165	0
1	O	1620	0	1575	165	0
2	B	1576	0	1554	203	0
2	D	1576	0	1554	167	0
2	F	1586	0	1567	209	0
2	H	1576	0	1554	239	0
2	J	1576	0	1554	206	0
2	L	1572	0	1551	209	0
2	N	1576	0	1554	139	0
2	P	1576	0	1554	172	0
3	A	34	0	0	4	0
3	B	29	0	0	3	0
3	C	25	0	0	6	0
3	D	27	0	0	0	0
3	E	26	0	0	2	0
3	F	18	0	0	2	0
3	G	23	0	0	3	0
3	H	31	0	0	2	0
3	I	21	0	0	2	0
3	J	17	0	0	2	0
3	K	21	0	0	3	0
3	L	20	0	0	3	0
3	M	23	0	0	4	0
3	N	31	0	0	2	0
3	O	22	0	0	1	0
3	P	23	0	0	0	0
All	All	25973	0	25049	2857	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 56.

All (2857) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LEU:CD2	1:A:104:LEU:HD22	1.56	1.32
1:A:11:LEU:CD2	1:A:104:LEU:CD2	2.20	1.18
2:J:2:VAL:HG21	2:J:94:LYS:HZ3	1.09	1.15
1:E:199:GLN:HA	1:I:199:GLN:HE22	1.12	1.15
2:H:150:VAL:HG22	2:H:151:THR:H	1.11	1.14
1:O:113:PRO:HB3	1:O:139:PHE:HB3	1.29	1.13
1:I:32:TYR:HB3	1:I:91:SER:HB2	1.29	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:68:THR:HB	2:H:81:GLU:HB3	1.30	1.11
1:G:7:SER:HB3	1:G:8:PRO:HD2	1.26	1.11
2:L:119:PRO:HB3	2:L:145:TYR:HB3	1.25	1.11
2:D:17:SER:HB3	2:D:82(A):SER:HA	1.34	1.10
2:P:126:PRO:HG3	2:P:138:LEU:HB3	1.34	1.09
2:B:159:LEU:HD21	2:B:182:VAL:HG21	1.33	1.08
2:F:64:GLN:HG3	2:L:116:THR:HB	1.37	1.05
1:K:190:LYS:HG2	1:K:210:ASN:HB2	1.38	1.05
1:G:90:GLN:HE22	1:G:93:SER:HB3	1.17	1.05
2:N:126:PRO:HG3	2:N:138:LEU:HB3	1.39	1.05
2:H:199:ASN:HD22	2:H:200:HIS:N	1.56	1.04
1:E:199:GLN:HA	1:I:199:GLN:NE2	1.72	1.04
2:F:87:THR:HG23	2:F:110:THR:HA	1.37	1.04
2:H:124:LEU:HD21	2:H:141:LEU:HB2	1.35	1.04
2:L:38:ARG:NH2	2:L:86:ASP:HA	1.73	1.03
2:H:153:SER:HB2	2:H:197:ASN:HB2	1.42	1.02
2:F:145:TYR:HE1	2:F:150:VAL:HB	1.25	1.01
1:E:151:ASP:O	1:E:152:ASN:HB2	1.59	1.01
1:K:142:ARG:HH12	1:K:163:VAL:HG11	1.22	1.01
1:A:211:ARG:HB2	1:A:211:ARG:HH11	1.26	1.00
2:H:124:LEU:HB2	2:H:139:GLY:HA3	1.40	1.00
2:J:83:ARG:HB3	2:J:85:GLU:HG3	1.41	1.00
1:A:46:LEU:HD23	1:A:55:GLN:HE21	1.26	1.00
1:K:123:GLU:CD	1:K:123:GLU:H	1.66	0.99
2:J:61:GLN:H	2:J:61:GLN:NE2	1.59	0.98
2:L:163:VAL:HG22	2:L:182:VAL:HB	1.44	0.98
1:C:34:ASN:HD22	1:C:89:GLN:HE21	1.07	0.98
2:F:2:VAL:HG21	2:F:32:TYR:HE1	1.24	0.98
2:D:17:SER:CB	2:D:82(A):SER:HA	1.94	0.97
2:D:94:LYS:HD3	2:D:102:VAL:HG11	1.46	0.97
1:A:11:LEU:HD22	1:A:104:LEU:CD2	1.92	0.97
2:H:124:LEU:HD21	2:H:141:LEU:CB	1.94	0.96
2:J:61:GLN:HE21	2:J:61:GLN:N	1.60	0.96
1:A:11:LEU:HD23	1:A:104:LEU:HD22	1.43	0.96
2:L:3:GLN:H	2:L:25:SER:HB3	1.30	0.96
2:D:12:LYS:HG3	2:D:18:VAL:HB	1.45	0.96
2:P:51:ILE:HB	2:P:57:ALA:HB2	1.45	0.96
2:D:163:VAL:HG22	2:D:182:VAL:HB	1.45	0.96
2:J:4:LEU:HB3	2:J:24:ALA:HB2	1.48	0.96
1:O:37:GLN:HB2	1:O:47:LEU:HD11	1.47	0.96
2:B:192:GLN:NE2	2:B:193:THR:H	1.65	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:ASN:HD22	2:B:200:HIS:N	1.64	0.95
1:K:179:LEU:HD12	1:K:180:THR:N	1.82	0.94
1:A:11:LEU:HD23	1:A:104:LEU:CD2	1.94	0.94
2:N:1:GLN:HG3	2:N:2:VAL:H	1.30	0.94
2:B:123:PRO:HD3	2:B:209:LYS:HE2	1.49	0.93
2:L:152:VAL:HG11	2:L:180:SER:CB	1.98	0.93
1:I:185:ASP:HA	1:I:188:LYS:HD2	1.50	0.93
2:J:17:SER:HB3	2:J:82(A):SER:HA	1.51	0.93
2:F:24:ALA:HB3	2:F:76:SER:HB2	1.51	0.93
1:G:113:PRO:HB3	1:G:139:PHE:CD1	2.03	0.93
1:E:116:PHE:HB2	1:E:135:LEU:HB3	1.50	0.92
2:B:138:LEU:H	2:B:138:LEU:HD23	1.34	0.92
2:J:131:THR:HG22	2:J:136:ALA:HA	1.48	0.92
2:L:126:PRO:HG3	2:L:138:LEU:HB3	1.52	0.92
2:J:2:VAL:HG21	2:J:94:LYS:NZ	1.83	0.92
2:D:165:THR:HG23	2:D:180:SER:HB2	1.50	0.92
2:F:29:PHE:HZ	2:F:71:ALA:HB1	1.31	0.92
1:I:38:GLN:O	1:I:84:ALA:HB1	1.69	0.92
2:P:201:LYS:HB3	2:P:202:PRO:HD3	1.52	0.91
1:I:2:ILE:CD1	1:I:93:SER:HB2	2.00	0.91
1:A:158:ASN:HD22	1:A:158:ASN:H	1.13	0.91
2:B:2:VAL:HA	2:B:26:GLY:HA3	1.52	0.91
1:K:210:ASN:N	1:K:210:ASN:HD22	1.66	0.91
2:F:199:ASN:HD22	2:F:199:ASN:C	1.74	0.91
2:F:32:TYR:HB3	2:F:94:LYS:HG3	1.53	0.91
2:L:94:LYS:HB3	2:L:102:VAL:HG13	1.51	0.90
1:E:11:LEU:HD12	1:E:104:LEU:HD22	1.52	0.90
1:O:167:ASP:OD1	1:O:169:LYS:HG2	1.71	0.90
2:D:18:VAL:HG12	2:D:82(C):LEU:HD11	1.51	0.90
1:G:116:PHE:CD2	2:H:130:SER:HA	2.05	0.90
2:H:150:VAL:HG22	2:H:151:THR:N	1.87	0.90
1:A:158:ASN:ND2	1:A:158:ASN:H	1.67	0.90
1:E:199:GLN:CA	1:I:199:GLN:HE22	1.83	0.89
1:G:136:LEU:HD11	1:G:196:VAL:HG21	1.54	0.89
1:E:147:GLN:HE22	1:I:11:LEU:CD2	1.84	0.89
2:F:24:ALA:CB	2:F:29:PHE:HB2	2.03	0.89
1:G:107:LYS:HA	1:G:140:TYR:OH	1.72	0.89
2:H:68:THR:CB	2:H:81:GLU:HB3	2.03	0.89
1:I:142:ARG:HH11	1:I:142:ARG:HG2	1.36	0.89
1:O:124:GLN:NE2	1:O:131:SER:OG	2.05	0.89
1:G:47:LEU:HD23	1:G:48:ILE:HG13	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:90:GLN:NE2	1:G:93:SER:HB3	1.86	0.88
2:H:73:GLU:H	2:H:73:GLU:CD	1.77	0.88
1:O:66:GLY:HA3	1:O:71:PHE:HA	1.54	0.88
1:C:11:LEU:HD21	1:O:154:LEU:HD12	1.54	0.88
1:G:7:SER:CB	1:G:8:PRO:HD2	1.95	0.88
1:I:2:ILE:HD11	1:I:93:SER:HB2	1.54	0.88
1:G:123:GLU:H	1:G:123:GLU:CD	1.76	0.88
2:J:11:VAL:HG21	2:J:147:PRO:HG3	1.56	0.88
2:B:192:GLN:HE21	2:B:193:THR:H	0.90	0.87
2:P:192:GLN:HE21	2:P:193:THR:H	1.21	0.87
1:A:20:THR:HG23	1:A:74:THR:HG23	1.56	0.87
2:D:171:GLN:HE21	2:D:177:SER:HB2	1.38	0.87
1:C:183:LYS:O	1:C:187:GLU:HG3	1.74	0.87
2:B:192:GLN:HE21	2:B:193:THR:N	1.73	0.87
1:I:61:ARG:CZ	1:I:79:GLN:HG3	2.05	0.86
2:J:126:PRO:HG3	2:J:138:LEU:HB3	1.57	0.86
2:N:52(A):PRO:O	2:N:53:VAL:HB	1.75	0.86
1:K:190:LYS:O	1:K:210:ASN:HA	1.76	0.86
1:M:175:LEU:HD23	1:M:176:SER:N	1.89	0.86
1:A:11:LEU:HD21	1:A:104:LEU:HD22	1.55	0.86
2:H:119:PRO:HB3	2:H:145:TYR:HB3	1.58	0.86
1:I:210:ASN:HD22	1:I:210:ASN:N	1.72	0.86
2:L:119:PRO:CB	2:L:145:TYR:HB3	2.04	0.86
1:M:4:MET:CB	1:M:99:GLY:HA2	2.06	0.86
2:P:34:ILE:HG21	2:P:78:THR:HG21	1.55	0.85
2:P:29:PHE:HB3	2:P:76:SER:HB2	1.58	0.85
2:B:87:THR:HG23	2:B:110:THR:HA	1.56	0.85
1:M:4:MET:HB2	1:M:99:GLY:HA2	1.58	0.85
1:E:61:ARG:CZ	1:E:79:GLN:HG3	2.07	0.85
2:H:186:SER:O	2:H:189:LEU:HG	1.75	0.85
2:F:13:LYS:HD3	2:F:113:SER:HA	1.56	0.85
2:F:126:PRO:HD2	2:F:213:PRO:HA	1.57	0.85
1:C:29:ILE:HD11	1:C:33:LEU:HB2	1.58	0.85
2:H:19:LYS:HA	2:H:80:MET:O	1.77	0.85
2:P:197:ASN:HA	2:P:208:ASP:OD2	1.76	0.85
2:B:40:ALA:HB3	2:B:43:GLN:HE21	1.41	0.84
2:J:123:PRO:HD3	2:J:209:LYS:HG2	1.58	0.84
2:N:200:HIS:HB3	2:N:205:THR:OG1	1.77	0.84
2:H:200:HIS:CE1	2:H:202:PRO:HD2	2.12	0.84
1:C:212:GLY:O	1:C:213:GLU:HG3	1.76	0.84
2:N:154:TRP:CZ3	2:N:196:CYS:HB3	2.11	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:62:LYS:HA	2:N:83:ARG:HH22	1.41	0.84
1:K:19:VAL:HG23	1:K:78:LEU:HD21	1.58	0.84
1:A:201:LEU:HD13	1:A:205:VAL:HG23	1.58	0.84
1:C:4:MET:HB2	1:C:98:PHE:O	1.77	0.84
2:H:124:LEU:HB2	2:H:139:GLY:CA	2.07	0.84
2:F:121:VAL:HG11	2:F:198:VAL:HG21	1.58	0.84
2:F:64:GLN:CG	2:L:116:THR:HB	2.07	0.84
1:E:48:ILE:HD12	1:E:73:LEU:HD13	1.58	0.83
2:D:126:PRO:HG3	2:D:138:LEU:HB3	1.60	0.83
1:K:11:LEU:HD12	1:K:104:LEU:HD22	1.60	0.83
2:P:2:VAL:HG22	2:P:3:GLN:H	1.41	0.83
2:F:2:VAL:HG21	2:F:32:TYR:CE1	2.13	0.83
1:M:33:LEU:HD11	1:M:35:TRP:NE1	1.94	0.83
1:M:18:ARG:HH11	1:M:18:ARG:HB2	1.41	0.83
2:D:6:GLN:HA	2:D:21:SER:O	1.79	0.83
2:F:61:GLN:HG3	2:F:62:LYS:H	1.42	0.83
2:L:138:LEU:HD12	2:L:138:LEU:C	1.99	0.83
1:E:110:VAL:HG22	1:E:141:PRO:HD3	1.61	0.83
1:I:54:LEU:HD12	1:I:55:GLN:N	1.93	0.83
1:A:198:HIS:ND1	1:A:200:GLY:N	2.27	0.82
2:F:29:PHE:CZ	2:F:71:ALA:HB1	2.13	0.82
2:H:150:VAL:CG2	2:H:151:THR:H	1.90	0.82
1:M:33:LEU:HD11	1:M:35:TRP:HE1	1.44	0.82
1:A:89:GLN:HB2	1:A:98:PHE:CE2	2.15	0.82
2:H:52(A):PRO:HG3	2:H:71:ALA:CB	2.10	0.82
1:M:67:SER:HA	1:M:71:PHE:CE2	2.14	0.82
1:C:12:SER:HA	1:C:105:GLU:HG3	1.61	0.82
1:C:50:ALA:HB3	1:C:53:SER:HB3	1.61	0.82
2:H:165:THR:HG23	2:H:180:SER:HB2	1.62	0.82
1:A:158:ASN:HD22	1:A:158:ASN:N	1.76	0.82
1:E:11:LEU:HD23	1:I:156:SER:HB2	1.61	0.82
1:C:38:GLN:O	1:C:84:ALA:HB1	1.80	0.82
1:E:39:LYS:HG2	1:E:84:ALA:HB2	1.61	0.81
2:L:87:THR:HA	2:L:109:VAL:O	1.80	0.81
1:K:186:TYR:CE2	1:K:211:ARG:HD3	2.14	0.81
1:O:39:LYS:HB3	1:O:40:PRO:CD	2.09	0.81
1:G:11:LEU:HD12	1:G:104:LEU:CD2	2.09	0.81
2:J:64:GLN:HB3	2:L:204:ASN:OD1	1.79	0.81
2:J:4:LEU:HA	2:J:24:ALA:HA	1.63	0.81
2:P:5:LEU:O	2:P:22:CYS:HA	1.80	0.81
1:A:33:LEU:HD11	1:A:35:TRP:NE1	1.96	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:123:GLU:N	1:M:123:GLU:OE2	2.12	0.81
2:B:30:SER:O	2:B:53:VAL:HG22	1.81	0.81
1:O:135:LEU:CD1	2:P:181:VAL:HG21	2.11	0.81
2:H:19:LYS:HE3	2:H:79:TYR:HB3	1.63	0.80
2:P:50:GLY:O	2:P:57:ALA:HB1	1.79	0.80
1:I:73:LEU:HD12	1:I:74:THR:H	1.47	0.80
2:N:153:SER:OG	2:N:197:ASN:HB2	1.80	0.80
1:A:189:HIS:O	1:A:211:ARG:HD3	1.81	0.80
2:H:36:TRP:CE3	2:H:80:MET:HG3	2.16	0.80
2:D:163:VAL:CG2	2:D:182:VAL:HB	2.11	0.80
1:I:73:LEU:HD12	1:I:74:THR:N	1.96	0.80
1:O:124:GLN:O	1:O:127:SER:HB2	1.82	0.80
1:I:48:ILE:HD13	1:I:64:GLY:N	1.96	0.80
2:N:118:GLY:HA3	2:N:205:THR:HG21	1.62	0.80
2:B:200:HIS:CE1	2:B:202:PRO:HB2	2.17	0.79
2:F:89:VAL:HG22	2:F:108:THR:HG23	1.64	0.79
2:H:130:SER:HB2	2:H:137:ALA:HB3	1.63	0.79
1:K:4:MET:HB2	1:K:98:PHE:O	1.81	0.79
2:H:200:HIS:ND1	2:H:202:PRO:HD2	1.97	0.79
2:P:126:PRO:CG	2:P:138:LEU:HB3	2.10	0.79
2:H:36:TRP:HB2	2:H:69:ILE:HD11	1.63	0.79
2:P:131:THR:HG22	2:P:136:ALA:HB2	1.63	0.79
1:K:163:VAL:O	2:L:167:PRO:HG2	1.82	0.79
1:M:179:LEU:HD12	1:M:180:THR:N	1.97	0.79
2:J:6:GLN:HB2	2:J:105:GLN:HG2	1.65	0.79
2:P:60:ALA:O	2:P:64:GLN:HG3	1.81	0.79
2:F:141:LEU:HD12	2:F:178:LEU:O	1.83	0.79
1:I:29:ILE:HA	1:I:92:TYR:CD2	2.17	0.79
2:L:119:PRO:HD2	2:L:205:THR:HG21	1.63	0.78
2:N:119:PRO:HB2	2:N:142:VAL:HG13	1.62	0.78
1:K:152:ASN:HD22	1:K:152:ASN:N	1.79	0.78
1:A:135:LEU:HG	1:A:136:LEU:N	1.98	0.78
2:B:69:ILE:HG12	2:B:80:MET:HG2	1.63	0.78
1:C:116:PHE:HD2	2:D:130:SER:HB2	1.48	0.78
1:G:113:PRO:HB3	1:G:139:PHE:HD1	1.47	0.78
1:K:29:ILE:HB	1:K:92:TYR:HB2	1.65	0.78
1:A:193:ALA:HB2	1:A:208:SER:HB3	1.65	0.78
1:K:164:THR:CG2	1:K:174:SER:H	1.96	0.78
2:H:7:SER:HB3	2:H:21:SER:H	1.49	0.78
1:I:142:ARG:HG3	1:I:163:VAL:HG11	1.66	0.78
1:M:209:PHE:C	1:M:210:ASN:HD22	1.86	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:126:LYS:N	1:I:126:LYS:HD2	1.99	0.78
2:D:138:LEU:HD11	2:D:182:VAL:HG13	1.67	0.77
2:F:145:TYR:CE1	2:F:150:VAL:HB	2.16	0.77
1:M:142:ARG:HH12	1:M:163:VAL:HG21	1.48	0.77
1:O:7:SER:CB	1:O:8:PRO:HD3	2.15	0.77
1:O:11:LEU:HB3	1:O:104:LEU:HD22	1.64	0.77
1:A:124:GLN:HE22	1:A:131:SER:H	1.32	0.77
1:E:20:THR:HG23	1:E:74:THR:OG1	1.84	0.77
1:K:156:SER:O	1:K:158:ASN:N	2.18	0.77
1:K:98:PHE:HE1	2:L:47:TRP:HB2	1.49	0.77
2:H:51:ILE:HB	2:H:57:ALA:HB2	1.66	0.77
2:F:17:SER:CB	2:F:82(A):SER:HA	2.15	0.77
2:B:188:SER:HA	2:B:191:THR:HG23	1.67	0.77
2:L:87:THR:HG23	2:L:110:THR:HA	1.66	0.77
1:C:185:ASP:O	1:C:188:LYS:HB2	1.84	0.76
1:A:90:GLN:HG3	1:A:97:THR:H	1.50	0.76
2:F:111:VAL:O	2:F:111:VAL:HG12	1.85	0.76
2:P:29:PHE:CB	2:P:76:SER:HB2	2.15	0.76
2:F:37:VAL:HG22	2:F:47:TRP:HA	1.65	0.76
2:L:182:VAL:HG22	2:L:184:VAL:HG13	1.66	0.76
2:B:170:LEU:HD13	2:B:176:TYR:CE1	2.21	0.76
2:D:51:ILE:HG12	2:D:52:ILE:H	1.49	0.76
2:H:53:VAL:HB	2:H:54:PHE:CE1	2.20	0.76
1:I:54:LEU:HD11	1:I:58:VAL:HB	1.67	0.76
1:M:193:ALA:CB	1:M:208:SER:HB3	2.16	0.76
1:A:19:VAL:HG13	1:M:154:LEU:HB2	1.66	0.76
2:P:192:GLN:HE21	2:P:193:THR:N	1.83	0.76
2:P:200:HIS:HD2	2:P:202:PRO:HD2	1.51	0.76
1:A:46:LEU:CD2	1:A:55:GLN:HE21	1.99	0.76
1:E:154:LEU:H	1:E:154:LEU:HD22	1.48	0.76
2:F:94:LYS:HZ3	2:F:95:GLY:HA2	1.50	0.76
2:J:63:PHE:O	2:J:67:VAL:HG12	1.86	0.76
2:P:70:THR:OG1	2:P:79:TYR:HB2	1.85	0.76
2:D:51:ILE:HG12	2:D:52:ILE:N	2.01	0.76
1:G:175:LEU:HD23	1:G:175:LEU:C	2.05	0.76
2:B:199:ASN:HD22	2:B:199:ASN:C	1.85	0.75
2:H:141:LEU:HD12	2:H:142:VAL:N	2.02	0.75
1:C:124:GLN:HG2	1:C:129:THR:O	1.87	0.75
1:I:184:ALA:O	1:I:188:LYS:HG3	1.86	0.75
2:L:151:THR:OG1	2:L:199:ASN:HB3	1.87	0.75
2:N:94:LYS:HB3	2:N:102:VAL:HG13	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ILE:HG23	1:A:117:ILE:O	1.87	0.75
1:E:198:HIS:CE1	1:E:200:GLY:H	2.05	0.75
1:E:209:PHE:C	1:E:210:ASN:HD22	1.90	0.75
1:A:183:LYS:O	1:A:187:GLU:HG3	1.87	0.75
2:H:117:LYS:HD3	2:H:118:GLY:O	1.87	0.75
1:M:198:HIS:HD2	1:M:199:GLN:H	1.32	0.75
2:D:71:ALA:HB2	2:D:78:THR:HG22	1.69	0.75
2:F:200:HIS:CD2	2:F:202:PRO:HD2	2.22	0.75
1:K:210:ASN:N	1:K:210:ASN:ND2	2.33	0.75
2:L:123:PRO:CB	2:L:211:VAL:HG22	2.17	0.74
1:C:29:ILE:O	1:C:29:ILE:HG13	1.85	0.74
1:G:122:ASP:O	1:G:126:LYS:HD3	1.86	0.74
2:B:23:LYS:HD3	2:B:24:ALA:N	2.02	0.74
1:G:163:VAL:HG22	1:G:175:LEU:HB2	1.68	0.74
2:H:154:TRP:O	2:H:155:ASN:HB2	1.85	0.74
2:B:126:PRO:HG3	2:B:138:LEU:HB3	1.66	0.74
1:C:62:PHE:O	1:C:63:SER:HB3	1.87	0.74
1:E:61:ARG:NE	1:E:79:GLN:HG3	2.01	0.74
1:I:139:PHE:HD2	1:I:198:HIS:NE2	1.85	0.74
2:N:126:PRO:HG3	2:N:138:LEU:CB	2.14	0.74
2:F:2:VAL:HG23	2:F:27:GLY:H	1.52	0.74
1:K:29:ILE:HG21	1:K:90:GLN:HG3	1.66	0.74
2:P:189:LEU:HD13	2:P:213:PRO:HG3	1.69	0.74
2:L:6:GLN:HA	2:L:21:SER:O	1.87	0.74
2:N:154:TRP:CH2	2:N:196:CYS:HB3	2.22	0.74
2:N:3:GLN:C	2:N:4:LEU:HD23	2.08	0.74
1:C:46:LEU:HD22	2:D:100(L):MET:H	1.51	0.74
1:E:147:GLN:HE22	1:I:11:LEU:HD21	1.53	0.74
2:D:64:GLN:HG3	2:N:116:THR:HB	1.70	0.74
2:D:36:TRP:CE2	2:D:80:MET:HB2	2.23	0.74
2:L:50:GLY:O	2:L:57:ALA:HB1	1.87	0.74
1:M:149:LYS:HG3	1:M:154:LEU:HD13	1.68	0.74
2:H:153:SER:HB2	2:H:197:ASN:CB	2.17	0.74
1:M:39:LYS:HG2	1:M:84:ALA:HB2	1.68	0.74
1:O:39:LYS:HB3	1:O:40:PRO:HD2	1.68	0.74
1:A:117:ILE:HD13	1:A:208:SER:HA	1.70	0.73
1:K:195:GLU:HB2	1:K:206:THR:HG23	1.68	0.73
2:B:131:THR:HG22	2:B:136:ALA:CB	2.18	0.73
1:C:116:PHE:HB3	2:D:130:SER:HB2	1.70	0.73
2:N:61:GLN:O	2:N:64:GLN:HB2	1.88	0.73
1:A:124:GLN:NE2	1:A:131:SER:H	1.84	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ILE:O	1:A:30:SER:HB3	1.88	0.73
1:A:162:SER:OG	2:B:167:PRO:HD2	1.87	0.73
2:J:30:SER:HA	2:J:52(A):PRO:HB2	1.70	0.73
2:L:13:LYS:HD3	2:L:113:SER:HA	1.69	0.73
2:J:12:LYS:HD2	2:J:18:VAL:HB	1.71	0.73
1:A:11:LEU:CD2	1:A:104:LEU:HD23	2.18	0.73
2:J:2:VAL:CG2	2:J:94:LYS:HZ3	1.96	0.73
1:I:2:ILE:HB	1:I:90:GLN:HE21	1.54	0.73
2:H:146:PHE:HB2	2:H:175:LEU:HD22	1.69	0.72
1:O:54:LEU:HD12	1:O:55:GLN:H	1.52	0.72
2:H:150:VAL:HG23	2:H:199:ASN:O	1.89	0.72
1:A:54:LEU:HD12	1:A:54:LEU:H	1.54	0.72
1:C:112:ALA:HB1	1:C:201:LEU:HG	1.71	0.72
1:G:7:SER:CB	1:G:8:PRO:CD	2.60	0.72
1:G:33:LEU:HD21	1:G:88:CYS:HB2	1.72	0.72
2:L:127:SER:O	2:L:131:THR:HG23	1.89	0.72
2:P:61:GLN:HA	2:P:64:GLN:OE1	1.90	0.72
2:L:170:LEU:HD12	2:L:171:GLN:H	1.53	0.72
2:D:210:LYS:HE2	2:D:212:GLU:HG3	1.69	0.72
1:I:138:ASN:HA	1:I:173:TYR:O	1.89	0.72
1:M:19:VAL:HG12	1:M:20:THR:N	2.04	0.72
1:M:33:LEU:HD22	1:M:34:ASN:N	2.04	0.72
2:H:136:ALA:O	2:H:183:THR:HA	1.88	0.72
2:J:94:LYS:HG2	2:J:95:GLY:N	2.04	0.72
1:I:167:ASP:OD1	1:I:169:LYS:HD3	1.89	0.72
1:K:111:ALA:O	1:K:139:PHE:HA	1.89	0.72
2:L:30:SER:O	2:L:53:VAL:HG23	1.90	0.72
1:A:133:VAL:HG22	1:A:178:THR:HG23	1.72	0.72
2:D:117:LYS:HG3	2:D:118:GLY:O	1.90	0.72
1:E:210:ASN:ND2	1:E:210:ASN:N	2.38	0.72
2:F:57:ALA:HB1	2:F:59:TYR:HE2	1.54	0.72
1:I:65:SER:HB2	1:I:72:THR:HG22	1.72	0.72
1:G:116:PHE:HD2	2:H:130:SER:HA	1.52	0.71
1:G:121:SER:HB2	1:G:123:GLU:OE1	1.90	0.71
2:H:134:GLY:O	2:H:186:SER:N	2.23	0.71
1:I:209:PHE:C	1:I:210:ASN:HD22	1.93	0.71
2:L:3:GLN:N	2:L:25:SER:HB3	2.04	0.71
2:N:156:SER:HA	2:N:197:ASN:HD21	1.54	0.71
2:P:200:HIS:CD2	2:P:202:PRO:HD2	2.24	0.71
1:A:136:LEU:HD21	1:A:196:VAL:HG11	1.72	0.71
1:I:117:ILE:HD12	1:I:207:LYS:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:159:LEU:HD21	2:N:182:VAL:HG21	1.72	0.71
2:P:4:LEU:HD11	2:P:94:LYS:HB2	1.71	0.71
2:B:40:ALA:CB	2:B:43:GLN:HE21	2.02	0.71
2:F:2:VAL:CG2	2:F:27:GLY:H	2.03	0.71
2:B:94:LYS:HD2	2:B:102:VAL:CG1	2.20	0.71
1:E:114:SER:HB2	1:E:137:ASN:HB3	1.72	0.71
2:F:83:ARG:HH12	2:J:62:LYS:HB3	1.56	0.71
1:O:182:SER:O	1:O:184:ALA:N	2.23	0.71
2:B:92:CYS:SG	2:B:92:CYS:O	2.49	0.71
1:G:73:LEU:HD23	1:G:73:LEU:C	2.11	0.71
1:K:167:ASP:OD1	1:K:169:LYS:HG2	1.90	0.71
1:O:200:GLY:O	1:O:201:LEU:HD23	1.91	0.71
2:L:38:ARG:HH22	2:L:86:ASP:HA	1.56	0.71
1:M:190:LYS:O	1:M:210:ASN:HA	1.90	0.71
1:M:210:ASN:HD22	1:M:210:ASN:N	1.85	0.71
1:A:28:SER:HA	1:A:69:THR:HG22	1.72	0.71
1:E:210:ASN:N	1:E:210:ASN:HD22	1.89	0.71
1:E:162:SER:OG	2:F:167:PRO:HD2	1.90	0.71
1:G:184:ALA:O	1:G:188:LYS:HG3	1.90	0.71
1:I:113:PRO:HB3	1:I:139:PHE:HB3	1.72	0.71
1:M:191:VAL:HG22	1:M:210:ASN:ND2	2.06	0.71
2:H:94:LYS:HE2	2:H:95:GLY:C	2.12	0.70
1:I:54:LEU:HD12	1:I:55:GLN:H	1.54	0.70
1:E:201:LEU:HD13	1:E:205:VAL:HG23	1.72	0.70
2:F:171:GLN:NE2	2:F:177:SER:HB2	2.05	0.70
2:L:152:VAL:HG11	2:L:180:SER:HB2	1.72	0.70
2:N:178:LEU:HD12	2:N:179:SER:N	2.05	0.70
2:D:72:ASP:OD1	2:D:74:ALA:HB3	1.91	0.70
1:E:32:TYR:HD1	1:E:92:TYR:CD1	2.10	0.70
2:L:159:LEU:HD12	2:L:160:THR:N	2.05	0.70
1:M:176:SER:HB3	2:N:166:PHE:CE1	2.27	0.70
1:G:106:ILE:HD12	1:G:106:ILE:H	1.57	0.70
2:H:124:LEU:HG	2:H:141:LEU:H	1.56	0.70
1:E:120:PRO:HB3	1:E:131:SER:H	1.56	0.70
1:G:201:LEU:HD13	1:G:205:VAL:HG23	1.73	0.70
1:O:94:THR:HG23	1:O:95:SER:N	2.07	0.70
1:C:34:ASN:HD22	1:C:89:GLN:NE2	1.86	0.70
2:H:29:PHE:CG	2:H:76:SER:HB2	2.27	0.70
2:N:63:PHE:HB3	2:N:67:VAL:HG11	1.71	0.70
2:J:151:THR:O	2:J:152:VAL:HG23	1.91	0.70
2:L:202:PRO:O	2:L:203:SER:HB3	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:113:PRO:HB3	1:M:139:PHE:HB3	1.73	0.70
2:D:65:GLY:HA3	2:N:203:SER:HB2	1.74	0.70
1:O:135:LEU:HD11	2:P:181:VAL:HG21	1.72	0.70
2:F:71:ALA:HA	2:F:77:THR:O	1.91	0.70
1:K:29:ILE:O	1:K:30:SER:HB3	1.90	0.70
1:M:19:VAL:HG12	1:M:20:THR:H	1.57	0.70
1:A:89:GLN:HB2	1:A:98:PHE:CD2	2.27	0.70
1:C:142:ARG:HH22	1:C:163:VAL:HG21	1.55	0.70
2:F:24:ALA:HB1	3:F:222:HOH:O	1.90	0.70
2:F:94:LYS:HE2	2:F:95:GLY:C	2.10	0.70
1:G:79:GLN:HA	1:G:79:GLN:HE21	1.56	0.70
2:H:193:THR:HG23	2:H:210:LYS:HE3	1.74	0.70
2:J:67:VAL:HG22	2:J:68:THR:N	2.07	0.70
1:K:38:GLN:O	1:K:84:ALA:HB1	1.92	0.70
2:L:63:PHE:HB3	2:L:67:VAL:HG11	1.74	0.70
1:M:140:TYR:HA	1:M:141:PRO:O	1.92	0.70
2:J:51:ILE:CD1	2:J:57:ALA:HB2	2.22	0.70
1:M:198:HIS:CD2	1:M:199:GLN:H	2.09	0.70
2:N:178:LEU:HD12	2:N:178:LEU:C	2.12	0.70
2:N:121:VAL:HG21	2:N:198:VAL:HG21	1.72	0.70
1:C:34:ASN:ND2	1:C:89:GLN:HE21	1.86	0.69
1:G:138:ASN:HA	1:G:172:THR:HB	1.74	0.69
2:H:19:LYS:HE2	2:H:79:TYR:CD2	2.27	0.69
1:A:14:SER:HB2	1:A:17:ASP:OD1	1.91	0.69
2:B:209:LYS:HG3	2:B:210:LYS:H	1.58	0.69
2:F:105:GLN:HG2	2:F:106:GLY:N	2.07	0.69
2:H:138:LEU:HD12	2:H:139:GLY:N	2.06	0.69
1:I:143:GLU:O	1:I:198:HIS:HD2	1.74	0.69
2:H:29:PHE:O	2:H:31:SER:N	2.25	0.69
2:H:94:LYS:HE2	2:H:95:GLY:O	1.91	0.69
1:I:30:SER:HA	3:I:226:HOH:O	1.91	0.69
1:I:6:GLN:HE22	1:I:87:TYR:HA	1.56	0.69
2:N:63:PHE:HB3	2:N:67:VAL:CG1	2.22	0.69
2:L:6:GLN:OE1	2:L:91:PHE:HA	1.91	0.69
1:O:170:ASP:O	1:O:172:THR:HG23	1.91	0.69
2:F:47:TRP:CH2	2:F:49:GLY:HA2	2.27	0.69
1:I:142:ARG:NH1	1:I:142:ARG:HG2	2.05	0.69
1:K:121:SER:O	1:K:124:GLN:HB3	1.92	0.69
1:M:193:ALA:HB2	1:M:208:SER:HB3	1.75	0.69
2:J:4:LEU:O	2:J:4:LEU:HD12	1.93	0.69
1:K:140:TYR:HA	1:K:141:PRO:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:116:THR:CG2	2:L:203:SER:HB3	2.23	0.69
2:B:51:ILE:HG12	2:B:52:ILE:N	2.08	0.69
1:C:14:SER:HB2	1:C:17:ASP:OD1	1.91	0.69
1:C:116:PHE:CD2	2:D:130:SER:HB2	2.26	0.69
2:P:143:LYS:HA	2:P:177:SER:OG	1.92	0.69
1:G:179:LEU:HG	1:G:181:LEU:HD11	1.74	0.69
2:P:51:ILE:HB	2:P:57:ALA:CB	2.20	0.69
2:D:18:VAL:HG22	2:D:19:LYS:N	2.07	0.69
2:H:38:ARG:HB3	2:H:90:TYR:CD2	2.27	0.69
2:J:17:SER:HB3	2:J:82(A):SER:CA	2.23	0.69
2:B:119:PRO:HB3	2:B:145:TYR:CD2	2.28	0.69
1:G:39:LYS:HD3	1:G:84:ALA:HB2	1.73	0.69
2:L:200:HIS:HB3	2:L:205:THR:HB	1.75	0.69
2:D:85:GLU:H	2:D:85:GLU:CD	1.97	0.69
2:L:116:THR:HG22	2:L:203:SER:HB3	1.75	0.69
1:G:132:VAL:HB	1:G:179:LEU:HB3	1.75	0.68
1:K:52:SER:O	1:K:53:SER:C	2.30	0.68
1:K:175:LEU:HD23	1:K:176:SER:N	2.09	0.68
1:A:116:PHE:CD1	1:A:135:LEU:HD23	2.27	0.68
1:C:6:GLN:O	1:C:7:SER:O	2.11	0.68
1:M:151:ASP:O	1:M:153:ALA:N	2.26	0.68
1:E:119:PRO:HB3	1:E:209:PHE:CZ	2.28	0.68
2:J:67:VAL:HG22	2:J:68:THR:H	1.57	0.68
1:K:26:SER:OG	1:K:27:GLN:OE1	2.05	0.68
1:M:29:ILE:HD11	1:M:33:LEU:HB2	1.75	0.68
2:H:51:ILE:HD11	2:H:55:GLY:HA2	1.74	0.68
1:C:7:SER:HB2	1:C:102:THR:OG1	1.94	0.68
2:F:24:ALA:HB1	2:F:29:PHE:HB2	1.73	0.68
1:M:113:PRO:HD3	1:M:198:HIS:ND1	2.09	0.68
1:A:18:ARG:HH11	1:A:18:ARG:HB2	1.58	0.68
2:F:68:THR:HB	2:F:81:GLU:HB3	1.74	0.68
1:A:33:LEU:HD13	1:A:33:LEU:C	2.13	0.68
2:F:63:PHE:HB3	2:F:67:VAL:HG12	1.75	0.68
1:I:193:ALA:HB2	1:I:208:SER:HB3	1.74	0.68
1:M:197:THR:HG22	1:M:204:PRO:HG3	1.74	0.68
2:N:156:SER:HA	2:N:197:ASN:ND2	2.08	0.68
2:H:67:VAL:HG22	2:H:68:THR:N	2.09	0.68
1:A:158:ASN:HA	1:M:24:ARG:HH21	1.57	0.68
2:B:51:ILE:HG12	2:B:52:ILE:H	1.58	0.68
1:I:32:TYR:CB	1:I:92:TYR:H	2.07	0.68
2:N:28:THR:HA	3:N:217:HOH:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:53:VAL:HG12	2:P:54:PHE:HD2	1.59	0.68
2:F:5:LEU:HB2	2:F:23:LYS:HB2	1.75	0.67
2:F:57:ALA:HB1	2:F:59:TYR:CE2	2.28	0.67
2:L:62:LYS:HG3	2:L:63:PHE:N	2.10	0.67
2:N:36:TRP:HE1	2:N:78:THR:HG21	1.58	0.67
2:H:154:TRP:CH2	2:H:196:CYS:HB3	2.29	0.67
1:M:17:ASP:O	1:M:78:LEU:HD22	1.94	0.67
2:N:94:LYS:HB3	2:N:102:VAL:CG1	2.24	0.67
1:A:48:ILE:HG22	1:A:49:TYR:N	2.10	0.67
1:I:114:SER:HB2	1:I:137:ASN:HB3	1.76	0.67
1:I:210:ASN:N	1:I:210:ASN:ND2	2.42	0.67
1:K:164:THR:HG22	1:K:174:SER:H	1.59	0.67
2:N:47:TRP:CH2	2:N:49:GLY:HA2	2.29	0.67
1:O:169:LYS:HG3	1:O:170:ASP:OD1	1.94	0.67
1:A:108:ARG:HD3	1:A:171:SER:O	1.94	0.67
1:A:124:GLN:HE22	1:A:131:SER:N	1.92	0.67
1:E:39:LYS:HG2	1:E:84:ALA:CB	2.23	0.67
2:F:94:LYS:HD3	2:F:94:LYS:C	2.14	0.67
2:J:171:GLN:NE2	2:J:177:SER:CB	2.58	0.67
1:A:33:LEU:HD21	1:A:88:CYS:HB2	1.77	0.67
2:J:119:PRO:HB3	2:J:145:TYR:HB3	1.76	0.67
1:E:93:SER:OG	1:E:94:THR:N	2.25	0.67
1:M:29:ILE:O	1:M:30:SER:HB3	1.94	0.67
2:P:6:GLN:NE2	2:P:106:GLY:HA2	2.09	0.67
2:B:119:PRO:HB3	2:B:145:TYR:HB3	1.76	0.67
1:E:18:ARG:NH1	1:E:76:SER:HA	2.09	0.67
1:K:19:VAL:O	1:K:74:THR:HG23	1.95	0.67
2:B:54:PHE:HD1	2:B:54:PHE:N	1.92	0.67
2:J:11:VAL:CG2	2:J:147:PRO:HG3	2.25	0.67
1:K:201:LEU:HD13	1:K:205:VAL:CG2	2.25	0.67
1:M:3:GLN:HB3	1:M:26:SER:HB3	1.75	0.67
2:D:197:ASN:HD22	2:D:208:ASP:CG	1.98	0.67
1:K:142:ARG:O	1:K:142:ARG:HG2	1.95	0.67
1:O:195:GLU:HA	1:O:206:THR:HA	1.77	0.67
2:B:29:PHE:O	2:B:31:SER:N	2.28	0.67
2:B:59:TYR:HE2	2:B:69:ILE:H	1.42	0.67
2:B:19:LYS:HE2	2:B:79:TYR:CD2	2.30	0.66
2:H:29:PHE:CB	2:H:76:SER:HB2	2.25	0.66
1:I:193:ALA:CB	1:I:208:SER:HB3	2.24	0.66
2:P:145:TYR:O	2:P:146:PHE:HB2	1.94	0.66
1:A:32:TYR:HB2	1:A:92:TYR:HB2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:105:GLN:HG2	2:F:106:GLY:H	1.60	0.66
2:F:185:PRO:HB2	2:F:188:SER:HB3	1.77	0.66
2:B:2:VAL:HA	2:B:26:GLY:CA	2.24	0.66
1:I:110:VAL:HG12	1:I:111:ALA:N	2.11	0.66
1:I:126:LYS:H	1:I:126:LYS:HD2	1.59	0.66
1:K:124:GLN:O	1:K:126:LYS:N	2.28	0.66
2:N:184:VAL:HG21	2:N:194:TYR:OH	1.95	0.66
1:G:139:PHE:HB2	1:G:198:HIS:CE1	2.30	0.66
1:M:193:ALA:HB2	1:M:208:SER:CB	2.25	0.66
1:G:123:GLU:N	1:G:123:GLU:CD	2.46	0.66
2:J:12:LYS:NZ	2:J:18:VAL:HA	2.11	0.66
2:P:176:TYR:O	2:P:177:SER:HB2	1.95	0.66
1:C:161:GLU:HB2	1:C:176:SER:O	1.96	0.66
2:F:5:LEU:HB2	2:F:23:LYS:CB	2.25	0.66
2:J:51:ILE:HD12	2:J:57:ALA:HB2	1.76	0.66
1:M:38:GLN:O	1:M:84:ALA:HB1	1.96	0.66
1:M:4:MET:HB3	1:M:99:GLY:HA2	1.77	0.66
2:P:2:VAL:HG21	2:P:32:TYR:HE1	1.60	0.66
1:A:8:PRO:HG3	1:A:100:GLN:OE1	1.94	0.66
1:C:90:GLN:NE2	1:C:97:THR:HB	2.11	0.66
1:E:54:LEU:HD21	1:E:59:PRO:O	1.94	0.66
2:F:199:ASN:C	2:F:199:ASN:ND2	2.48	0.66
2:B:51:ILE:HB	2:B:57:ALA:HB2	1.78	0.66
1:G:35:TRP:CE2	1:G:73:LEU:HB2	2.31	0.66
2:H:61:GLN:O	2:H:64:GLN:HB2	1.96	0.66
1:I:6:GLN:HB3	1:I:99:GLY:HA3	1.76	0.66
1:G:134:CYS:HB2	1:G:148:TRP:CH2	2.31	0.66
1:K:143:GLU:OE2	1:K:143:GLU:N	2.29	0.66
2:N:30:SER:O	2:N:53:VAL:HG23	1.96	0.66
2:P:203:SER:O	2:P:205:THR:N	2.29	0.66
1:A:90:GLN:HE22	1:A:93:SER:H	1.44	0.65
1:G:176:SER:HB3	2:H:166:PHE:CE1	2.31	0.65
1:G:175:LEU:HD23	1:G:176:SER:N	2.11	0.65
1:M:122:ASP:O	1:M:126:LYS:HD3	1.96	0.65
1:C:154:LEU:HD23	1:O:18:ARG:O	1.96	0.65
1:A:158:ASN:HA	1:M:24:ARG:NH2	2.11	0.65
1:A:46:LEU:HD23	1:A:55:GLN:NE2	2.07	0.65
2:F:140:CYS:O	2:F:179:SER:HA	1.96	0.65
2:H:35:SER:O	2:H:92:CYS:HA	1.96	0.65
2:H:52(A):PRO:HG3	2:H:71:ALA:HB1	1.76	0.65
1:O:163:VAL:HG12	1:O:164:THR:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:PRO:HB3	1:C:139:PHE:HB3	1.78	0.65
2:D:210:LYS:HE2	2:D:212:GLU:CG	2.25	0.65
2:H:62:LYS:HE2	2:H:63:PHE:CE1	2.32	0.65
2:L:35:SER:OG	2:L:47:TRP:NE1	2.30	0.65
1:M:29:ILE:HG21	1:M:90:GLN:HG3	1.77	0.65
2:H:7:SER:HB3	2:H:21:SER:OG	1.96	0.65
2:J:130:SER:HB3	2:J:137:ALA:O	1.96	0.65
2:J:41:PRO:HD3	2:J:87:THR:O	1.95	0.65
2:B:131:THR:HG22	2:B:136:ALA:HA	1.78	0.65
2:D:121:VAL:CG2	2:D:198:VAL:HG21	2.27	0.65
2:D:59:TYR:CD2	2:D:67:VAL:HG13	2.30	0.65
1:I:50:ALA:O	1:I:51:ALA:HB3	1.96	0.65
2:B:37:VAL:HG11	2:B:45:LEU:HB3	1.78	0.65
1:E:33:LEU:HD22	1:E:34:ASN:H	1.62	0.65
2:F:17:SER:HB3	2:F:82(A):SER:HA	1.79	0.65
2:H:36:TRP:CB	2:H:69:ILE:HD11	2.27	0.65
1:A:169:LYS:HG3	1:A:170:ASP:OD1	1.97	0.65
2:F:158:ALA:O	2:F:160:THR:HG23	1.96	0.65
2:F:70:THR:OG1	2:F:79:TYR:HB2	1.97	0.65
2:H:5:LEU:O	2:H:22:CYS:HA	1.95	0.65
2:L:155:ASN:HD21	2:L:194:TYR:HD1	1.43	0.65
2:L:71:ALA:O	2:L:72:ASP:HB2	1.97	0.65
1:O:11:LEU:O	1:O:104:LEU:HA	1.97	0.65
2:D:138:LEU:CD1	2:D:182:VAL:HG13	2.27	0.65
2:F:12:LYS:HG3	2:F:18:VAL:HB	1.78	0.65
2:J:13:LYS:HD2	2:J:113:SER:HA	1.79	0.65
2:J:19:LYS:HA	2:J:80:MET:O	1.96	0.65
1:K:100:GLN:HG2	1:K:101:GLY:N	2.12	0.65
2:N:32:TYR:CD2	2:N:94:LYS:HE3	2.32	0.65
1:I:197:THR:HG22	1:I:204:PRO:HB3	1.79	0.64
1:C:184:ALA:O	1:C:185:ASP:C	2.35	0.64
2:H:176:TYR:CD2	2:H:176:TYR:N	2.66	0.64
1:G:150:VAL:HG22	1:G:192:TYR:HD1	1.62	0.64
1:K:33:LEU:HG	1:K:71:PHE:CG	2.32	0.64
1:M:198:HIS:CD2	1:M:199:GLN:N	2.65	0.64
1:A:40:PRO:O	1:A:42:LYS:N	2.30	0.64
1:K:179:LEU:C	1:K:179:LEU:HD12	2.16	0.64
2:B:59:TYR:CD2	2:B:67:VAL:HG13	2.32	0.64
2:F:121:VAL:CG1	2:F:198:VAL:HG21	2.28	0.64
2:H:199:ASN:C	2:H:199:ASN:HD22	1.98	0.64
2:L:11:VAL:HG22	2:L:110:THR:HB	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:113:PRO:HB3	1:O:139:PHE:CB	2.18	0.64
2:B:54:PHE:CD1	2:B:54:PHE:N	2.63	0.64
1:I:12:SER:O	1:I:13:ALA:HB2	1.97	0.64
1:K:147:GLN:O	1:K:194:CYS:HA	1.97	0.64
2:N:90:TYR:HE1	2:N:109:VAL:HB	1.63	0.64
2:P:2:VAL:HG22	2:P:3:GLN:N	2.12	0.64
2:B:35:SER:OG	2:B:47:TRP:NE1	2.31	0.64
2:J:86:ASP:O	2:J:88:ALA:N	2.30	0.64
1:O:38:GLN:HA	3:O:217:HOH:O	1.98	0.64
2:B:124:LEU:HD12	2:B:139:GLY:C	2.18	0.64
2:J:4:LEU:HD21	2:J:102:VAL:HG13	1.79	0.64
2:L:138:LEU:HD12	2:L:139:GLY:N	2.11	0.64
2:L:164:HIS:HB2	2:L:181:VAL:CG2	2.28	0.64
2:P:201:LYS:HB3	2:P:202:PRO:CD	2.23	0.64
2:H:4:LEU:HD12	2:H:102:VAL:HG13	1.79	0.64
1:I:2:ILE:HB	1:I:90:GLN:NE2	2.11	0.64
1:K:96:HIS:O	2:L:47:TRP:HB3	1.98	0.64
1:O:46:LEU:HD23	1:O:55:GLN:OE1	1.98	0.64
2:P:30:SER:O	2:P:52(A):PRO:HB2	1.97	0.64
2:B:63:PHE:O	2:B:67:VAL:HG12	1.97	0.64
1:C:170:ASP:OD2	1:C:172:THR:HG23	1.98	0.64
1:E:175:LEU:HD23	1:E:176:SER:N	2.13	0.64
2:J:6:GLN:HE22	2:J:91:PHE:HA	1.63	0.64
2:L:159:LEU:HD12	2:L:160:THR:H	1.62	0.64
2:L:18:VAL:O	2:L:81:GLU:HA	1.98	0.64
2:N:90:TYR:CE1	2:N:109:VAL:HB	2.32	0.64
1:G:121:SER:O	1:G:124:GLN:HB3	1.97	0.63
2:L:115:SER:HB3	2:L:117:LYS:HE2	1.79	0.63
2:L:36:TRP:HE1	2:L:78:THR:HG21	1.64	0.63
2:P:36:TRP:CG	2:P:80:MET:HG3	2.32	0.63
2:P:67:VAL:HG22	2:P:68:THR:H	1.63	0.63
2:B:188:SER:HA	2:B:191:THR:CG2	2.28	0.63
2:H:197:ASN:O	2:H:198:VAL:C	2.37	0.63
2:H:51:ILE:HB	2:H:57:ALA:CB	2.28	0.63
1:I:6:GLN:NE2	1:I:86:TYR:O	2.30	0.63
2:J:171:GLN:NE2	2:J:177:SER:HB2	2.14	0.63
2:J:19:LYS:HB2	2:J:81:GLU:OE1	1.98	0.63
2:L:11:VAL:HG22	2:L:110:THR:CB	2.28	0.63
1:C:136:LEU:HD11	1:C:146:VAL:CG2	2.28	0.63
1:E:32:TYR:HD1	1:E:92:TYR:HD1	1.46	0.63
1:E:90:GLN:OE1	1:E:97:THR:N	2.25	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:120:SER:HB3	2:H:122:PHE:CE1	2.33	0.63
1:I:121:SER:O	1:I:124:GLN:N	2.31	0.63
2:N:1:GLN:HG3	2:N:2:VAL:N	2.09	0.63
1:O:8:PRO:CD	1:O:10:SER:H	2.11	0.63
1:G:111:ALA:O	1:G:139:PHE:HA	1.98	0.63
2:H:164:HIS:HB2	2:H:181:VAL:HG22	1.79	0.63
1:M:187:GLU:HG2	1:M:211:ARG:HD2	1.81	0.63
1:M:211:ARG:HH11	1:M:211:ARG:HG2	1.64	0.63
2:P:40:ALA:HA	2:P:88:ALA:HB2	1.80	0.63
2:D:34:ILE:HG21	2:D:78:THR:HG21	1.79	0.63
2:H:131:THR:HG22	2:H:136:ALA:HA	1.81	0.63
2:H:119:PRO:HD3	2:H:200:HIS:CD2	2.34	0.63
1:K:47:LEU:HD11	1:K:86:TYR:HE2	1.63	0.63
2:N:19:LYS:HA	2:N:80:MET:O	1.99	0.63
1:O:83:PHE:CE1	1:O:106:ILE:HD13	2.34	0.63
2:L:126:PRO:HD2	2:L:213:PRO:HA	1.80	0.63
2:D:2:VAL:HG22	2:D:2:VAL:O	1.99	0.63
2:J:29:PHE:O	2:J:52(A):PRO:HG2	1.98	0.63
2:L:84:SER:HB2	2:L:85:GLU:OE2	1.99	0.63
1:A:124:GLN:CD	1:A:130:ALA:HA	2.18	0.63
1:E:54:LEU:HD11	1:E:58:VAL:HG11	1.81	0.63
2:H:199:ASN:HD22	2:H:200:HIS:H	1.43	0.63
1:I:32:TYR:HB3	1:I:91:SER:CB	2.18	0.63
1:K:96:HIS:HB2	2:L:47:TRP:CD2	2.34	0.63
2:N:55:GLY:O	2:N:56:SER:HB3	1.99	0.63
2:H:7:SER:OG	2:H:20:VAL:HG13	1.99	0.63
2:J:62:LYS:C	2:J:64:GLN:H	2.02	0.63
2:P:32:TYR:HD2	2:P:32:TYR:H	1.47	0.63
2:P:6:GLN:HE22	2:P:106:GLY:HA2	1.64	0.63
2:D:108:THR:HG23	2:D:108:THR:O	1.99	0.62
2:D:93:ALA:HB1	2:D:100(L):MET:HG2	1.81	0.62
2:H:121:VAL:HG21	2:H:207:VAL:HG11	1.81	0.62
1:O:35:TRP:CG	1:O:73:LEU:HD13	2.34	0.62
2:D:13:LYS:HA	2:D:112:ALA:O	1.99	0.62
2:P:170:LEU:HD12	2:P:171:GLN:N	2.14	0.62
1:A:118:PHE:CD2	2:B:124:LEU:HB3	2.34	0.62
1:G:174:SER:O	2:H:166:PHE:HE2	1.82	0.62
1:I:139:PHE:CD2	1:I:198:HIS:NE2	2.66	0.62
1:O:210:ASN:O	1:O:213:GLU:HB3	1.99	0.62
1:A:54:LEU:N	1:A:54:LEU:HD12	2.14	0.62
2:B:50:GLY:O	2:B:57:ALA:HB1	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:LEU:HD21	1:C:130:ALA:HB2	1.82	0.62
1:E:54:LEU:HD11	1:E:58:VAL:CG1	2.30	0.62
1:G:47:LEU:CD2	1:G:48:ILE:HG13	2.28	0.62
2:H:138:LEU:HD11	2:H:154:TRP:CH2	2.34	0.62
2:J:148:GLU:HG2	2:J:149:PRO:HA	1.80	0.62
1:M:185:ASP:O	1:M:188:LYS:HB2	1.98	0.62
2:P:39:GLN:O	2:P:88:ALA:HB1	1.98	0.62
1:G:134:CYS:HB2	1:G:148:TRP:CZ2	2.35	0.62
2:J:150:VAL:HG23	2:J:200:HIS:CD2	2.35	0.62
1:K:151:ASP:OD2	1:K:189:HIS:HB3	2.00	0.62
2:L:85:GLU:CD	2:L:85:GLU:H	2.03	0.62
1:E:110:VAL:HG22	1:E:141:PRO:CD	2.29	0.62
1:E:154:LEU:H	1:E:154:LEU:CD2	2.13	0.62
1:E:2:ILE:N	1:E:26:SER:HG	1.97	0.62
1:O:146:VAL:HG13	1:O:196:VAL:HG22	1.82	0.62
2:P:47:TRP:CH2	2:P:49:GLY:HA2	2.34	0.62
1:A:11:LEU:HD23	1:A:104:LEU:HD23	1.75	0.62
1:G:176:SER:HB3	2:H:166:PHE:CZ	2.35	0.62
2:H:119:PRO:HB3	2:H:145:TYR:CB	2.29	0.62
2:H:138:LEU:HD11	2:H:154:TRP:CZ2	2.35	0.62
2:N:100(J):HIS:CG	2:N:100(K):GLY:H	2.18	0.62
2:B:4:LEU:HD12	2:B:103:TRP:C	2.21	0.62
2:D:121:VAL:HG21	2:D:198:VAL:HG21	1.81	0.62
2:F:93:ALA:HB3	2:F:100(L):MET:SD	2.39	0.62
1:G:164:THR:HG23	1:G:174:SER:O	1.99	0.62
2:J:93:ALA:HA	2:J:102:VAL:O	1.99	0.62
2:J:94:LYS:HE2	2:J:96:GLY:HA2	1.82	0.62
1:K:8:PRO:HA	1:K:101:GLY:O	2.00	0.62
2:N:52:ILE:HG22	2:N:52(A):PRO:O	2.00	0.62
2:F:121:VAL:HG21	2:F:198:VAL:HG21	1.81	0.62
1:G:164:THR:HG21	1:G:174:SER:HB2	1.82	0.62
1:G:186:TYR:CE1	1:G:192:TYR:HE2	2.18	0.62
2:H:54:PHE:CD1	2:H:54:PHE:N	2.68	0.62
1:E:11:LEU:HD21	1:I:154:LEU:HD12	1.82	0.62
2:J:87:THR:HG23	2:J:110:THR:HA	1.82	0.62
1:O:54:LEU:HD12	1:O:55:GLN:N	2.15	0.62
1:O:89:GLN:HG3	1:O:98:PHE:CE2	2.35	0.62
2:P:23:LYS:HB2	2:P:77:THR:OG1	2.00	0.62
2:B:126:PRO:HD3	2:B:211:VAL:HG12	1.82	0.61
2:D:12:LYS:HB3	2:D:16:SER:OG	1.99	0.61
1:E:151:ASP:O	1:E:152:ASN:CB	2.43	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:105:GLN:N	2:F:105:GLN:OE1	2.28	0.61
2:F:20:VAL:HG12	2:F:21:SER:H	1.65	0.61
2:H:32:TYR:CG	2:H:94:LYS:HE3	2.35	0.61
1:K:26:SER:HG	1:K:27:GLN:CD	2.01	0.61
1:K:19:VAL:CG2	1:K:78:LEU:HD21	2.28	0.61
2:D:6:GLN:N	2:D:105:GLN:OE1	2.27	0.61
2:F:126:PRO:HG3	2:F:138:LEU:HB3	1.82	0.61
1:K:11:LEU:HB3	1:K:104:LEU:HD23	1.83	0.61
1:O:61:ARG:HG3	1:O:62:PHE:CE1	2.35	0.61
1:A:54:LEU:CD1	1:A:54:LEU:H	2.14	0.61
2:H:130:SER:O	2:H:137:ALA:N	2.31	0.61
1:K:136:LEU:HD21	1:K:196:VAL:CG1	2.30	0.61
1:O:138:ASN:N	1:O:138:ASN:ND2	2.48	0.61
1:O:7:SER:HB3	1:O:8:PRO:HD3	1.81	0.61
1:E:130:ALA:N	1:E:181:LEU:O	2.23	0.61
1:G:61:ARG:CZ	1:G:79:GLN:HG3	2.29	0.61
1:I:169:LYS:HE2	1:I:170:ASP:OD1	2.01	0.61
2:L:34:ILE:N	2:L:34:ILE:HD12	2.16	0.61
1:M:3:GLN:CB	1:M:26:SER:HB3	2.30	0.61
1:M:30:SER:O	1:M:71:PHE:HZ	1.84	0.61
1:O:210:ASN:HB2	1:O:213:GLU:OE1	2.00	0.61
1:G:118:PHE:N	1:G:118:PHE:CD2	2.67	0.61
1:A:33:LEU:HD13	1:A:34:ASN:N	2.16	0.61
2:B:126:PRO:HG3	2:B:138:LEU:CB	2.31	0.61
2:D:171:GLN:HB2	2:D:175:LEU:O	2.01	0.61
1:E:81:GLU:OE1	1:E:81:GLU:N	2.33	0.61
2:H:84:SER:C	2:H:86:ASP:H	2.04	0.61
1:C:154:LEU:N	1:C:154:LEU:HD22	2.14	0.61
2:D:39:GLN:NE2	2:D:43:GLN:O	2.33	0.61
1:I:175:LEU:HD23	1:I:176:SER:N	2.16	0.61
2:J:136:ALA:O	2:J:183:THR:HA	2.01	0.61
2:L:55:GLY:O	2:L:56:SER:CB	2.48	0.61
1:M:61:ARG:NH2	3:M:228:HOH:O	2.33	0.61
2:N:109:VAL:HG12	2:N:109:VAL:O	2.00	0.61
1:A:20:THR:CG2	1:A:74:THR:HG23	2.29	0.61
2:B:34:ILE:HG21	2:B:78:THR:HG21	1.81	0.61
2:H:22:CYS:C	2:H:77:THR:HG23	2.21	0.61
1:O:155:GLN:OE1	1:O:158:ASN:ND2	2.34	0.61
1:O:37:GLN:HG2	1:O:38:GLN:N	2.15	0.61
1:O:61:ARG:O	1:O:75:ILE:HA	2.01	0.61
2:B:199:ASN:C	2:B:199:ASN:ND2	2.52	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:33:LEU:HD13	1:E:34:ASN:N	2.16	0.61
2:F:143:LYS:HE2	2:F:171:GLN:OE1	2.01	0.61
2:H:124:LEU:HB2	2:H:139:GLY:C	2.21	0.61
1:I:143:GLU:O	1:I:198:HIS:CD2	2.54	0.61
1:K:201:LEU:HD13	1:K:205:VAL:HG21	1.81	0.61
1:K:59:PRO:HB3	1:K:61:ARG:NH1	2.16	0.61
1:I:125:LEU:HD22	1:I:183:LYS:HG3	1.81	0.61
2:L:152:VAL:HG11	2:L:180:SER:OG	2.01	0.61
2:B:94:LYS:HD2	2:B:102:VAL:HG12	1.81	0.60
2:B:94:LYS:HE2	2:B:96:GLY:N	2.16	0.60
2:D:171:GLN:NE2	2:D:177:SER:HB2	2.14	0.60
2:H:172:SER:O	1:K:26:SER:HA	2.01	0.60
1:E:11:LEU:CD2	1:I:156:SER:HB2	2.29	0.60
1:I:184:ALA:HB1	1:I:188:LYS:HE3	1.83	0.60
2:J:94:LYS:HE2	2:J:96:GLY:CA	2.31	0.60
1:K:49:TYR:N	1:K:49:TYR:CD2	2.68	0.60
1:C:150:VAL:HG22	1:C:192:TYR:HD1	1.66	0.60
1:C:186:TYR:O	1:C:192:TYR:OH	2.19	0.60
1:E:192:TYR:O	1:E:208:SER:HB2	2.00	0.60
1:I:80:PRO:O	1:I:83:PHE:HD1	1.84	0.60
2:L:82(A):SER:O	2:L:82(B):SER:HB2	2.01	0.60
1:A:135:LEU:CD1	2:B:181:VAL:HG21	2.31	0.60
2:B:53:VAL:C	2:B:54:PHE:HD1	2.04	0.60
2:F:37:VAL:HG13	2:F:46:GLU:C	2.21	0.60
1:G:165:GLU:HB3	3:G:216:HOH:O	2.00	0.60
2:H:51:ILE:HD12	2:H:57:ALA:HB2	1.83	0.60
2:J:162:GLY:C	2:J:182:VAL:HG23	2.22	0.60
2:L:143:LYS:HA	2:L:177:SER:OG	2.01	0.60
2:L:47:TRP:CH2	2:L:49:GLY:HA2	2.36	0.60
2:H:2:VAL:HG22	2:H:2:VAL:O	1.99	0.60
1:I:33:LEU:HG	1:I:71:PHE:CD2	2.36	0.60
2:L:131:THR:HA	2:L:135:THR:O	2.01	0.60
2:L:61:GLN:O	2:L:64:GLN:HB2	2.01	0.60
2:L:73:GLU:C	2:L:75:THR:H	2.05	0.60
1:M:161:GLU:HB2	1:M:175:LEU:HD21	1.83	0.60
1:O:191:VAL:HG22	1:O:210:ASN:OD1	2.02	0.60
2:B:39:GLN:HG3	2:B:43:GLN:O	2.01	0.60
2:D:95:GLY:O	2:D:96:GLY:C	2.39	0.60
2:J:2:VAL:O	2:J:2:VAL:HG13	2.01	0.60
1:K:195:GLU:HA	1:K:205:VAL:O	2.01	0.60
2:N:17:SER:HB3	2:N:82(A):SER:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:67:VAL:HG22	2:P:68:THR:N	2.15	0.60
2:P:29:PHE:HE1	2:P:73:GLU:HG3	1.66	0.60
1:A:47:LEU:HD11	1:A:86:TYR:HE2	1.66	0.60
2:B:163:VAL:HG22	2:B:182:VAL:HB	1.84	0.60
1:C:35:TRP:CE2	1:C:73:LEU:HB2	2.36	0.60
1:C:87:TYR:OH	2:D:44:GLY:HA2	2.02	0.60
2:H:61:GLN:HA	2:H:64:GLN:OE1	2.02	0.60
2:J:83:ARG:HB3	2:J:85:GLU:CG	2.25	0.60
1:G:186:TYR:C	1:G:188:LYS:H	2.05	0.60
2:H:102:VAL:HG23	3:H:221:HOH:O	2.02	0.60
2:J:30:SER:O	2:J:52(A):PRO:HB2	2.02	0.60
1:A:18:ARG:NH2	1:A:76:SER:HA	2.16	0.60
1:C:133:VAL:HG22	1:C:178:THR:HG23	1.83	0.60
2:J:109:VAL:HG12	2:J:109:VAL:O	2.01	0.60
2:J:201:LYS:HB2	2:J:202:PRO:HD3	1.83	0.60
2:D:18:VAL:CG2	2:D:19:LYS:N	2.65	0.60
2:F:37:VAL:HA	2:F:46:GLU:O	2.02	0.60
2:H:146:PHE:HB2	2:H:175:LEU:CD2	2.32	0.60
1:K:33:LEU:HD13	1:K:34:ASN:N	2.17	0.60
2:N:36:TRP:HE1	2:N:78:THR:CG2	2.14	0.60
2:F:89:VAL:CG2	2:F:108:THR:HG23	2.31	0.60
1:G:61:ARG:O	1:G:75:ILE:HA	2.02	0.60
1:I:83:PHE:CZ	1:I:106:ILE:HG12	2.37	0.60
2:N:115:SER:O	2:N:146:PHE:HB3	2.02	0.60
2:N:51:ILE:HG13	2:N:56:SER:O	2.02	0.60
2:P:38:ARG:HG3	2:P:46:GLU:HB3	1.82	0.60
2:B:77:THR:HG22	2:B:78:THR:N	2.16	0.59
2:F:182:VAL:O	2:F:182:VAL:HG22	2.00	0.59
1:G:11:LEU:HD12	1:G:104:LEU:HD23	1.84	0.59
1:K:118:PHE:CB	2:L:124:LEU:HD22	2.31	0.59
1:A:211:ARG:CB	1:A:211:ARG:HH11	2.09	0.59
1:E:154:LEU:HD22	1:E:154:LEU:N	2.16	0.59
2:F:29:PHE:CD1	2:F:30:SER:N	2.70	0.59
2:H:29:PHE:HB2	2:H:76:SER:HB2	1.84	0.59
2:N:163:VAL:HG12	2:N:164:HIS:N	2.17	0.59
2:P:171:GLN:HG3	2:P:175:LEU:O	2.02	0.59
1:E:198:HIS:HB3	1:E:201:LEU:HD12	1.84	0.59
1:G:209:PHE:CD1	1:G:209:PHE:C	2.74	0.59
2:J:131:THR:HG22	2:J:136:ALA:CA	2.28	0.59
1:K:124:GLN:O	1:K:125:LEU:C	2.39	0.59
1:K:3:GLN:O	1:K:25:ALA:HA	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:30:SER:HA	2:L:52(A):PRO:HB2	1.83	0.59
2:F:199:ASN:HD22	2:F:200:HIS:N	2.01	0.59
1:G:180:THR:HG21	2:H:143:LYS:CE	2.32	0.59
2:H:36:TRP:CG	2:H:69:ILE:HD11	2.37	0.59
2:L:136:ALA:HB2	2:L:186:SER:HB3	1.82	0.59
2:P:21:SER:O	2:P:22:CYS:HB3	2.01	0.59
2:P:2:VAL:HG21	2:P:32:TYR:CE1	2.36	0.59
2:P:36:TRP:CE2	2:P:80:MET:HB2	2.37	0.59
1:C:150:VAL:HG22	1:C:192:TYR:CD1	2.38	0.59
2:D:111:VAL:HG12	2:D:111:VAL:O	2.01	0.59
2:F:32:TYR:HB3	2:F:94:LYS:CG	2.31	0.59
1:G:186:TYR:O	1:G:188:LYS:N	2.36	0.59
2:H:143:LYS:HA	2:H:177:SER:OG	2.02	0.59
2:J:53:VAL:HG12	2:J:53:VAL:O	2.02	0.59
1:K:182:SER:OG	1:K:184:ALA:HB3	2.02	0.59
2:P:10:GLU:O	2:P:109:VAL:HA	2.02	0.59
2:P:38:ARG:N	2:P:46:GLU:O	2.33	0.59
1:G:83:PHE:CD1	1:G:106:ILE:HG13	2.37	0.59
1:K:202:SER:O	1:K:203:SER:CB	2.51	0.59
2:L:162:GLY:O	2:L:182:VAL:HA	2.02	0.59
2:P:53:VAL:HG12	2:P:53:VAL:O	2.02	0.59
2:B:52(A):PRO:O	2:B:55:GLY:N	2.31	0.59
1:C:116:PHE:CD2	2:D:137:ALA:HB3	2.38	0.59
1:E:8:PRO:HA	1:E:102:THR:HA	1.85	0.59
1:I:139:PHE:HD2	1:I:198:HIS:CE1	2.20	0.59
1:I:117:ILE:CD1	1:I:207:LYS:O	2.51	0.59
2:J:161:SER:C	2:J:163:VAL:H	2.06	0.59
2:L:202:PRO:O	2:L:203:SER:CB	2.48	0.59
1:A:119:PRO:HB3	1:A:209:PHE:CE2	2.37	0.59
2:H:134:GLY:O	2:H:185:PRO:HA	2.03	0.59
2:J:94:LYS:HB3	2:J:102:VAL:CG1	2.33	0.59
1:M:136:LEU:HG	1:M:196:VAL:HG21	1.85	0.59
1:M:151:ASP:C	1:M:153:ALA:H	2.04	0.59
1:M:19:VAL:O	1:M:74:THR:HG23	2.02	0.59
2:B:68:THR:HB	2:B:81:GLU:HB3	1.84	0.59
2:H:87:THR:HG23	2:H:109:VAL:O	2.03	0.59
1:M:136:LEU:N	1:M:136:LEU:HD12	2.17	0.59
2:N:192:GLN:HG2	2:N:194:TYR:CZ	2.38	0.59
2:P:195:ILE:HG12	2:P:210:LYS:HA	1.83	0.59
1:A:76:SER:OG	1:A:77:SER:N	2.35	0.59
2:B:36:TRP:HE1	2:B:78:THR:HG21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:110:THR:O	2:D:110:THR:HG22	2.03	0.59
1:E:175:LEU:C	1:E:175:LEU:HD23	2.23	0.59
1:I:88:CYS:O	1:I:98:PHE:HD2	1.85	0.59
2:J:17:SER:CB	2:J:82(A):SER:HA	2.28	0.59
2:L:18:VAL:HG22	2:L:19:LYS:N	2.17	0.59
1:M:210:ASN:ND2	1:M:210:ASN:N	2.51	0.59
1:M:93:SER:OG	1:M:94:THR:N	2.36	0.59
2:N:83:ARG:O	2:N:111:VAL:HG11	2.02	0.59
1:A:123:GLU:N	1:A:123:GLU:OE2	2.36	0.58
2:B:36:TRP:HE1	2:B:78:THR:CG2	2.15	0.58
2:D:17:SER:HB2	2:D:82(A):SER:HA	1.84	0.58
2:J:207:VAL:HG12	2:J:208:ASP:N	2.17	0.58
2:J:208:ASP:N	2:J:208:ASP:OD1	2.36	0.58
2:B:62:LYS:HA	2:N:83:ARG:NH2	2.17	0.58
1:E:18:ARG:HH12	1:E:76:SER:HB3	1.68	0.58
2:H:170:LEU:HD12	2:H:171:GLN:H	1.68	0.58
1:K:142:ARG:NH1	1:K:163:VAL:HG11	2.06	0.58
1:K:46:LEU:HB3	3:K:225:HOH:O	2.03	0.58
1:M:67:SER:HA	1:M:71:PHE:CZ	2.37	0.58
2:N:138:LEU:HD12	2:N:139:GLY:N	2.18	0.58
1:O:138:ASN:HD22	1:O:138:ASN:N	2.00	0.58
1:O:183:LYS:O	1:O:187:GLU:HG3	2.03	0.58
1:A:115:VAL:HG12	1:A:116:PHE:N	2.18	0.58
1:A:151:ASP:HB2	3:A:232:HOH:O	2.01	0.58
2:B:124:LEU:HD12	2:B:140:CYS:N	2.19	0.58
1:C:116:PHE:HD2	2:D:130:SER:CB	2.15	0.58
1:C:210:ASN:HD22	1:C:210:ASN:N	2.00	0.58
2:F:148:GLU:HG2	2:F:176:TYR:CD2	2.38	0.58
2:F:40:ALA:O	2:F:43:GLN:HB2	2.03	0.58
1:K:152:ASN:ND2	1:K:152:ASN:N	2.51	0.58
1:K:79:GLN:HB3	1:K:80:PRO:HD2	1.84	0.58
1:M:24:ARG:NH1	3:M:221:HOH:O	2.36	0.58
1:O:161:GLU:HA	1:O:176:SER:O	2.03	0.58
1:O:183:LYS:HA	1:O:186:TYR:HB3	1.84	0.58
1:O:195:GLU:CD	1:O:204:PRO:HB3	2.23	0.58
2:P:21:SER:O	2:P:22:CYS:CB	2.51	0.58
1:A:124:GLN:NE2	1:A:131:SER:N	2.51	0.58
1:I:122:ASP:HA	1:I:125:LEU:HD12	1.86	0.58
2:J:150:VAL:HG23	2:J:200:HIS:HD2	1.68	0.58
2:J:171:GLN:NE2	2:J:177:SER:HB3	2.18	0.58
1:M:181:LEU:HD12	1:M:181:LEU:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:154:LEU:H	1:G:154:LEU:HD22	1.69	0.58
2:H:19:LYS:CE	2:H:79:TYR:HB3	2.32	0.58
1:I:142:ARG:HG2	1:I:142:ARG:O	2.03	0.58
1:M:201:LEU:HD13	1:M:205:VAL:HG23	1.85	0.58
1:A:90:GLN:NE2	1:A:93:SER:HB3	2.18	0.58
1:K:11:LEU:HD12	1:K:104:LEU:CD2	2.31	0.58
1:A:34:ASN:ND2	1:A:91:SER:HB2	2.19	0.58
1:C:142:ARG:HH11	1:C:142:ARG:HG2	1.69	0.58
1:G:151:ASP:OD2	1:G:189:HIS:ND1	2.36	0.58
1:I:54:LEU:HD21	1:I:59:PRO:O	2.02	0.58
2:P:18:VAL:HG12	2:P:82(C):LEU:HD11	1.85	0.58
1:A:90:GLN:HE22	1:A:93:SER:HB3	1.68	0.58
1:G:83:PHE:CE1	1:G:106:ILE:HG13	2.38	0.58
2:P:131:THR:HG22	2:P:136:ALA:CB	2.32	0.58
1:A:142:ARG:HG3	1:A:142:ARG:O	2.02	0.58
2:D:138:LEU:HD12	2:D:138:LEU:C	2.24	0.58
1:E:65:SER:OG	1:E:72:THR:HG23	2.04	0.58
1:G:180:THR:HG21	2:H:143:LYS:HE2	1.85	0.58
2:J:171:GLN:C	2:J:173:SER:H	2.07	0.58
1:K:52:SER:HB3	1:K:64:GLY:O	2.04	0.58
1:K:27:GLN:O	1:K:69:THR:HG22	2.03	0.58
2:P:119:PRO:HD3	2:P:200:HIS:ND1	2.19	0.58
2:B:68:THR:O	2:B:81:GLU:HB3	2.04	0.58
2:H:184:VAL:HG21	2:H:194:TYR:CZ	2.39	0.58
1:O:170:ASP:O	1:O:172:THR:N	2.37	0.58
1:O:138:ASN:HA	1:O:173:TYR:O	2.04	0.58
1:A:18:ARG:NH1	1:A:18:ARG:HB2	2.19	0.57
2:B:52(A):PRO:O	2:B:54:PHE:N	2.37	0.57
2:D:197:ASN:ND2	2:D:208:ASP:OD1	2.37	0.57
1:E:110:VAL:HG13	1:E:140:TYR:O	2.04	0.57
2:F:131:THR:HG22	2:F:136:ALA:HA	1.85	0.57
1:M:197:THR:HG22	1:M:204:PRO:CG	2.33	0.57
1:M:79:GLN:HB3	1:M:81:GLU:OE2	2.04	0.57
2:B:184:VAL:HB	2:B:185:PRO:CD	2.34	0.57
2:F:182:VAL:O	2:F:184:VAL:HG13	2.04	0.57
2:H:67:VAL:HA	2:H:81:GLU:O	2.04	0.57
1:I:89:GLN:HB2	1:I:98:PHE:CE2	2.39	0.57
1:K:179:LEU:HD11	1:K:181:LEU:HD13	1.85	0.57
1:O:25:ALA:O	1:O:69:THR:HG22	2.04	0.57
1:O:83:PHE:CZ	1:O:106:ILE:HD13	2.40	0.57
2:P:146:PHE:C	2:P:146:PHE:CD2	2.77	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:75:ILE:CG2	1:C:78:LEU:HD12	2.34	0.57
1:C:39:LYS:HG2	1:C:84:ALA:HB2	1.87	0.57
1:E:66:GLY:O	1:E:67:SER:HB3	2.04	0.57
2:H:170:LEU:HD12	2:H:171:GLN:N	2.19	0.57
2:P:127:SER:O	2:P:131:THR:HG23	2.04	0.57
2:F:24:ALA:HB3	2:F:29:PHE:HB2	1.86	0.57
2:H:124:LEU:HD21	2:H:141:LEU:HB3	1.82	0.57
1:I:110:VAL:HG12	1:I:111:ALA:H	1.69	0.57
2:J:171:GLN:HE21	2:J:177:SER:HB3	1.69	0.57
1:K:136:LEU:HD21	1:K:196:VAL:HG11	1.85	0.57
2:L:63:PHE:HB3	2:L:67:VAL:CG1	2.34	0.57
2:P:82(A):SER:O	2:P:82(B):SER:C	2.42	0.57
2:B:69:ILE:HA	2:B:79:TYR:O	2.05	0.57
1:C:35:TRP:CZ3	1:C:88:CYS:HB3	2.39	0.57
2:D:18:VAL:HG12	2:D:82(C):LEU:CD1	2.29	0.57
2:F:155:ASN:HD22	2:F:159:LEU:HB2	1.70	0.57
2:H:69:ILE:HG13	2:H:80:MET:HG2	1.86	0.57
2:J:61:GLN:H	2:J:61:GLN:HE21	0.78	0.57
2:L:90:TYR:HE1	2:L:109:VAL:HB	1.70	0.57
2:N:28:THR:HG22	2:N:28:THR:O	2.03	0.57
1:O:135:LEU:HD13	2:P:181:VAL:HG21	1.84	0.57
2:P:146:PHE:H	2:P:200:HIS:HE1	1.52	0.57
2:P:94:LYS:HD3	2:P:94:LYS:C	2.25	0.57
1:C:32:TYR:HB3	1:C:91:SER:HB3	1.85	0.57
1:E:14:SER:HB2	1:E:17:ASP:OD1	2.04	0.57
2:H:48:MET:HE3	2:H:63:PHE:HE2	1.69	0.57
2:L:193:THR:HG22	2:L:194:TYR:N	2.20	0.57
2:N:150:VAL:HG23	2:N:199:ASN:O	2.04	0.57
2:F:185:PRO:HB2	2:F:188:SER:CB	2.34	0.57
2:H:138:LEU:CD1	2:H:139:GLY:N	2.68	0.57
1:M:112:ALA:HB2	1:M:200:GLY:O	2.03	0.57
2:P:199:ASN:HD22	2:P:200:HIS:N	2.02	0.57
2:B:169:VAL:O	2:B:176:TYR:HA	2.05	0.57
1:C:45:LYS:HG2	1:C:47:LEU:HD23	1.86	0.57
2:D:17:SER:HB2	2:D:82:LEU:O	2.05	0.57
2:J:189:LEU:C	2:J:191:THR:H	2.08	0.57
1:K:55:GLN:O	1:K:58:VAL:HG23	2.05	0.57
2:L:37:VAL:HG12	2:L:38:ARG:N	2.19	0.57
2:L:40:ALA:HA	2:L:88:ALA:HB2	1.86	0.57
1:O:27:GLN:O	1:O:29:ILE:HG23	2.04	0.57
1:C:199:GLN:HA	1:O:199:GLN:NE2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:165:THR:HG23	2:D:180:SER:CB	2.31	0.57
2:H:193:THR:HG22	2:H:194:TYR:N	2.20	0.57
1:I:27:GLN:O	1:I:29:ILE:HG23	2.05	0.57
1:O:94:THR:CG2	1:O:95:SER:N	2.68	0.57
1:A:3:GLN:O	1:A:4:MET:SD	2.62	0.57
1:C:145:LYS:HD3	1:C:197:THR:CG2	2.35	0.57
1:E:30:SER:OG	1:E:31:SER:N	2.38	0.57
2:H:48:MET:HE3	2:H:63:PHE:CE2	2.40	0.57
1:M:26:SER:HB2	1:M:27:GLN:NE2	2.20	0.57
2:B:131:THR:HG22	2:B:136:ALA:CA	2.35	0.56
1:C:161:GLU:HA	3:C:214:HOH:O	2.03	0.56
1:C:168:SER:OG	1:C:169:LYS:N	2.38	0.56
2:F:30:SER:HA	2:F:52(A):PRO:CB	2.35	0.56
1:G:164:THR:CG2	1:G:174:SER:HB2	2.35	0.56
2:H:84:SER:O	2:H:86:ASP:N	2.38	0.56
1:K:47:LEU:C	1:K:48:ILE:HG13	2.25	0.56
1:K:47:LEU:O	1:K:55:GLN:HB3	2.05	0.56
1:C:199:GLN:NE2	1:O:199:GLN:HA	2.20	0.56
2:B:146:PHE:HB2	2:B:175:LEU:HD23	1.86	0.56
1:C:61:ARG:HD3	1:C:79:GLN:HE21	1.69	0.56
2:F:168:ALA:HA	2:F:178:LEU:HB3	1.88	0.56
1:I:6:GLN:HE22	1:I:87:TYR:CA	2.18	0.56
2:J:47:TRP:HE1	2:J:100(L):MET:HE1	1.70	0.56
1:K:164:THR:HG21	1:K:174:SER:HB2	1.87	0.56
1:K:164:THR:HG22	1:K:174:SER:O	2.05	0.56
2:P:145:TYR:O	2:P:146:PHE:CB	2.52	0.56
2:B:51:ILE:HD11	2:B:55:GLY:O	2.04	0.56
1:C:45:LYS:HG2	1:C:47:LEU:CD2	2.35	0.56
1:C:90:GLN:OE1	1:C:93:SER:HB3	2.06	0.56
1:E:116:PHE:HD2	2:F:130:SER:CA	2.19	0.56
2:J:145:TYR:O	2:J:146:PHE:HB2	2.05	0.56
1:K:55:GLN:HB3	1:K:58:VAL:HG21	1.87	0.56
2:L:154:TRP:CZ3	2:L:196:CYS:HB3	2.40	0.56
2:L:170:LEU:HD12	2:L:171:GLN:N	2.20	0.56
1:M:192:TYR:O	1:M:208:SER:HB2	2.06	0.56
2:P:89:VAL:HA	2:P:107:THR:O	2.05	0.56
1:G:48:ILE:HD12	1:G:64:GLY:HA3	1.86	0.56
1:G:162:SER:OG	2:H:167:PRO:HD2	2.05	0.56
2:H:39:GLN:C	2:H:88:ALA:HB1	2.26	0.56
1:M:124:GLN:HE22	1:M:131:SER:HB2	1.69	0.56
1:M:62:PHE:HE2	1:M:86:TYR:HE2	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:VAL:HG12	1:A:192:TYR:N	2.20	0.56
1:C:130:ALA:N	1:C:181:LEU:O	2.31	0.56
2:F:54:PHE:O	2:F:55:GLY:C	2.44	0.56
1:G:11:LEU:HD12	1:G:104:LEU:HD21	1.87	0.56
1:G:96:HIS:HB2	2:H:47:TRP:CE2	2.40	0.56
2:H:1:GLN:O	2:H:26:GLY:HA3	2.06	0.56
2:H:30:SER:O	2:H:53:VAL:HG23	2.06	0.56
2:J:171:GLN:HE21	2:J:177:SER:CB	2.18	0.56
2:L:1:GLN:CD	2:L:1:GLN:H3	2.08	0.56
1:O:142:ARG:HG2	1:O:142:ARG:O	2.06	0.56
1:C:167:ASP:HA	3:C:221:HOH:O	2.05	0.56
2:D:84:SER:HB2	2:D:85:GLU:OE2	2.05	0.56
2:F:100(J):HIS:N	3:F:225:HOH:O	2.39	0.56
2:F:4:LEU:HA	2:F:23:LYS:O	2.05	0.56
2:F:4:LEU:HD22	2:F:22:CYS:SG	2.46	0.56
1:G:14:SER:HB2	1:G:17:ASP:OD1	2.04	0.56
2:H:111:VAL:O	2:H:112:ALA:HB2	2.05	0.56
1:M:164:THR:HB	1:M:174:SER:H	1.70	0.56
1:A:117:ILE:HG22	2:B:129:LYS:HB3	1.88	0.56
1:E:47:LEU:O	1:E:48:ILE:HG13	2.05	0.56
2:F:11:VAL:HA	2:F:110:THR:O	2.05	0.56
2:D:145:TYR:CE1	2:D:176:TYR:HB2	2.41	0.56
2:D:63:PHE:HB3	2:D:67:VAL:HG12	1.86	0.56
2:F:201:LYS:N	2:F:202:PRO:CD	2.68	0.56
1:G:48:ILE:CD1	1:G:64:GLY:HA3	2.35	0.56
2:J:91:PHE:CD1	2:J:91:PHE:N	2.74	0.56
1:K:6:GLN:O	1:K:100:GLN:NE2	2.39	0.56
1:K:123:GLU:N	1:K:123:GLU:CD	2.46	0.56
1:A:147:GLN:OE1	1:A:147:GLN:HA	2.06	0.56
1:C:142:ARG:NH2	1:C:163:VAL:HG21	2.20	0.56
2:H:19:LYS:HE2	2:H:79:TYR:HD2	1.70	0.56
2:L:19:LYS:HG2	3:L:215:HOH:O	2.05	0.56
1:O:119:PRO:HB3	1:O:209:PHE:CZ	2.41	0.56
2:P:28:THR:N	2:P:32:TYR:OH	2.38	0.56
2:P:2:VAL:O	2:P:3:GLN:HB2	2.06	0.56
1:A:90:GLN:HG3	1:A:97:THR:N	2.20	0.56
1:C:195:GLU:HA	1:C:205:VAL:O	2.06	0.56
1:C:28:SER:HA	1:C:68:GLY:O	2.06	0.56
2:D:10:GLU:O	2:D:109:VAL:HA	2.05	0.56
2:F:7:SER:N	2:F:21:SER:OG	2.38	0.56
2:B:192:GLN:HG3	2:B:193:THR:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:ALA:HA	1:O:18:ARG:HB3	1.88	0.56
1:E:55:GLN:OE1	1:E:56:SER:N	2.37	0.56
1:G:150:VAL:HG22	1:G:192:TYR:CD1	2.41	0.56
1:G:151:ASP:O	1:G:152:ASN:HB2	2.05	0.56
1:G:61:ARG:NE	1:G:82:ASP:OD2	2.38	0.56
2:H:1:GLN:O	2:H:25:SER:O	2.24	0.56
1:G:11:LEU:HB3	1:G:104:LEU:HD23	1.88	0.55
2:H:7:SER:CB	2:H:21:SER:H	2.19	0.55
1:I:13:ALA:N	1:I:107:LYS:HB2	2.21	0.55
1:I:120:PRO:HD3	1:I:132:VAL:HG22	1.88	0.55
1:O:133:VAL:HG22	1:O:178:THR:HG23	1.87	0.55
1:A:169:LYS:HG3	1:A:170:ASP:H	1.71	0.55
1:A:167:ASP:O	1:A:171:SER:HA	2.06	0.55
1:C:83:PHE:HA	1:C:104:LEU:HB3	1.87	0.55
1:G:136:LEU:HD11	1:G:196:VAL:CG2	2.34	0.55
1:I:184:ALA:C	1:I:188:LYS:HE3	2.26	0.55
1:E:154:LEU:HD23	1:I:18:ARG:O	2.05	0.55
1:I:83:PHE:CE1	1:I:106:ILE:HG12	2.40	0.55
2:J:30:SER:O	2:J:53:VAL:HG23	2.06	0.55
2:J:80:MET:HE1	2:J:82:LEU:HB2	1.89	0.55
1:K:128:GLY:HA2	3:K:218:HOH:O	2.06	0.55
1:K:30:SER:O	1:K:71:PHE:HZ	1.89	0.55
2:L:35:SER:HG	2:L:47:TRP:HE1	1.55	0.55
1:M:18:ARG:NH1	1:M:18:ARG:HB2	2.15	0.55
1:C:52:SER:HB2	3:C:220:HOH:O	2.06	0.55
1:E:26:SER:HB2	1:E:27:GLN:NE2	2.21	0.55
2:H:168:ALA:HA	2:H:178:LEU:HB3	1.88	0.55
2:H:37:VAL:HG13	2:H:47:TRP:HA	1.88	0.55
1:M:125:LEU:HD22	1:M:183:LYS:HG3	1.87	0.55
1:M:186:TYR:CE1	1:M:192:TYR:CE2	2.95	0.55
1:O:158:ASN:N	1:O:158:ASN:OD1	2.33	0.55
2:P:70:THR:O	2:P:78:THR:HG23	2.07	0.55
2:D:33:ALA:HB3	2:D:95:GLY:HA3	1.87	0.55
1:G:110:VAL:CG1	1:G:111:ALA:N	2.69	0.55
2:H:124:LEU:HG	2:H:141:LEU:N	2.19	0.55
1:I:11:LEU:O	1:I:104:LEU:HA	2.06	0.55
2:L:115:SER:O	2:L:117:LYS:HG2	2.06	0.55
1:K:118:PHE:CD1	2:L:124:LEU:HB3	2.41	0.55
2:L:165:THR:HG22	2:L:165:THR:O	2.05	0.55
2:L:6:GLN:NE2	2:L:90:TYR:O	2.40	0.55
1:O:61:ARG:NE	1:O:79:GLN:HG3	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:39:GLN:NE2	2:D:44:GLY:HA2	2.21	0.55
1:E:38:GLN:HB3	1:E:85:THR:HG22	1.89	0.55
1:K:122:ASP:C	1:K:124:GLN:N	2.58	0.55
1:K:170:ASP:OD1	1:K:170:ASP:N	2.40	0.55
1:K:4:MET:CB	1:K:98:PHE:O	2.53	0.55
2:N:20:VAL:HG12	2:N:36:TRP:CH2	2.42	0.55
1:A:135:LEU:HD13	2:B:181:VAL:HG11	1.89	0.55
2:H:164:HIS:O	2:H:180:SER:HA	2.07	0.55
1:I:13:ALA:H	1:I:107:LYS:HB2	1.71	0.55
2:J:155:ASN:O	2:J:158:ALA:HB3	2.06	0.55
1:E:119:PRO:HB3	1:E:209:PHE:CE1	2.42	0.55
1:E:205:VAL:HG12	1:E:206:THR:N	2.22	0.55
1:G:142:ARG:O	1:G:144:ALA:N	2.40	0.55
2:H:10:GLU:O	2:H:109:VAL:HA	2.06	0.55
2:J:82:LEU:HD23	2:J:82(C):LEU:CD2	2.37	0.55
1:G:158:ASN:HD22	1:K:22:THR:HG21	1.71	0.55
1:O:48:ILE:HD13	1:O:64:GLY:HA3	1.88	0.55
1:C:124:GLN:HB2	3:C:223:HOH:O	2.07	0.55
1:C:62:PHE:CD1	1:C:62:PHE:N	2.73	0.55
1:G:110:VAL:HG12	1:G:111:ALA:N	2.20	0.55
1:G:118:PHE:CE2	2:H:130:SER:HB3	2.42	0.55
2:H:119:PRO:HD3	2:H:200:HIS:HD2	1.72	0.55
1:I:150:VAL:HG23	1:I:155:GLN:HG3	1.89	0.55
1:I:79:GLN:HB2	1:I:82:ASP:OD2	2.06	0.55
2:J:35:SER:HB3	2:J:100(L):MET:HE1	1.89	0.55
2:B:14:PRO:HG2	2:B:113:SER:N	2.22	0.55
2:D:192:GLN:HG2	2:D:194:TYR:CZ	2.41	0.55
2:D:32:TYR:HB2	2:D:34:ILE:CD1	2.37	0.55
2:F:71:ALA:HB2	2:F:78:THR:HG23	1.87	0.55
1:M:29:ILE:CG2	1:M:90:GLN:HG3	2.37	0.55
1:M:43:VAL:HG11	2:N:103:TRP:HB2	1.88	0.55
2:N:30:SER:C	2:N:53:VAL:HG23	2.27	0.55
2:P:155:ASN:HB2	2:P:158:ALA:HB3	1.89	0.55
2:B:51:ILE:CG1	2:B:52:ILE:H	2.20	0.55
2:B:73:GLU:C	2:B:75:THR:H	2.10	0.55
2:D:61:GLN:O	2:D:64:GLN:HB2	2.07	0.55
1:G:132:VAL:HG12	1:G:148:TRP:CH2	2.42	0.55
1:G:6:GLN:C	1:G:7:SER:O	2.44	0.55
1:I:142:ARG:HB2	1:I:173:TYR:CE2	2.42	0.55
1:E:199:GLN:OE1	1:I:199:GLN:HA	2.06	0.55
1:I:20:THR:HG23	1:I:74:THR:OG1	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:30:SER:HB2	2:N:53:VAL:HG23	1.89	0.55
2:P:29:PHE:HB3	2:P:76:SER:CB	2.32	0.55
1:I:195:GLU:HA	1:I:205:VAL:O	2.07	0.54
2:J:170:LEU:HD12	2:J:171:GLN:N	2.22	0.54
2:J:4:LEU:HD13	2:J:22:CYS:SG	2.47	0.54
2:J:48:MET:O	2:J:60:ALA:HB2	2.06	0.54
1:K:179:LEU:HD12	1:K:180:THR:H	1.71	0.54
2:N:121:VAL:HA	2:N:141:LEU:O	2.06	0.54
1:O:203:SER:O	1:O:204:PRO:O	2.24	0.54
2:P:19:LYS:HA	2:P:81:GLU:HA	1.87	0.54
2:B:19:LYS:HE2	2:B:79:TYR:CG	2.41	0.54
2:B:87:THR:O	2:B:88:ALA:HB2	2.08	0.54
2:D:122:PHE:HB2	2:D:141:LEU:HB3	1.89	0.54
2:D:184:VAL:HB	2:D:185:PRO:CD	2.37	0.54
2:F:18:VAL:HG22	2:F:19:LYS:N	2.22	0.54
2:J:52:ILE:C	2:J:53:VAL:H	2.10	0.54
1:K:54:LEU:HD12	1:K:55:GLN:H	1.72	0.54
2:L:6:GLN:N	2:L:105:GLN:HE22	2.05	0.54
1:M:159:SER:HA	1:M:178:THR:O	2.08	0.54
2:N:117:LYS:NZ	2:N:144:ASP:HB2	2.22	0.54
2:F:94:LYS:HE2	2:F:95:GLY:CA	2.37	0.54
1:G:35:TRP:HB2	1:G:48:ILE:HB	1.89	0.54
1:I:95:SER:O	1:I:96:HIS:HD2	1.91	0.54
1:K:12:SER:HA	1:K:105:GLU:O	2.07	0.54
2:L:163:VAL:CG2	2:L:182:VAL:HB	2.30	0.54
2:N:163:VAL:HG12	2:N:164:HIS:H	1.72	0.54
1:E:124:GLN:HE22	1:E:131:SER:HB2	1.73	0.54
1:E:168:SER:OG	1:E:169:LYS:N	2.40	0.54
2:H:208:ASP:O	2:H:209:LYS:HB2	2.08	0.54
1:I:86:TYR:O	1:I:101:GLY:HA2	2.07	0.54
1:K:11:LEU:HB3	1:K:104:LEU:CD2	2.38	0.54
2:N:64:GLN:N	3:N:229:HOH:O	2.40	0.54
2:B:150:VAL:O	2:B:150:VAL:HG13	2.06	0.54
1:E:12:SER:HA	1:E:105:GLU:HG3	1.89	0.54
2:H:94:LYS:HD3	2:H:94:LYS:C	2.27	0.54
1:I:4:MET:SD	1:I:90:GLN:HB2	2.48	0.54
2:L:29:PHE:HA	2:L:32:TYR:CD1	2.42	0.54
2:N:201:LYS:O	2:N:203:SER:N	2.41	0.54
1:A:119:PRO:HB3	1:A:209:PHE:CZ	2.43	0.54
1:G:137:ASN:HD22	1:G:138:ASN:CG	2.11	0.54
2:J:105:GLN:HA	3:J:219:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:7:SER:OG	2:L:20:VAL:HG13	2.08	0.54
2:P:51:ILE:CB	2:P:57:ALA:HB2	2.29	0.54
2:B:19:LYS:HE2	2:B:79:TYR:HB3	1.90	0.54
1:C:11:LEU:HD22	1:C:11:LEU:C	2.28	0.54
2:D:29:PHE:CD1	2:D:30:SER:N	2.76	0.54
1:E:124:GLN:HB2	3:E:216:HOH:O	2.07	0.54
1:G:137:ASN:ND2	1:G:138:ASN:CG	2.61	0.54
2:H:191:THR:OG1	2:H:192:GLN:N	2.41	0.54
1:K:37:GLN:HG3	1:K:86:TYR:CE2	2.43	0.54
1:M:28:SER:HA	1:M:69:THR:HG22	1.90	0.54
1:G:61:ARG:HE	1:G:82:ASP:CG	2.10	0.54
2:H:141:LEU:HD11	2:H:143:LYS:HB2	1.90	0.54
2:H:119:PRO:CB	2:H:145:TYR:HB3	2.33	0.54
1:I:32:TYR:CD1	1:I:92:TYR:HD1	2.25	0.54
1:K:34:ASN:HD22	1:K:89:GLN:HE22	1.55	0.54
1:K:52:SER:O	1:K:54:LEU:N	2.40	0.54
1:M:24:ARG:HA	1:M:69:THR:O	2.08	0.54
1:A:136:LEU:HD13	1:A:175:LEU:HD22	1.90	0.54
1:E:179:LEU:HD11	1:E:181:LEU:HD21	1.89	0.54
1:E:61:ARG:O	1:E:75:ILE:HA	2.07	0.54
2:F:201:LYS:H	2:F:202:PRO:CD	2.21	0.54
1:G:118:PHE:HD2	1:G:118:PHE:N	2.04	0.54
1:G:158:ASN:O	1:G:179:LEU:HD12	2.07	0.54
1:G:182:SER:O	1:G:183:LYS:C	2.46	0.54
1:G:32:TYR:HB3	1:G:91:SER:HB2	1.90	0.54
2:J:77:THR:HB	2:J:79:TYR:HE1	1.73	0.54
1:M:19:VAL:CG1	1:M:20:THR:H	2.20	0.54
2:P:141:LEU:CD1	2:P:179:SER:HB3	2.38	0.54
1:C:148:TRP:CG	1:C:179:LEU:HD12	2.43	0.54
2:D:210:LYS:HE2	2:D:212:GLU:OE2	2.08	0.54
2:F:105:GLN:CG	2:F:106:GLY:H	2.21	0.54
1:G:136:LEU:HB3	1:G:139:PHE:CE1	2.43	0.54
2:H:3:GLN:OE1	2:H:5:LEU:HG	2.08	0.54
2:J:39:GLN:HE21	2:J:45:LEU:HD23	1.72	0.54
2:J:39:GLN:NE2	2:J:45:LEU:HD23	2.22	0.54
1:K:164:THR:CG2	1:K:174:SER:N	2.67	0.54
2:N:171:GLN:NE2	2:N:177:SER:HB2	2.23	0.54
1:C:140:TYR:CD2	1:C:173:TYR:HE2	2.26	0.53
1:C:93:SER:C	1:C:95:SER:H	2.10	0.53
1:I:185:ASP:O	1:I:188:LYS:HB2	2.08	0.53
2:J:94:LYS:CG	2:J:95:GLY:N	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:126:LYS:HA	1:K:126:LYS:HE3	1.90	0.53
2:L:87:THR:HG23	2:L:109:VAL:O	2.08	0.53
2:N:143:LYS:HA	2:N:177:SER:OG	2.08	0.53
1:C:125:LEU:CD2	1:C:130:ALA:HB2	2.38	0.53
1:C:140:TYR:HD2	1:C:173:TYR:HE2	1.55	0.53
1:G:2:ILE:HD13	3:H:236:HOH:O	2.07	0.53
2:L:73:GLU:OE2	2:L:73:GLU:N	2.36	0.53
2:P:29:PHE:CE1	2:P:52(A):PRO:HB3	2.43	0.53
2:D:52:ILE:O	2:D:53:VAL:N	2.41	0.53
1:G:124:GLN:O	1:G:127:SER:N	2.40	0.53
2:H:145:TYR:CE2	2:H:177:SER:HA	2.43	0.53
2:N:158:ALA:O	2:N:160:THR:HG23	2.09	0.53
1:O:93:SER:OG	1:O:94:THR:N	2.40	0.53
1:A:125:LEU:HD23	1:A:130:ALA:HB2	1.89	0.53
1:G:93:SER:HG	1:G:95:SER:HG	1.55	0.53
2:J:83:ARG:CB	2:J:85:GLU:HG3	2.28	0.53
2:N:30:SER:HB2	2:N:53:VAL:CG2	2.38	0.53
1:O:18:ARG:NH2	1:O:76:SER:HB2	2.23	0.53
2:P:134:GLY:O	2:P:186:SER:N	2.40	0.53
1:A:120:PRO:HD3	1:A:132:VAL:HG22	1.90	0.53
1:G:142:ARG:HG3	1:G:143:GLU:N	2.24	0.53
1:K:146:VAL:HG11	1:K:177:SER:CB	2.38	0.53
1:M:151:ASP:OD2	1:M:189:HIS:HB3	2.08	0.53
2:B:137:ALA:CB	2:B:183:THR:HA	2.38	0.53
1:G:148:TRP:CE3	1:G:194:CYS:HB3	2.44	0.53
2:H:176:TYR:HD2	2:H:176:TYR:N	2.07	0.53
1:I:50:ALA:O	1:I:51:ALA:CB	2.57	0.53
2:L:155:ASN:OD1	2:L:194:TYR:HA	2.09	0.53
1:M:26:SER:HB2	1:M:27:GLN:HE22	1.72	0.53
1:A:198:HIS:O	1:M:199:GLN:NE2	2.26	0.53
2:B:138:LEU:H	2:B:138:LEU:CD2	2.16	0.53
2:B:40:ALA:HA	2:B:88:ALA:HB2	1.90	0.53
2:D:71:ALA:HA	2:D:77:THR:O	2.09	0.53
2:F:24:ALA:O	2:F:26:GLY:N	2.38	0.53
2:H:131:THR:HB	2:H:135:THR:O	2.09	0.53
2:H:51:ILE:HG23	2:H:51:ILE:O	2.09	0.53
1:I:185:ASP:HA	1:I:188:LYS:CD	2.33	0.53
2:J:152:VAL:HG22	2:J:198:VAL:HG22	1.91	0.53
2:J:64:GLN:O	2:J:66:ARG:N	2.42	0.53
2:J:67:VAL:CG2	2:J:80:MET:SD	2.97	0.53
2:L:145:TYR:O	2:L:176:TYR:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:29:PHE:CE1	2:P:73:GLU:HG3	2.44	0.53
1:C:142:ARG:HD2	3:C:225:HOH:O	2.09	0.53
1:C:145:LYS:NZ	1:C:147:GLN:HE21	2.06	0.53
2:D:201:LYS:O	2:D:203:SER:N	2.42	0.53
1:E:122:ASP:O	1:E:126:LYS:HD2	2.09	0.53
1:G:130:ALA:O	1:G:180:THR:HA	2.08	0.53
2:H:7:SER:O	2:H:107:THR:HG23	2.08	0.53
1:I:54:LEU:HD11	1:I:58:VAL:CB	2.39	0.53
2:J:153:SER:OG	2:J:197:ASN:HB2	2.09	0.53
2:L:93:ALA:HB1	2:L:100(L):MET:HB3	1.91	0.53
1:C:12:SER:OG	1:C:105:GLU:OE1	2.22	0.53
2:F:30:SER:HA	2:F:52(A):PRO:HB2	1.91	0.53
2:H:38:ARG:HB3	2:H:90:TYR:CE2	2.43	0.53
2:L:36:TRP:CD1	2:L:69:ILE:HD13	2.43	0.53
2:P:100(L):MET:CE	2:P:100(L):MET:H	2.22	0.53
1:A:124:GLN:OE1	1:A:130:ALA:HA	2.09	0.53
1:A:143:GLU:OE2	1:A:143:GLU:N	2.41	0.53
1:A:61:ARG:HA	1:A:76:SER:HB3	1.91	0.53
2:B:119:PRO:HB3	2:B:145:TYR:HD2	1.74	0.53
1:C:135:LEU:HD12	1:C:175:LEU:O	2.09	0.53
1:G:39:LYS:HD3	1:G:84:ALA:CB	2.39	0.53
2:J:207:VAL:CG1	2:J:208:ASP:N	2.72	0.53
1:M:158:ASN:N	1:M:158:ASN:OD1	2.42	0.53
1:O:108:ARG:HH11	1:O:172:THR:HG22	1.74	0.53
1:O:61:ARG:HG3	1:O:62:PHE:CD1	2.44	0.53
1:O:67:SER:N	1:O:70:ASP:O	2.41	0.53
2:B:186:SER:O	2:B:189:LEU:HG	2.09	0.52
2:B:53:VAL:HG23	2:B:54:PHE:CD1	2.43	0.52
1:C:164:THR:HG22	1:C:173:TYR:HA	1.92	0.52
2:F:145:TYR:N	2:F:145:TYR:HD2	2.07	0.52
2:H:53:VAL:HB	2:H:54:PHE:CD1	2.44	0.52
1:K:202:SER:O	1:K:203:SER:HB3	2.08	0.52
2:N:116:THR:HG22	2:N:116:THR:O	2.09	0.52
2:N:4:LEU:HD23	2:N:4:LEU:N	2.24	0.52
2:P:40:ALA:HB3	2:P:43:GLN:CG	2.40	0.52
1:A:90:GLN:HE22	1:A:93:SER:CB	2.22	0.52
2:D:83:ARG:HD2	2:P:61:GLN:OE1	2.08	0.52
2:F:34:ILE:HG21	2:F:78:THR:HG21	1.92	0.52
1:I:12:SER:HB3	1:I:107:LYS:HG3	1.90	0.52
2:J:199:ASN:HD22	2:J:200:HIS:N	2.08	0.52
1:K:145:LYS:HD3	1:K:197:THR:HG21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:193:THR:CG2	2:L:195:ILE:HD11	2.40	0.52
2:N:159:LEU:CD2	2:N:182:VAL:HG21	2.39	0.52
1:O:56:SER:C	1:O:58:VAL:H	2.12	0.52
2:P:39:GLN:C	2:P:88:ALA:HB1	2.29	0.52
1:A:199:GLN:HB2	3:A:219:HOH:O	2.08	0.52
1:C:163:VAL:HG12	1:C:164:THR:H	1.75	0.52
2:D:145:TYR:C	2:D:145:TYR:CD1	2.82	0.52
1:E:49:TYR:H	1:E:49:TYR:HD2	1.57	0.52
2:F:105:GLN:CG	2:F:106:GLY:N	2.72	0.52
2:F:62:LYS:HG3	2:F:63:PHE:CD1	2.45	0.52
1:G:124:GLN:OE1	1:G:131:SER:HB2	2.09	0.52
2:J:201:LYS:C	2:J:203:SER:H	2.13	0.52
2:J:35:SER:OG	2:J:47:TRP:NE1	2.42	0.52
1:K:156:SER:C	1:K:158:ASN:H	2.13	0.52
2:L:66:ARG:HG3	2:L:82:LEU:HD12	1.90	0.52
2:N:6:GLN:OE1	2:N:91:PHE:HA	2.09	0.52
2:P:17:SER:O	2:P:18:VAL:HB	2.09	0.52
1:A:164:THR:HG21	2:B:164:HIS:CD2	2.45	0.52
2:B:2:VAL:HG23	2:B:26:GLY:HA3	1.91	0.52
2:B:51:ILE:CG1	2:B:52:ILE:N	2.72	0.52
2:D:178:LEU:HD12	2:D:178:LEU:C	2.30	0.52
1:E:110:VAL:CG1	1:E:111:ALA:N	2.73	0.52
2:F:13:LYS:CD	2:F:113:SER:HA	2.35	0.52
2:F:1:GLN:HG2	2:N:3:GLN:NE2	2.24	0.52
2:H:124:LEU:CD2	2:H:141:LEU:HB2	2.24	0.52
2:J:163:VAL:HG12	2:J:164:HIS:N	2.24	0.52
1:K:195:GLU:CG	1:K:204:PRO:HB3	2.39	0.52
2:B:141:LEU:HD12	2:B:141:LEU:C	2.30	0.52
2:B:48:MET:HE1	2:B:82:LEU:HD22	1.91	0.52
2:F:184:VAL:HB	2:F:185:PRO:CD	2.39	0.52
2:F:51:ILE:O	2:F:52(A):PRO:HD3	2.09	0.52
1:G:185:ASP:O	1:G:188:LYS:HB2	2.09	0.52
2:H:84:SER:C	2:H:86:ASP:N	2.62	0.52
1:E:199:GLN:N	1:I:199:GLN:HE22	2.07	0.52
1:I:49:TYR:O	1:I:50:ALA:HB3	2.10	0.52
1:I:32:TYR:CB	1:I:91:SER:HB2	2.20	0.52
2:J:62:LYS:O	2:J:64:GLN:N	2.43	0.52
1:K:136:LEU:HD11	1:K:196:VAL:CG2	2.40	0.52
1:K:190:LYS:HG2	1:K:210:ASN:CB	2.27	0.52
2:N:20:VAL:HG12	2:N:36:TRP:HH2	1.75	0.52
1:A:210:ASN:O	1:A:213:GLU:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:SER:HA	1:C:105:GLU:CG	2.37	0.52
2:D:12:LYS:CG	2:D:18:VAL:HB	2.30	0.52
1:E:116:PHE:HD2	2:F:130:SER:HA	1.73	0.52
1:G:124:GLN:HE22	1:G:131:SER:CB	2.22	0.52
2:J:3:GLN:HB2	3:J:224:HOH:O	2.10	0.52
1:K:185:ASP:O	1:K:188:LYS:HB2	2.09	0.52
1:M:66:GLY:O	1:M:71:PHE:CE2	2.63	0.52
1:M:95:SER:HA	2:N:47:TRP:CZ3	2.45	0.52
2:P:93:ALA:HB1	2:P:100(L):MET:HB3	1.91	0.52
1:A:150:VAL:HG23	1:A:155:GLN:CG	2.40	0.52
1:C:2:ILE:HG22	1:C:3:GLN:N	2.25	0.52
2:F:103:TRP:CD1	2:F:103:TRP:N	2.78	0.52
1:G:159:SER:HB3	1:G:179:LEU:HD13	1.92	0.52
1:G:181:LEU:N	1:G:181:LEU:HD12	2.25	0.52
2:H:123:PRO:HD3	2:H:209:LYS:HE2	1.91	0.52
2:H:192:GLN:NE2	2:H:193:THR:N	2.58	0.52
2:J:12:LYS:HZ2	2:J:18:VAL:HA	1.73	0.52
1:M:110:VAL:HG22	1:M:141:PRO:HD3	1.90	0.52
2:N:201:LYS:C	2:N:203:SER:H	2.13	0.52
1:A:151:ASP:OD2	1:A:189:HIS:HA	2.10	0.52
1:A:39:LYS:HE3	1:A:81:GLU:O	2.10	0.52
1:A:71:PHE:CD1	1:A:71:PHE:N	2.78	0.52
2:F:145:TYR:CE2	2:F:176:TYR:HB2	2.45	0.52
1:G:162:SER:OG	2:H:166:PHE:HB3	2.10	0.52
1:M:89:GLN:HE21	1:M:96:HIS:HB3	1.75	0.52
1:O:14:SER:O	1:O:15:VAL:O	2.27	0.52
1:A:135:LEU:HD13	2:B:181:VAL:HG21	1.91	0.52
2:B:201:LYS:N	2:B:202:PRO:CD	2.73	0.52
1:C:17:ASP:O	1:C:77:SER:HA	2.10	0.52
2:D:62:LYS:HE2	2:D:63:PHE:CE1	2.45	0.52
2:F:163:VAL:HG12	2:F:164:HIS:N	2.25	0.52
2:F:121:VAL:CG2	2:F:198:VAL:HG11	2.40	0.52
1:I:37:GLN:HG2	1:I:38:GLN:N	2.25	0.52
1:K:34:ASN:HD22	1:K:89:GLN:NE2	2.08	0.52
2:J:64:GLN:CB	2:L:204:ASN:OD1	2.55	0.52
1:O:138:ASN:H	1:O:138:ASN:HD22	1.57	0.52
1:O:89:GLN:HE22	2:P:100(L):MET:CE	2.22	0.52
1:A:116:PHE:HD1	1:A:135:LEU:HD23	1.70	0.52
1:A:211:ARG:HB2	1:A:211:ARG:NH1	2.10	0.52
1:A:61:ARG:CB	1:A:76:SER:OG	2.58	0.52
2:D:36:TRP:CD2	2:D:80:MET:HB2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:23:LYS:N	2:H:77:THR:HG23	2.25	0.52
2:H:59:TYR:O	2:H:64:GLN:NE2	2.43	0.52
2:H:75:THR:O	2:H:76:SER:C	2.49	0.52
1:I:201:LEU:O	1:I:202:SER:C	2.48	0.52
2:J:178:LEU:HD12	2:J:178:LEU:C	2.30	0.52
1:K:6:GLN:C	1:K:100:GLN:NE2	2.64	0.52
1:O:108:ARG:NH1	1:O:172:THR:HG22	2.24	0.52
1:A:18:ARG:NH1	1:A:76:SER:O	2.42	0.51
2:B:137:ALA:HB2	2:B:183:THR:HA	1.92	0.51
1:E:18:ARG:NH1	1:E:76:SER:CA	2.72	0.51
2:F:125:ALA:HB1	2:F:213:PRO:O	2.10	0.51
1:I:175:LEU:C	1:I:175:LEU:HD23	2.30	0.51
1:I:195:GLU:HG2	1:I:196:VAL:N	2.23	0.51
2:J:145:TYR:O	2:J:146:PHE:CB	2.57	0.51
1:K:33:LEU:HG	1:K:71:PHE:CB	2.39	0.51
1:M:39:LYS:HG2	1:M:84:ALA:CB	2.38	0.51
2:N:40:ALA:O	2:N:41:PRO:C	2.49	0.51
1:O:15:VAL:HG13	1:O:78:LEU:O	2.09	0.51
1:A:164:THR:HG21	2:B:164:HIS:HD2	1.75	0.51
1:G:138:ASN:HB3	1:G:172:THR:HG21	1.92	0.51
1:G:211:ARG:HH11	1:G:211:ARG:HG2	1.74	0.51
1:C:128:GLY:C	1:C:129:THR:HG22	2.30	0.51
1:G:169:LYS:HG3	1:G:170:ASP:H	1.76	0.51
1:G:113:PRO:HD3	1:G:198:HIS:ND1	2.25	0.51
2:H:95:GLY:HA2	2:H:101:ASP:OD2	2.09	0.51
2:H:14:PRO:HA	2:H:82(C):LEU:O	2.11	0.51
1:I:184:ALA:HB1	1:I:188:LYS:CE	2.40	0.51
1:I:90:GLN:OE1	1:I:90:GLN:O	2.28	0.51
2:J:119:PRO:HB2	2:J:142:VAL:HG13	1.92	0.51
2:L:40:ALA:HA	2:L:88:ALA:CB	2.40	0.51
2:N:165:THR:HG23	2:N:180:SER:HB2	1.92	0.51
1:A:208:SER:O	2:B:129:LYS:HD3	2.11	0.51
2:B:131:THR:HG22	2:B:136:ALA:HB2	1.90	0.51
2:F:18:VAL:HG12	2:F:82(C):LEU:HD11	1.92	0.51
1:G:143:GLU:H	1:G:143:GLU:CD	2.14	0.51
2:H:32:TYR:CD2	2:H:94:LYS:HE3	2.46	0.51
2:L:127:SER:OG	2:L:129:LYS:HB2	2.10	0.51
2:L:141:LEU:HD12	2:L:141:LEU:C	2.31	0.51
2:L:164:HIS:HB2	2:L:181:VAL:HG23	1.92	0.51
2:L:18:VAL:O	2:L:81:GLU:HG3	2.11	0.51
2:N:94:LYS:O	2:N:100(L):MET:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:94:LYS:HG2	2:N:95:GLY:N	2.26	0.51
1:O:36:TYR:CE2	1:O:46:LEU:HD13	2.45	0.51
1:A:117:ILE:CG2	1:A:117:ILE:O	2.57	0.51
1:C:136:LEU:N	1:C:136:LEU:HD12	2.25	0.51
1:C:90:GLN:HE22	1:C:97:THR:HB	1.75	0.51
2:F:171:GLN:HE21	2:F:177:SER:HB2	1.74	0.51
2:F:94:LYS:NZ	2:F:96:GLY:N	2.59	0.51
1:E:24:ARG:HH12	1:I:158:ASN:HA	1.75	0.51
2:J:34:ILE:HG22	2:J:35:SER:N	2.24	0.51
2:B:77:THR:CG2	2:B:78:THR:N	2.74	0.51
2:F:52:ILE:O	2:F:52(A):PRO:C	2.48	0.51
2:H:116:THR:CG2	2:H:117:LYS:N	2.73	0.51
1:K:122:ASP:O	1:K:126:LYS:HD2	2.11	0.51
1:K:62:PHE:CE2	1:K:75:ILE:HG12	2.46	0.51
2:L:11:VAL:HA	2:L:110:THR:O	2.11	0.51
2:L:145:TYR:HD1	2:L:200:HIS:CD2	2.29	0.51
2:L:40:ALA:O	2:L:43:GLN:HB2	2.11	0.51
1:O:130:ALA:O	1:O:180:THR:HG23	2.10	0.51
2:P:53:VAL:HG12	2:P:54:PHE:CD2	2.44	0.51
2:P:73:GLU:CD	2:P:73:GLU:H	2.12	0.51
2:B:20:VAL:O	2:B:79:TYR:HA	2.11	0.51
2:D:63:PHE:HB3	2:D:67:VAL:CG1	2.41	0.51
1:G:32:TYR:CD1	1:G:32:TYR:N	2.79	0.51
1:I:61:ARG:NE	1:I:82:ASP:OD2	2.38	0.51
2:J:139:GLY:HA3	2:J:180:SER:O	2.11	0.51
1:O:182:SER:O	1:O:183:LYS:C	2.49	0.51
1:O:205:VAL:HG12	1:O:205:VAL:O	2.09	0.51
1:O:33:LEU:HD22	1:O:34:ASN:H	1.75	0.51
1:A:39:LYS:CE	1:A:81:GLU:O	2.59	0.51
2:B:107:THR:HG22	2:B:109:VAL:HG23	1.92	0.51
2:B:82(A):SER:O	2:B:82(B):SER:C	2.50	0.51
2:D:201:LYS:C	2:D:203:SER:H	2.14	0.51
2:F:4:LEU:HD13	2:F:92:CYS:O	2.10	0.51
1:G:117:ILE:HG21	1:G:207:LYS:HG3	1.93	0.51
2:H:193:THR:HG22	2:H:194:TYR:H	1.76	0.51
1:I:2:ILE:N	3:I:220:HOH:O	2.42	0.51
1:I:32:TYR:HB2	1:I:92:TYR:H	1.73	0.51
1:K:29:ILE:O	1:K:30:SER:CB	2.59	0.51
2:L:63:PHE:O	2:L:67:VAL:HG12	2.10	0.51
2:N:94:LYS:HG2	2:N:95:GLY:H	1.74	0.51
2:B:73:GLU:C	2:B:75:THR:N	2.62	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:3:GLN:HG2	2:D:4:LEU:N	2.26	0.51
2:H:51:ILE:CB	2:H:57:ALA:HB2	2.37	0.51
1:I:136:LEU:N	1:I:136:LEU:HD12	2.26	0.51
1:I:48:ILE:HG21	1:I:64:GLY:HA3	1.91	0.51
1:M:19:VAL:CG1	1:M:20:THR:N	2.72	0.51
1:O:124:GLN:HG2	1:O:129:THR:O	2.11	0.51
1:O:20:THR:HG23	1:O:72:THR:CG2	2.41	0.51
1:A:184:ALA:HB1	1:A:188:LYS:HE3	1.92	0.51
2:B:19:LYS:HA	2:B:80:MET:O	2.11	0.51
1:I:81:GLU:N	1:I:81:GLU:OE1	2.44	0.51
2:J:90:TYR:CD1	2:J:90:TYR:N	2.79	0.51
2:L:123:PRO:HB2	2:L:211:VAL:HG22	1.92	0.51
1:O:112:ALA:HB1	1:O:201:LEU:HD21	1.92	0.51
1:C:78:LEU:HD21	1:C:104:LEU:HD11	1.92	0.50
1:C:154:LEU:CD2	1:C:154:LEU:H	2.23	0.50
1:E:210:ASN:O	1:E:211:ARG:C	2.50	0.50
1:E:42:LYS:O	1:E:43:VAL:C	2.48	0.50
2:B:94:LYS:C	2:B:94:LYS:HD3	2.31	0.50
2:D:138:LEU:C	2:D:138:LEU:CD1	2.80	0.50
2:F:35:SER:O	2:F:92:CYS:HA	2.10	0.50
2:H:162:GLY:O	2:H:182:VAL:HA	2.11	0.50
2:H:12:LYS:HE3	2:H:18:VAL:HG23	1.93	0.50
2:L:141:LEU:HD12	2:L:142:VAL:N	2.26	0.50
2:P:28:THR:O	2:P:30:SER:N	2.44	0.50
2:P:29:PHE:O	2:P:52(A):PRO:HG2	2.11	0.50
1:A:188:LYS:O	1:A:189:HIS:CG	2.64	0.50
2:B:53:VAL:C	2:B:54:PHE:CD1	2.85	0.50
2:F:85:GLU:N	2:F:85:GLU:CD	2.64	0.50
1:G:197:THR:HG22	1:G:204:PRO:HG3	1.94	0.50
1:G:63:SER:OG	1:G:74:THR:HB	2.10	0.50
2:H:36:TRP:HB2	2:H:69:ILE:CD1	2.38	0.50
2:H:67:VAL:CG2	2:H:68:THR:N	2.74	0.50
2:L:24:ALA:HB3	2:L:76:SER:HB3	1.94	0.50
2:P:159:LEU:HD12	2:P:160:THR:N	2.26	0.50
1:C:136:LEU:HD11	1:C:146:VAL:HG21	1.92	0.50
1:C:162:SER:OG	2:D:167:PRO:HD2	2.11	0.50
1:C:167:ASP:OD1	1:C:169:LYS:HG2	2.11	0.50
1:C:145:LYS:HD3	1:C:197:THR:HG23	1.94	0.50
2:D:159:LEU:HD12	2:D:160:THR:N	2.27	0.50
1:E:3:GLN:N	1:E:26:SER:OG	2.44	0.50
1:E:90:GLN:NE2	1:E:97:THR:OG1	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:50:ALA:HB3	1:K:53:SER:OG	2.12	0.50
1:K:79:GLN:O	1:K:82:ASP:HB2	2.12	0.50
1:M:75:ILE:HD11	1:M:86:TYR:CE2	2.46	0.50
1:O:148:TRP:CE3	1:O:194:CYS:HB3	2.46	0.50
2:B:51:ILE:CG1	2:B:57:ALA:HB2	2.41	0.50
1:C:154:LEU:N	1:C:154:LEU:CD2	2.75	0.50
2:D:82:LEU:HG	2:D:82(C):LEU:CD2	2.41	0.50
1:G:161:GLU:HA	1:G:176:SER:O	2.11	0.50
2:H:62:LYS:HG3	2:H:63:PHE:HD1	1.76	0.50
1:E:154:LEU:HD21	1:I:17:ASP:HB3	1.93	0.50
1:K:169:LYS:HG3	1:K:170:ASP:OD1	2.12	0.50
1:O:11:LEU:HB3	1:O:104:LEU:CD2	2.38	0.50
1:O:94:THR:CG2	1:O:95:SER:H	2.25	0.50
1:C:192:TYR:O	1:C:208:SER:HB2	2.11	0.50
1:E:36:TYR:CE2	1:E:46:LEU:HD13	2.47	0.50
1:G:154:LEU:HD22	1:G:154:LEU:N	2.27	0.50
2:J:123:PRO:HG3	2:J:209:LYS:HZ1	1.75	0.50
2:J:73:GLU:O	2:J:76:SER:N	2.44	0.50
1:M:150:VAL:HG11	1:M:189:HIS:CD2	2.46	0.50
1:A:158:ASN:CA	1:M:24:ARG:HH21	2.24	0.50
1:O:48:ILE:HD12	1:O:73:LEU:HD12	1.94	0.50
1:O:95:SER:HA	2:P:47:TRP:CZ3	2.47	0.50
1:A:118:PHE:HZ	2:B:137:ALA:O	1.95	0.50
2:D:27:GLY:O	2:D:29:PHE:N	2.45	0.50
2:F:145:TYR:N	2:F:145:TYR:CD2	2.77	0.50
2:F:201:LYS:H	2:F:202:PRO:HD3	1.76	0.50
2:F:24:ALA:HB2	2:F:29:PHE:HD2	1.76	0.50
1:G:35:TRP:CZ3	1:G:88:CYS:HB3	2.47	0.50
1:G:39:LYS:NZ	1:G:81:GLU:O	2.42	0.50
1:G:89:GLN:HG3	1:G:98:PHE:CE2	2.46	0.50
1:I:32:TYR:HB3	1:I:92:TYR:H	1.74	0.50
1:K:161:GLU:HA	1:K:177:SER:HA	1.93	0.50
2:L:11:VAL:HG22	2:L:110:THR:OG1	2.11	0.50
2:N:89:VAL:HG12	2:N:91:PHE:CE1	2.46	0.50
2:P:185:PRO:O	2:P:186:SER:C	2.50	0.50
1:A:142:ARG:CG	1:A:142:ARG:O	2.60	0.50
2:B:2:VAL:HG21	2:B:32:TYR:CE1	2.47	0.50
1:E:113:PRO:HB3	1:E:139:PHE:CD1	2.47	0.50
1:E:150:VAL:C	1:E:152:ASN:H	2.15	0.50
2:F:11:VAL:HG22	2:F:110:THR:HB	1.94	0.50
2:F:34:ILE:HD12	2:F:94:LYS:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:119:PRO:HB3	1:I:209:PHE:CZ	2.47	0.50
2:N:119:PRO:HB2	2:N:142:VAL:CG1	2.36	0.50
1:C:212:GLY:O	1:C:213:GLU:CG	2.54	0.50
2:F:117:LYS:HE3	2:F:144:ASP:HB3	1.94	0.50
1:G:52:SER:HB3	1:G:65:SER:HA	1.94	0.50
2:H:150:VAL:HA	2:H:199:ASN:O	2.12	0.50
1:K:96:HIS:HB2	2:L:47:TRP:CE2	2.47	0.50
1:O:86:TYR:O	1:O:101:GLY:HA2	2.12	0.50
2:P:134:GLY:O	2:P:185:PRO:HA	2.12	0.50
2:P:189:LEU:HD13	2:P:213:PRO:CG	2.39	0.50
2:P:19:LYS:HA	2:P:80:MET:O	2.12	0.50
2:P:38:ARG:CG	2:P:46:GLU:HB3	2.42	0.50
1:A:118:PHE:HE1	2:B:130:SER:OG	1.95	0.49
1:A:174:SER:O	2:B:166:PHE:HE2	1.95	0.49
2:B:153:SER:O	2:B:197:ASN:HB2	2.12	0.49
2:B:23:LYS:HD3	2:B:24:ALA:H	1.76	0.49
1:E:190:LYS:O	1:E:210:ASN:HA	2.11	0.49
2:F:126:PRO:HB2	2:F:189:LEU:HD13	1.94	0.49
1:G:175:LEU:C	1:G:175:LEU:CD2	2.78	0.49
2:H:68:THR:HB	2:H:81:GLU:CB	2.21	0.49
1:I:140:TYR:O	1:I:198:HIS:HE1	1.94	0.49
2:J:178:LEU:HD12	2:J:178:LEU:O	2.12	0.49
2:J:72:ASP:O	2:J:76:SER:N	2.45	0.49
2:L:8:GLY:O	2:L:9:ALA:C	2.51	0.49
2:N:154:TRP:CZ3	2:N:196:CYS:CB	2.91	0.49
2:P:36:TRP:CD2	2:P:80:MET:HG3	2.47	0.49
1:A:164:THR:HG22	1:A:174:SER:H	1.77	0.49
2:B:124:LEU:HD21	2:B:141:LEU:HB2	1.94	0.49
1:E:15:VAL:HG11	1:E:80:PRO:HD3	1.94	0.49
2:F:52(A):PRO:O	2:F:53:VAL:C	2.50	0.49
2:F:68:THR:HB	2:F:81:GLU:CG	2.43	0.49
1:G:115:VAL:HG12	1:G:116:PHE:N	2.28	0.49
1:C:26:SER:O	1:C:27:GLN:NE2	2.46	0.49
2:D:82:LEU:HG	2:D:82(C):LEU:HD23	1.93	0.49
1:G:186:TYR:C	1:G:188:LYS:N	2.64	0.49
2:J:168:ALA:HA	2:J:178:LEU:HB3	1.95	0.49
1:K:179:LEU:HD11	1:K:181:LEU:CD1	2.42	0.49
2:L:1:GLN:N	2:L:1:GLN:CD	2.66	0.49
1:O:145:LYS:HB3	1:O:197:THR:OG1	2.13	0.49
2:B:89:VAL:HA	2:B:107:THR:O	2.12	0.49
1:A:87:TYR:CE2	2:B:44:GLY:HA2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:ILE:O	1:C:31:SER:N	2.46	0.49
1:C:48:ILE:HD12	1:C:73:LEU:CD1	2.43	0.49
1:C:90:GLN:HE22	1:C:97:THR:N	2.11	0.49
2:D:201:LYS:N	2:D:202:PRO:CD	2.75	0.49
2:D:6:GLN:CA	2:D:21:SER:O	2.57	0.49
2:D:24:ALA:HB3	2:D:76:SER:HB3	1.94	0.49
2:D:52(A):PRO:O	2:D:53:VAL:C	2.50	0.49
1:E:170:ASP:OD2	1:E:170:ASP:C	2.51	0.49
1:E:34:ASN:OD1	1:E:49:TYR:CB	2.61	0.49
1:E:116:PHE:CD2	2:F:130:SER:HA	2.46	0.49
2:L:86:ASP:HB2	2:L:111:VAL:HG21	1.94	0.49
1:M:66:GLY:O	1:M:71:PHE:CD2	2.65	0.49
2:P:159:LEU:HD12	2:P:160:THR:H	1.77	0.49
1:C:30:SER:HG	1:C:92:TYR:HE1	1.61	0.49
1:C:39:LYS:HG2	1:C:84:ALA:CB	2.42	0.49
2:D:119:PRO:HB3	2:D:145:TYR:CD2	2.47	0.49
2:F:94:LYS:C	2:F:94:LYS:CD	2.78	0.49
2:H:6:GLN:OE1	2:H:104:GLY:HA3	2.13	0.49
1:K:48:ILE:HG12	1:K:54:LEU:HD13	1.94	0.49
2:L:34:ILE:N	2:L:34:ILE:CD1	2.76	0.49
2:N:87:THR:HG23	2:N:110:THR:HA	1.93	0.49
2:N:171:GLN:HE21	2:N:177:SER:HB2	1.77	0.49
2:N:201:LYS:C	2:N:203:SER:N	2.65	0.49
2:N:3:GLN:O	2:N:4:LEU:HD23	2.13	0.49
2:N:85:GLU:O	2:N:87:THR:N	2.45	0.49
2:P:29:PHE:O	2:P:29:PHE:CG	2.66	0.49
1:A:48:ILE:HG22	1:A:49:TYR:H	1.78	0.49
1:C:155:GLN:O	1:C:156:SER:HB2	2.13	0.49
2:D:154:TRP:CZ2	2:D:196:CYS:HB3	2.47	0.49
1:K:107:LYS:O	1:K:108:ARG:HB3	2.12	0.49
1:C:54:LEU:HD23	1:C:55:GLN:N	2.28	0.49
2:F:131:THR:HG22	2:F:136:ALA:CB	2.42	0.49
2:F:163:VAL:CG1	2:F:164:HIS:N	2.75	0.49
2:F:1:GLN:O	2:F:2:VAL:C	2.51	0.49
1:G:130:ALA:N	1:G:181:LEU:O	2.46	0.49
1:G:55:GLN:CD	1:G:56:SER:N	2.66	0.49
1:G:79:GLN:HB3	1:G:81:GLU:OE1	2.13	0.49
1:I:148:TRP:CE3	1:I:194:CYS:HB3	2.47	0.49
2:J:22:CYS:HB3	2:J:78:THR:HB	1.94	0.49
2:J:35:SER:OG	2:J:49:GLY:O	2.31	0.49
1:K:118:PHE:HB3	2:L:124:LEU:HD22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:112:ALA:HB3	2:L:146:PHE:HZ	1.77	0.49
2:L:152:VAL:HB	2:L:165:THR:OG1	2.13	0.49
2:B:158:ALA:O	2:B:160:THR:HG23	2.13	0.49
2:B:2:VAL:CA	2:B:26:GLY:HA3	2.36	0.49
2:D:152:VAL:HG12	2:D:153:SER:N	2.28	0.49
1:E:11:LEU:O	1:E:104:LEU:HA	2.12	0.49
1:E:123:GLU:OE2	1:E:123:GLU:N	2.28	0.49
1:G:19:VAL:HG12	1:G:20:THR:N	2.28	0.49
2:H:176:TYR:HD2	2:H:176:TYR:H	1.60	0.49
1:I:83:PHE:CE2	1:I:106:ILE:HG12	2.47	0.49
2:J:18:VAL:HG12	2:J:82(C):LEU:HD11	1.94	0.49
1:A:210:ASN:O	1:A:211:ARG:O	2.31	0.49
1:A:48:ILE:CG2	1:A:49:TYR:N	2.75	0.49
1:A:65:SER:OG	3:A:214:HOH:O	1.96	0.49
2:B:82(A):SER:O	2:B:82(C):LEU:N	2.45	0.49
1:C:167:ASP:OD1	1:C:169:LYS:CG	2.61	0.49
1:C:45:LYS:HD3	1:C:47:LEU:HD21	1.95	0.49
1:E:75:ILE:HG21	1:E:78:LEU:HD12	1.93	0.49
2:F:37:VAL:HG13	2:F:46:GLU:O	2.13	0.49
1:G:206:THR:HG22	1:G:207:LYS:N	2.27	0.49
2:H:72:ASP:O	2:H:76:SER:N	2.46	0.49
1:I:151:ASP:O	1:I:152:ASN:C	2.51	0.49
2:J:38:ARG:NH1	2:J:86:ASP:HA	2.26	0.49
1:K:145:LYS:HB3	1:K:197:THR:OG1	2.13	0.49
1:M:49:TYR:CE1	1:M:53:SER:OG	2.65	0.49
2:N:31:SER:O	2:N:32:TYR:C	2.51	0.49
1:A:115:VAL:CG1	1:A:116:PHE:N	2.76	0.49
1:C:184:ALA:O	1:C:187:GLU:N	2.46	0.49
2:D:154:TRP:CH2	2:D:196:CYS:HB3	2.48	0.49
1:E:18:ARG:HH12	1:E:76:SER:CB	2.26	0.49
2:H:20:VAL:HG12	2:H:36:TRP:HH2	1.77	0.49
2:H:62:LYS:HG3	2:H:63:PHE:CD1	2.48	0.49
1:I:18:ARG:NH1	1:I:76:SER:OG	2.45	0.49
1:I:97:THR:CG2	1:I:98:PHE:N	2.75	0.49
2:J:163:VAL:N	2:J:182:VAL:HG23	2.28	0.49
2:J:94:LYS:HD3	2:J:102:VAL:HG11	1.94	0.49
2:L:205:THR:O	2:L:205:THR:HG22	2.13	0.49
1:M:112:ALA:HB2	1:M:200:GLY:C	2.33	0.49
2:N:194:TYR:C	2:N:195:ILE:HG13	2.33	0.49
2:N:206:LYS:O	2:N:207:VAL:HG22	2.13	0.49
1:O:33:LEU:O	1:O:51:ALA:N	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:TRP:O	2:B:155:ASN:C	2.51	0.48
2:B:61:GLN:O	2:B:63:PHE:N	2.46	0.48
1:C:170:ASP:OD2	1:C:172:THR:CG2	2.60	0.48
2:F:20:VAL:HG12	2:F:21:SER:N	2.28	0.48
2:J:113:SER:O	2:J:114:ALA:C	2.51	0.48
2:J:188:SER:O	2:J:192:GLN:HB3	2.13	0.48
1:K:182:SER:O	1:K:185:ASP:N	2.46	0.48
2:L:154:TRP:HB2	2:L:159:LEU:HB3	1.95	0.48
2:N:184:VAL:HG21	2:N:194:TYR:CZ	2.48	0.48
2:P:7:SER:HB3	2:P:20:VAL:HG13	1.93	0.48
1:A:90:GLN:OE1	1:A:90:GLN:C	2.52	0.48
1:A:135:LEU:HD11	2:B:181:VAL:HG21	1.94	0.48
2:B:51:ILE:CB	2:B:57:ALA:HB2	2.43	0.48
1:C:36:TYR:CE1	1:C:89:GLN:NE2	2.81	0.48
2:D:20:VAL:HB	2:D:36:TRP:CZ3	2.49	0.48
2:D:29:PHE:CE1	2:D:76:SER:HA	2.47	0.48
1:G:162:SER:O	1:G:175:LEU:HA	2.14	0.48
2:H:40:ALA:HB3	2:H:43:GLN:HB2	1.95	0.48
2:H:87:THR:O	2:H:88:ALA:HB2	2.12	0.48
1:I:148:TRP:CZ3	1:I:194:CYS:HB3	2.48	0.48
2:J:156:SER:C	2:J:158:ALA:H	2.16	0.48
1:K:142:ARG:HH12	1:K:163:VAL:CG1	2.10	0.48
1:K:153:ALA:O	1:K:155:GLN:NE2	2.46	0.48
2:L:126:PRO:HG3	2:L:138:LEU:CB	2.36	0.48
2:L:130:SER:HB2	2:L:137:ALA:O	2.12	0.48
2:L:197:ASN:ND2	2:L:208:ASP:OD2	2.45	0.48
1:O:94:THR:HG23	1:O:95:SER:H	1.77	0.48
1:C:124:GLN:CB	3:C:223:HOH:O	2.61	0.48
1:M:124:GLN:HG2	1:M:129:THR:O	2.12	0.48
1:O:8:PRO:O	1:O:102:THR:HA	2.12	0.48
2:P:155:ASN:CB	2:P:158:ALA:HB3	2.44	0.48
2:B:10:GLU:O	2:B:109:VAL:HA	2.14	0.48
2:D:197:ASN:ND2	2:D:208:ASP:CG	2.66	0.48
2:D:210:LYS:CD	2:D:212:GLU:OE2	2.60	0.48
1:E:113:PRO:CA	1:E:139:PHE:HB3	2.44	0.48
1:E:19:VAL:HG22	1:I:154:LEU:CB	2.43	0.48
1:E:90:GLN:NE2	1:E:95:SER:O	2.46	0.48
2:F:121:VAL:HG11	2:F:198:VAL:CG2	2.36	0.48
2:F:121:VAL:HG21	2:F:198:VAL:HG11	1.95	0.48
1:G:29:ILE:O	1:G:30:SER:HB3	2.14	0.48
2:H:163:VAL:HA	2:H:181:VAL:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:117:LYS:O	2:L:145:TYR:HA	2.12	0.48
1:A:131:SER:OG	1:A:180:THR:HG23	2.13	0.48
1:A:43:VAL:HG13	1:A:44:PRO:HD2	1.94	0.48
2:B:17:SER:OG	2:B:18:VAL:N	2.44	0.48
2:B:200:HIS:CG	2:B:202:PRO:HD2	2.48	0.48
1:C:31:SER:O	1:C:33:LEU:N	2.43	0.48
1:C:74:THR:CG2	1:C:75:ILE:N	2.76	0.48
1:E:13:ALA:O	1:E:107:LYS:HB3	2.13	0.48
1:M:163:VAL:HG12	1:M:164:THR:H	1.79	0.48
1:A:193:ALA:HA	1:A:207:LYS:O	2.14	0.48
1:A:193:ALA:CB	1:A:208:SER:HB3	2.39	0.48
1:C:16:GLY:HA2	1:C:77:SER:OG	2.13	0.48
2:D:83:ARG:N	2:D:86:ASP:OD2	2.35	0.48
1:E:85:THR:HG21	1:E:87:TYR:CE1	2.48	0.48
2:F:94:LYS:HZ3	2:F:95:GLY:CA	2.23	0.48
2:H:18:VAL:HG12	2:H:82:LEU:HB3	1.96	0.48
1:I:85:THR:HA	1:I:102:THR:O	2.14	0.48
2:J:19:LYS:HE2	2:J:79:TYR:HB3	1.96	0.48
1:K:136:LEU:HD11	1:K:196:VAL:HG21	1.95	0.48
2:F:1:GLN:HG2	2:N:3:GLN:HE22	1.78	0.48
2:P:51:ILE:HG12	2:P:52:ILE:N	2.28	0.48
2:B:192:GLN:CG	2:B:193:THR:N	2.77	0.48
2:B:194:TYR:C	2:B:195:ILE:HD12	2.33	0.48
2:B:52(A):PRO:C	2:B:54:PHE:H	2.16	0.48
2:B:73:GLU:N	2:B:73:GLU:OE1	2.46	0.48
1:C:49:TYR:CD2	1:C:53:SER:O	2.66	0.48
2:D:210:LYS:HD3	2:D:212:GLU:OE2	2.14	0.48
2:D:2:VAL:CG2	2:D:27:GLY:N	2.76	0.48
2:D:93:ALA:CB	2:D:100(L):MET:HG2	2.42	0.48
1:E:116:PHE:CD2	2:F:137:ALA:HB3	2.49	0.48
1:I:120:PRO:HG3	1:I:186:TYR:CZ	2.49	0.48
2:J:51:ILE:CG1	2:J:57:ALA:HB2	2.43	0.48
2:J:6:GLN:NE2	2:J:91:PHE:HA	2.27	0.48
2:L:83:ARG:HB3	2:L:85:GLU:OE1	2.13	0.48
1:M:117:ILE:HD12	1:M:208:SER:HA	1.95	0.48
2:N:204:ASN:OD1	2:P:64:GLN:CB	2.62	0.48
2:B:101:ASP:OD2	2:B:101:ASP:N	2.30	0.48
2:D:90:TYR:O	2:D:106:GLY:HA2	2.14	0.48
2:D:138:LEU:O	2:D:181:VAL:HB	2.14	0.48
1:E:39:LYS:HB3	1:E:40:PRO:HD2	1.96	0.48
1:E:96:HIS:O	2:F:47:TRP:CG	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:111:VAL:O	2:F:111:VAL:CG1	2.56	0.48
2:F:153:SER:O	2:F:196:CYS:HA	2.14	0.48
1:G:170:ASP:OD2	1:G:172:THR:HG23	2.13	0.48
2:H:187:SER:O	2:H:191:THR:HG21	2.14	0.48
2:H:199:ASN:ND2	2:H:199:ASN:C	2.66	0.48
2:H:199:ASN:ND2	2:H:200:HIS:N	2.41	0.48
1:I:203:SER:OG	1:I:204:PRO:HD2	2.14	0.48
1:K:195:GLU:HG3	1:K:204:PRO:HB3	1.96	0.48
2:L:125:ALA:HA	2:L:126:PRO:HD3	1.79	0.48
2:L:13:LYS:O	2:L:14:PRO:O	2.32	0.48
2:L:164:HIS:HB2	2:L:181:VAL:HG22	1.95	0.48
2:L:67:VAL:HA	2:L:81:GLU:O	2.13	0.48
1:M:163:VAL:HG12	1:M:164:THR:N	2.28	0.48
2:N:206:LYS:C	2:N:207:VAL:CG2	2.82	0.48
1:O:188:LYS:O	1:O:189:HIS:CG	2.66	0.48
1:A:182:SER:O	1:A:183:LYS:C	2.52	0.48
2:B:182:VAL:HG22	2:B:184:VAL:CG1	2.44	0.48
1:C:184:ALA:O	1:C:186:TYR:N	2.47	0.48
1:C:193:ALA:HB2	1:C:208:SER:CB	2.43	0.48
2:D:52:ILE:HG22	2:D:53:VAL:HG23	1.96	0.48
1:E:115:VAL:O	1:E:207:LYS:NZ	2.40	0.48
2:H:116:THR:HG22	2:H:117:LYS:N	2.27	0.48
2:H:138:LEU:HD12	2:H:138:LEU:C	2.34	0.48
2:H:18:VAL:HB	2:H:82(C):LEU:HD11	1.96	0.48
1:I:36:TYR:OH	2:J:100(L):MET:N	2.36	0.48
2:L:151:THR:HG1	2:L:199:ASN:HB3	1.78	0.48
1:M:140:TYR:CD1	1:M:141:PRO:HA	2.48	0.48
2:N:123:PRO:HB3	2:N:211:VAL:HG22	1.96	0.48
1:A:124:GLN:CD	1:A:131:SER:H	2.18	0.48
1:A:55:GLN:HA	1:A:55:GLN:OE1	2.13	0.48
2:B:120:SER:O	2:B:121:VAL:CG2	2.62	0.48
2:B:141:LEU:HA	2:B:179:SER:HB3	1.96	0.48
1:C:30:SER:O	1:C:68:GLY:N	2.36	0.48
1:E:136:LEU:HD11	1:E:196:VAL:HG22	1.96	0.48
2:F:2:VAL:HA	2:F:26:GLY:HA3	1.95	0.48
1:G:147:GLN:CG	1:G:154:LEU:HD12	2.44	0.48
2:J:141:LEU:C	2:J:141:LEU:HD12	2.34	0.48
2:J:67:VAL:CG2	2:J:68:THR:N	2.77	0.48
2:L:82(A):SER:O	2:L:82(B):SER:CB	2.62	0.48
2:N:156:SER:CA	2:N:197:ASN:HD21	2.26	0.48
1:O:62:PHE:N	1:O:62:PHE:CD1	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:14:PRO:HD3	2:P:112:ALA:O	2.14	0.48
2:B:37:VAL:CG1	2:B:45:LEU:HB3	2.42	0.47
1:C:152:ASN:O	1:C:154:LEU:HD22	2.14	0.47
2:F:83:ARG:O	2:F:111:VAL:HG11	2.13	0.47
1:G:180:THR:C	1:G:181:LEU:HD12	2.34	0.47
2:J:18:VAL:O	2:J:81:GLU:HA	2.14	0.47
1:K:195:GLU:HG2	1:K:195:GLU:O	2.12	0.47
1:K:212:GLY:C	1:K:213:GLU:HG3	2.35	0.47
1:K:32:TYR:N	1:K:32:TYR:CD1	2.81	0.47
2:L:105:GLN:N	2:L:105:GLN:OE1	2.47	0.47
2:B:95:GLY:HA2	2:B:101:ASP:OD2	2.14	0.47
1:C:6:GLN:OE1	1:C:99:GLY:HA3	2.13	0.47
2:D:71:ALA:HB2	2:D:78:THR:CG2	2.41	0.47
2:F:143:LYS:HG2	2:F:144:ASP:OD2	2.14	0.47
2:H:201:LYS:H	2:H:202:PRO:CD	2.26	0.47
1:I:79:GLN:O	1:I:82:ASP:HB2	2.13	0.47
2:J:70:THR:O	2:J:78:THR:HA	2.13	0.47
1:K:197:THR:HG22	1:K:204:PRO:HG3	1.97	0.47
1:K:32:TYR:N	1:K:32:TYR:HD1	2.12	0.47
1:K:62:PHE:CD2	1:K:75:ILE:HG23	2.50	0.47
2:L:184:VAL:HB	2:L:185:PRO:HD2	1.96	0.47
2:N:122:PHE:HB2	2:N:141:LEU:HB3	1.97	0.47
1:O:29:ILE:HD11	1:O:71:PHE:CE1	2.49	0.47
2:P:6:GLN:NE2	2:P:106:GLY:CA	2.76	0.47
1:A:125:LEU:CD2	1:A:130:ALA:HB2	2.44	0.47
1:A:191:VAL:CG1	1:A:192:TYR:N	2.77	0.47
1:E:128:GLY:O	1:E:129:THR:HG23	2.14	0.47
1:K:183:LYS:HA	1:K:186:TYR:HB3	1.95	0.47
1:K:4:MET:SD	1:K:25:ALA:HB2	2.54	0.47
1:K:62:PHE:CE2	1:K:75:ILE:HG23	2.49	0.47
2:L:18:VAL:CG2	2:L:19:LYS:N	2.77	0.47
1:M:108:ARG:HD2	1:M:171:SER:HB2	1.96	0.47
2:P:203:SER:C	2:P:205:THR:N	2.67	0.47
2:B:40:ALA:HB3	2:B:43:GLN:NE2	2.20	0.47
2:B:19:LYS:HE2	2:B:79:TYR:CB	2.44	0.47
1:C:151:ASP:OD2	1:C:189:HIS:HB3	2.14	0.47
1:E:143:GLU:CD	1:E:143:GLU:H	2.18	0.47
2:F:145:TYR:CE2	2:F:176:TYR:CB	2.97	0.47
2:F:40:ALA:HB3	2:F:43:GLN:HG3	1.96	0.47
1:G:29:ILE:HG12	1:G:68:GLY:O	2.15	0.47
1:G:34:ASN:N	1:G:34:ASN:ND2	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:96:HIS:HB2	2:J:47:TRP:CD1	2.50	0.47
2:J:64:GLN:C	2:J:66:ARG:H	2.18	0.47
1:M:4:MET:CB	1:M:99:GLY:CA	2.87	0.47
2:P:32:TYR:CD2	2:P:32:TYR:N	2.78	0.47
1:C:23:CYS:HB3	1:C:35:TRP:CH2	2.50	0.47
1:E:4:MET:HE1	1:E:33:LEU:HD23	1.97	0.47
2:F:5:LEU:HB2	2:F:23:LYS:HB3	1.95	0.47
1:G:118:PHE:HE1	2:H:138:LEU:O	1.97	0.47
1:K:201:LEU:HD13	1:K:205:VAL:HG23	1.95	0.47
1:M:96:HIS:CD2	1:M:96:HIS:N	2.81	0.47
1:O:179:LEU:O	1:O:179:LEU:HG	2.14	0.47
1:O:187:GLU:HA	1:O:211:ARG:CZ	2.45	0.47
1:A:85:THR:OG1	1:A:103:LYS:HG3	2.14	0.47
1:A:175:LEU:HD23	1:A:176:SER:N	2.29	0.47
1:A:40:PRO:C	1:A:42:LYS:H	2.18	0.47
2:B:35:SER:O	2:B:92:CYS:HA	2.14	0.47
1:C:154:LEU:HD22	1:C:154:LEU:H	1.79	0.47
1:C:48:ILE:HD12	1:C:73:LEU:HD12	1.96	0.47
2:F:121:VAL:CG2	2:F:198:VAL:HG21	2.44	0.47
2:F:18:VAL:CG2	2:F:19:LYS:N	2.77	0.47
1:G:154:LEU:C	1:G:155:GLN:HE21	2.16	0.47
1:G:69:THR:O	1:G:71:PHE:HD1	1.98	0.47
1:G:83:PHE:HD2	1:G:104:LEU:O	1.97	0.47
2:H:112:ALA:C	2:H:114:ALA:H	2.18	0.47
2:J:151:THR:O	2:J:198:VAL:HG13	2.15	0.47
2:J:51:ILE:HG13	2:J:57:ALA:HB2	1.95	0.47
1:K:135:LEU:HD12	1:K:136:LEU:O	2.14	0.47
1:K:210:ASN:HD22	1:K:210:ASN:H	1.52	0.47
1:K:174:SER:O	2:L:166:PHE:HE2	1.98	0.47
1:M:89:GLN:NE2	1:M:96:HIS:HB3	2.28	0.47
2:P:16:SER:OG	2:P:17:SER:N	2.45	0.47
2:P:119:PRO:HD2	2:P:205:THR:HG21	1.96	0.47
2:P:31:SER:O	2:P:32:TYR:C	2.52	0.47
1:A:135:LEU:HG	1:A:136:LEU:H	1.79	0.47
2:B:63:PHE:O	2:B:67:VAL:CG1	2.62	0.47
2:F:29:PHE:HD1	2:F:30:SER:N	2.12	0.47
2:F:71:ALA:CA	2:F:77:THR:O	2.61	0.47
2:H:141:LEU:HD12	2:H:142:VAL:H	1.80	0.47
1:I:55:GLN:HG3	1:I:56:SER:N	2.29	0.47
1:I:6:GLN:HB2	1:I:88:CYS:SG	2.55	0.47
1:M:151:ASP:C	1:M:153:ALA:N	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:184:ALA:O	1:O:188:LYS:HG3	2.15	0.47
1:O:140:TYR:O	1:O:198:HIS:CE1	2.68	0.47
1:A:6:GLN:HE22	1:A:101:GLY:HA2	1.80	0.47
2:B:83:ARG:NH2	3:B:222:HOH:O	2.47	0.47
2:D:80:MET:HE2	2:D:90:TYR:CD2	2.49	0.47
1:E:187:GLU:HA	1:E:211:ARG:NE	2.29	0.47
1:G:191:VAL:HG22	1:G:210:ASN:HD21	1.80	0.47
2:J:203:SER:O	2:J:205:THR:N	2.48	0.47
1:G:18:ARG:HD3	1:K:153:ALA:HB2	1.97	0.47
2:L:136:ALA:HB1	2:L:189:LEU:HD11	1.97	0.47
1:M:142:ARG:NH1	1:M:163:VAL:HG11	2.29	0.47
2:D:113:SER:O	2:D:114:ALA:C	2.53	0.47
2:D:188:SER:O	2:D:189:LEU:C	2.53	0.47
2:D:5:LEU:O	2:D:22:CYS:HA	2.15	0.47
1:G:208:SER:OG	1:G:209:PHE:N	2.48	0.47
2:H:187:SER:O	2:H:191:THR:CG2	2.62	0.47
1:I:192:TYR:O	1:I:208:SER:HA	2.15	0.47
1:K:149:LYS:HB2	1:K:149:LYS:HZ2	1.80	0.47
1:M:186:TYR:CD1	1:M:192:TYR:CZ	3.02	0.47
1:M:92:TYR:O	1:M:93:SER:O	2.33	0.47
2:N:166:PHE:HA	2:N:167:PRO:HD3	1.80	0.47
1:O:209:PHE:CD2	1:O:209:PHE:C	2.87	0.47
1:A:131:SER:HA	1:A:180:THR:HA	1.95	0.47
1:A:147:GLN:HG3	1:A:154:LEU:HD11	1.97	0.47
2:B:52(A):PRO:C	2:B:54:PHE:N	2.67	0.47
1:E:186:TYR:O	1:E:192:TYR:OH	2.29	0.47
1:G:182:SER:O	1:G:184:ALA:N	2.48	0.47
2:N:96:GLY:CA	2:N:101:ASP:HB2	2.45	0.47
1:O:32:TYR:HB2	1:O:92:TYR:HB2	1.96	0.47
1:A:124:GLN:NE2	1:A:131:SER:OG	2.48	0.47
1:C:124:GLN:HE22	1:C:131:SER:HB2	1.79	0.47
2:H:160:THR:HA	2:H:163:VAL:HG21	1.96	0.47
1:K:120:PRO:HD3	1:K:132:VAL:HG22	1.97	0.47
1:M:207:LYS:HD3	2:N:129:LYS:O	2.15	0.47
1:M:55:GLN:NE2	1:M:56:SER:H	2.12	0.47
2:N:1:GLN:O	2:N:3:GLN:HG3	2.15	0.47
1:O:62:PHE:N	1:O:62:PHE:HD1	2.12	0.47
1:A:113:PRO:HD3	1:A:198:HIS:CD2	2.49	0.46
2:B:117:LYS:NZ	2:B:144:ASP:HB3	2.31	0.46
2:B:14:PRO:CG	2:B:113:SER:N	2.79	0.46
1:C:142:ARG:HG2	1:C:142:ARG:NH1	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:THR:HG22	1:C:75:ILE:N	2.30	0.46
1:G:117:ILE:HG23	1:G:117:ILE:O	2.15	0.46
1:I:48:ILE:HD13	1:I:64:GLY:H	1.79	0.46
2:J:192:GLN:NE2	2:J:193:THR:O	2.38	0.46
1:K:182:SER:O	1:K:183:LYS:C	2.52	0.46
2:L:83:ARG:N	2:L:86:ASP:OD2	2.47	0.46
1:M:147:GLN:CG	1:M:154:LEU:HD12	2.45	0.46
1:M:165:GLU:OE2	1:M:165:GLU:HA	2.16	0.46
2:P:146:PHE:CD2	2:P:147:PRO:N	2.84	0.46
2:B:199:ASN:ND2	2:B:205:THR:O	2.49	0.46
1:C:29:ILE:HG12	1:C:71:PHE:CE1	2.50	0.46
1:C:38:GLN:HE21	1:C:44:PRO:HG3	1.80	0.46
2:H:115:SER:OG	2:H:116:THR:N	2.49	0.46
2:H:51:ILE:CG1	2:H:57:ALA:HB2	2.46	0.46
1:I:15:VAL:C	1:I:17:ASP:H	2.18	0.46
1:I:183:LYS:O	1:I:187:GLU:HG3	2.14	0.46
1:K:79:GLN:HB3	1:K:81:GLU:OE2	2.15	0.46
2:L:186:SER:O	2:L:188:SER:N	2.48	0.46
2:N:145:TYR:CE1	2:N:150:VAL:HG12	2.51	0.46
1:C:180:THR:HG22	1:O:24:ARG:HH22	1.79	0.46
2:P:32:TYR:HD2	2:P:32:TYR:N	2.13	0.46
1:A:61:ARG:HB3	1:A:76:SER:OG	2.15	0.46
1:E:110:VAL:HG12	1:E:111:ALA:N	2.30	0.46
1:E:126:LYS:HE3	1:E:126:LYS:N	2.31	0.46
2:F:52(A):PRO:O	2:F:54:PHE:N	2.48	0.46
1:K:100:GLN:HG2	1:K:101:GLY:H	1.81	0.46
1:K:185:ASP:O	1:K:188:LYS:N	2.44	0.46
2:L:186:SER:HA	2:L:189:LEU:HG	1.97	0.46
1:M:4:MET:HB2	1:M:99:GLY:CA	2.39	0.46
1:M:4:MET:HB2	1:M:98:PHE:O	2.14	0.46
1:O:150:VAL:O	1:O:151:ASP:C	2.53	0.46
2:B:100(J):HIS:HB3	2:B:100(K):GLY:H	1.52	0.46
2:D:18:VAL:H	2:D:82(C):LEU:HD11	1.79	0.46
1:E:34:ASN:OD1	1:E:49:TYR:HA	2.16	0.46
2:F:142:VAL:HB	2:F:178:LEU:HD12	1.98	0.46
2:H:68:THR:N	2:H:81:GLU:O	2.48	0.46
1:M:124:GLN:O	1:M:127:SER:N	2.45	0.46
2:N:193:THR:HG22	2:N:194:TYR:N	2.31	0.46
1:O:61:ARG:NE	1:O:79:GLN:CG	2.78	0.46
2:P:29:PHE:CD1	2:P:76:SER:HA	2.49	0.46
1:A:64:GLY:O	3:A:233:HOH:O	2.21	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:GLN:O	1:C:90:GLN:NE2	2.49	0.46
2:F:20:VAL:HG11	2:F:36:TRP:HZ3	1.81	0.46
2:F:94:LYS:CE	2:F:95:GLY:CA	2.94	0.46
1:G:147:GLN:HG3	1:G:154:LEU:HD12	1.98	0.46
1:I:110:VAL:CG1	1:I:111:ALA:N	2.78	0.46
1:I:35:TRP:CE2	1:I:73:LEU:HB2	2.51	0.46
1:K:62:PHE:HE2	1:K:75:ILE:HG12	1.81	0.46
2:L:138:LEU:CD1	2:L:138:LEU:C	2.71	0.46
1:M:124:GLN:CD	1:M:131:SER:H	2.18	0.46
2:D:52(A):PRO:O	2:D:53:VAL:O	2.34	0.46
1:E:8:PRO:HG3	1:E:100:GLN:OE1	2.15	0.46
2:F:2:VAL:CB	2:F:27:GLY:H	2.27	0.46
2:H:84:SER:HA	2:H:111:VAL:HB	1.96	0.46
1:E:154:LEU:HB2	1:I:19:VAL:HG22	1.97	0.46
1:M:47:LEU:HD13	1:M:62:PHE:CD2	2.51	0.46
2:N:125:ALA:HA	2:N:126:PRO:HD3	1.81	0.46
2:N:203:SER:OG	2:N:205:THR:HG23	2.16	0.46
1:O:83:PHE:CZ	1:O:106:ILE:HG23	2.51	0.46
1:O:144:ALA:HB3	1:O:175:LEU:HD13	1.98	0.46
2:P:41:PRO:HD3	2:P:87:THR:O	2.14	0.46
1:C:146:VAL:HG22	1:C:196:VAL:HG22	1.98	0.46
1:E:107:LYS:CG	1:E:108:ARG:N	2.79	0.46
2:F:112:ALA:HB3	2:F:146:PHE:CZ	2.50	0.46
1:G:2:ILE:N	1:G:26:SER:HG	2.14	0.46
2:H:207:VAL:HG12	2:H:208:ASP:N	2.30	0.46
2:H:32:TYR:HB3	2:H:94:LYS:CG	2.46	0.46
1:I:155:GLN:HB3	1:I:158:ASN:HD21	1.81	0.46
1:K:7:SER:HA	1:K:100:GLN:NE2	2.31	0.46
1:M:36:TYR:CE2	2:N:103:TRP:HZ2	2.34	0.46
1:O:127:SER:HG	2:P:122:PHE:HZ	1.63	0.46
1:A:183:LYS:NZ	1:A:187:GLU:OE2	2.48	0.46
1:A:47:LEU:HD11	1:A:86:TYR:CE2	2.49	0.46
1:A:90:GLN:O	1:A:90:GLN:HG3	2.16	0.46
2:B:36:TRP:CD1	2:B:69:ILE:HD13	2.51	0.46
2:D:18:VAL:CG2	2:D:19:LYS:H	2.27	0.46
1:E:107:LYS:HG2	1:E:108:ARG:N	2.31	0.46
1:G:188:LYS:O	1:G:189:HIS:CG	2.68	0.46
2:J:131:THR:HG22	2:J:135:THR:O	2.16	0.46
1:K:19:VAL:HG23	1:K:78:LEU:CD2	2.40	0.46
2:L:35:SER:O	2:L:92:CYS:HA	2.16	0.46
1:M:3:GLN:HB3	1:M:26:SER:CB	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:38:GLN:HE22	2:P:39:GLN:HE22	1.64	0.46
2:P:90:TYR:N	2:P:90:TYR:CD1	2.84	0.46
1:C:167:ASP:O	1:C:171:SER:HA	2.16	0.46
2:D:42:GLY:C	2:D:43:GLN:OE1	2.54	0.46
2:D:30:SER:HA	2:D:52(A):PRO:HB2	1.98	0.46
2:F:70:THR:O	2:F:71:ALA:HB2	2.16	0.46
2:H:155:ASN:O	2:H:156:SER:HB2	2.15	0.46
2:H:137:ALA:HA	2:H:182:VAL:O	2.15	0.46
1:I:7:SER:OG	1:I:100:GLN:NE2	2.49	0.46
2:J:39:GLN:NE2	2:J:45:LEU:CD2	2.79	0.46
2:J:47:TRP:HE1	2:J:100(L):MET:CE	2.28	0.46
1:K:136:LEU:HD21	1:K:196:VAL:HG13	1.98	0.46
2:L:115:SER:H	2:L:117:LYS:HE2	1.81	0.46
2:L:119:PRO:HD3	2:L:145:TYR:HB2	1.98	0.46
2:N:170:LEU:HD13	2:N:176:TYR:CE1	2.50	0.46
1:O:89:GLN:HG3	1:O:98:PHE:CD2	2.51	0.46
2:P:82(A):SER:OG	2:P:82(B):SER:N	2.49	0.46
2:B:125:ALA:HA	2:B:126:PRO:HD3	1.65	0.46
1:C:190:LYS:O	1:C:210:ASN:HA	2.15	0.46
1:C:62:PHE:O	1:C:63:SER:CB	2.60	0.46
1:E:212:GLY:O	1:E:213:GLU:HB2	2.16	0.46
2:F:155:ASN:ND2	2:F:159:LEU:HB2	2.30	0.46
2:F:67:VAL:CG2	2:F:68:THR:N	2.79	0.46
1:G:17:ASP:N	1:G:17:ASP:OD1	2.49	0.46
2:H:171:GLN:NE2	2:H:175:LEU:O	2.49	0.46
1:I:119:PRO:HB3	1:I:209:PHE:CE1	2.51	0.46
2:J:12:LYS:HZ1	2:J:18:VAL:HA	1.80	0.46
2:F:62:LYS:HA	2:J:83:ARG:NH1	2.31	0.46
1:E:60:SER:HB3	1:M:81:GLU:OE1	2.16	0.46
2:N:31:SER:O	2:N:32:TYR:O	2.34	0.46
1:O:142:ARG:HB2	1:O:173:TYR:CE2	2.51	0.46
1:O:8:PRO:CD	1:O:10:SER:N	2.77	0.46
2:P:53:VAL:CG1	2:P:53:VAL:O	2.63	0.46
2:D:35:SER:CB	2:D:49:GLY:O	2.65	0.45
2:D:73:GLU:H	2:D:73:GLU:CD	2.19	0.45
1:E:20:THR:CG2	1:E:72:THR:OG1	2.64	0.45
1:E:4:MET:CE	1:E:33:LEU:HD23	2.46	0.45
1:G:91:SER:O	1:G:92:TYR:C	2.54	0.45
2:H:119:PRO:HB2	2:H:142:VAL:CG1	2.46	0.45
2:H:144:ASP:HB3	2:H:175:LEU:HD12	1.98	0.45
1:I:193:ALA:HB1	1:I:206:THR:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:126:LYS:CA	1:K:126:LYS:HE3	2.46	0.45
1:K:37:GLN:HB2	1:K:47:LEU:HD11	1.98	0.45
2:L:171:GLN:NE2	2:L:173:SER:OG	2.49	0.45
2:L:181:VAL:C	2:L:182:VAL:HG12	2.36	0.45
1:M:135:LEU:HD12	1:M:175:LEU:O	2.16	0.45
1:M:79:GLN:O	1:M:82:ASP:HB2	2.16	0.45
1:O:83:PHE:CE2	1:O:106:ILE:HG23	2.51	0.45
1:A:138:ASN:HA	1:A:173:TYR:O	2.16	0.45
1:A:72:THR:HG22	1:A:72:THR:O	2.14	0.45
2:B:183:THR:O	2:B:183:THR:HG23	2.16	0.45
2:B:184:VAL:CB	2:B:185:PRO:CD	2.94	0.45
1:E:125:LEU:O	1:E:183:LYS:HD2	2.16	0.45
1:E:32:TYR:CD1	1:E:92:TYR:CD1	2.98	0.45
2:F:145:TYR:HE1	2:F:150:VAL:CB	2.13	0.45
1:E:98:PHE:CZ	2:F:37:VAL:HG11	2.50	0.45
1:K:146:VAL:HG11	1:K:177:SER:OG	2.16	0.45
1:K:47:LEU:HD11	1:K:86:TYR:CE2	2.46	0.45
2:L:193:THR:CG2	2:L:194:TYR:N	2.79	0.45
1:M:89:GLN:HG2	1:M:90:GLN:N	2.31	0.45
2:N:63:PHE:HB3	2:N:67:VAL:HG12	1.98	0.45
2:N:95:GLY:HA2	2:N:100(L):MET:HA	1.98	0.45
1:O:61:ARG:HG3	1:O:62:PHE:HE1	1.80	0.45
2:P:52:ILE:O	2:P:53:VAL:N	2.49	0.45
1:A:151:ASP:O	1:A:152:ASN:HB2	2.16	0.45
1:A:210:ASN:O	1:A:213:GLU:CG	2.64	0.45
2:D:126:PRO:HD2	2:D:213:PRO:HA	1.98	0.45
2:D:36:TRP:CZ2	2:D:80:MET:HB2	2.51	0.45
1:E:170:ASP:O	1:E:172:THR:HG23	2.15	0.45
1:E:55:GLN:O	1:E:58:VAL:HG23	2.16	0.45
2:H:32:TYR:HB3	2:H:94:LYS:HG2	1.99	0.45
1:E:24:ARG:NH1	1:I:158:ASN:HA	2.31	0.45
2:J:201:LYS:O	2:J:203:SER:N	2.49	0.45
2:L:73:GLU:C	2:L:75:THR:N	2.69	0.45
1:M:62:PHE:HE2	1:M:86:TYR:CE2	2.35	0.45
1:E:98:PHE:CE1	2:F:37:VAL:HG11	2.52	0.45
1:G:32:TYR:HB3	1:G:92:TYR:H	1.82	0.45
2:H:112:ALA:O	2:H:114:ALA:N	2.50	0.45
2:J:20:VAL:O	2:J:79:TYR:HA	2.16	0.45
1:K:183:LYS:HD2	3:K:218:HOH:O	2.16	0.45
1:O:120:PRO:HB3	1:O:131:SER:H	1.82	0.45
1:O:79:GLN:HB3	1:O:81:GLU:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:LEU:HD13	1:A:205:VAL:CG2	2.38	0.45
2:B:162:GLY:O	2:B:182:VAL:HA	2.16	0.45
2:B:38:ARG:CZ	2:B:63:PHE:HZ	2.30	0.45
1:C:185:ASP:HA	1:C:188:LYS:HD2	1.98	0.45
1:C:4:MET:CE	1:C:33:LEU:HD23	2.47	0.45
2:D:39:GLN:HE22	2:D:44:GLY:HA2	1.81	0.45
1:E:140:TYR:CG	1:E:141:PRO:HA	2.52	0.45
1:E:143:GLU:CD	1:E:143:GLU:N	2.70	0.45
1:E:66:GLY:O	1:E:67:SER:CB	2.64	0.45
2:F:214:LYS:OXT	2:F:214:LYS:CG	2.65	0.45
1:K:7:SER:OG	1:K:7:SER:O	2.29	0.45
2:P:12:LYS:HE3	2:P:18:VAL:CG2	2.47	0.45
1:A:90:GLN:HE22	1:A:93:SER:N	2.13	0.45
1:G:64:GLY:O	1:G:65:SER:HB3	2.16	0.45
1:G:74:THR:HG22	1:G:75:ILE:N	2.31	0.45
2:H:145:TYR:HE2	2:H:177:SER:HA	1.82	0.45
1:I:197:THR:HG22	1:I:204:PRO:CB	2.46	0.45
2:L:145:TYR:HE2	2:L:177:SER:HA	1.81	0.45
2:L:51:ILE:HG23	2:L:51:ILE:O	2.17	0.45
1:M:146:VAL:HG22	1:M:196:VAL:HG22	1.98	0.45
2:B:94:LYS:HB3	2:B:102:VAL:HG13	1.98	0.45
1:C:61:ARG:HG3	1:C:62:PHE:CD1	2.52	0.45
1:C:67:SER:HA	1:C:71:PHE:CE2	2.51	0.45
2:F:11:VAL:HG11	2:F:146:PHE:HZ	1.82	0.45
1:G:191:VAL:CG2	1:G:210:ASN:HD21	2.29	0.45
1:G:7:SER:HA	1:G:8:PRO:HD3	1.50	0.45
2:J:163:VAL:HG12	2:J:164:HIS:H	1.80	0.45
2:L:87:THR:O	2:L:88:ALA:HB2	2.16	0.45
1:M:211:ARG:HG2	1:M:211:ARG:NH1	2.28	0.45
1:M:28:SER:HA	1:M:69:THR:CG2	2.46	0.45
1:M:162:SER:OG	2:N:167:PRO:HD2	2.17	0.45
2:N:138:LEU:HD13	2:N:211:VAL:HG11	1.98	0.45
2:B:48:MET:SD	2:B:80:MET:HE2	2.57	0.45
2:F:32:TYR:CD2	2:F:94:LYS:HE3	2.51	0.45
2:F:68:THR:HB	2:F:81:GLU:CB	2.42	0.45
2:F:16:SER:O	2:F:82(C):LEU:HG	2.16	0.45
2:H:89:VAL:HG13	2:H:107:THR:H	1.82	0.45
2:J:181:VAL:O	2:J:182:VAL:HB	2.16	0.45
2:L:112:ALA:HB3	2:L:146:PHE:CZ	2.52	0.45
2:L:186:SER:C	2:L:188:SER:H	2.20	0.45
1:O:114:SER:HB2	1:O:137:ASN:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:141:LEU:HD12	2:P:179:SER:HB3	1.99	0.45
1:A:140:TYR:CG	1:A:141:PRO:HA	2.52	0.45
1:A:50:ALA:O	1:A:51:ALA:HB3	2.16	0.45
2:B:138:LEU:N	2:B:138:LEU:HD23	2.15	0.45
2:B:200:HIS:HE1	2:B:202:PRO:HB2	1.77	0.45
2:B:29:PHE:O	2:B:32:TYR:N	2.49	0.45
2:B:83:ARG:HD2	2:B:85:GLU:OE1	2.17	0.45
2:D:51:ILE:O	2:D:52:ILE:CG1	2.64	0.45
1:G:83:PHE:CE2	1:G:105:GLU:C	2.90	0.45
2:H:6:GLN:HA	2:H:21:SER:O	2.17	0.45
1:I:203:SER:OG	1:I:204:PRO:CD	2.65	0.45
1:M:29:ILE:O	1:M:30:SER:CB	2.63	0.45
2:N:40:ALA:O	2:N:43:GLN:HB2	2.16	0.45
1:O:13:ALA:O	1:O:107:LYS:N	2.34	0.45
1:O:148:TRP:CE3	1:O:193:ALA:O	2.70	0.45
1:O:199:GLN:HE21	1:O:199:GLN:CA	2.30	0.45
1:A:108:ARG:NH1	1:A:172:THR:CG2	2.80	0.45
1:A:114:SER:O	1:A:116:PHE:CE1	2.70	0.45
2:D:178:LEU:HD12	2:D:179:SER:N	2.32	0.45
1:G:14:SER:HB2	1:G:17:ASP:CG	2.37	0.45
2:H:138:LEU:CD1	2:H:154:TRP:CH2	2.98	0.45
1:I:32:TYR:CB	1:I:92:TYR:N	2.79	0.45
1:O:140:TYR:O	1:O:198:HIS:HE1	1.99	0.45
1:A:119:PRO:HB3	1:A:209:PHE:CD2	2.53	0.44
1:A:25:ALA:N	1:A:69:THR:O	2.49	0.44
2:D:17:SER:CB	2:D:82:LEU:O	2.65	0.44
1:I:106:ILE:N	1:I:166:GLN:OE1	2.48	0.44
1:K:126:LYS:C	1:K:128:GLY:N	2.68	0.44
1:K:33:LEU:C	1:K:33:LEU:HD13	2.37	0.44
2:L:154:TRP:CH2	2:L:196:CYS:HB3	2.53	0.44
1:M:29:ILE:CD1	1:M:33:LEU:HB2	2.46	0.44
2:N:32:TYR:O	2:N:52(A):PRO:HD2	2.17	0.44
2:N:47:TRP:CE3	2:N:60:ALA:HB2	2.52	0.44
2:P:12:LYS:HE3	2:P:18:VAL:HB	2.00	0.44
2:P:36:TRP:HD1	2:P:69:ILE:CD1	2.30	0.44
2:P:53:VAL:C	2:P:54:PHE:CD2	2.90	0.44
1:A:145:LYS:HB3	1:A:197:THR:CG2	2.47	0.44
1:A:174:SER:HB2	2:B:164:HIS:CD2	2.52	0.44
2:F:184:VAL:CB	2:F:185:PRO:CD	2.96	0.44
1:G:169:LYS:HG3	1:G:170:ASP:N	2.32	0.44
1:I:121:SER:O	1:I:124:GLN:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:6:GLN:NE2	1:I:87:TYR:HA	2.28	0.44
1:K:108:ARG:NH2	1:K:109:THR:OG1	2.51	0.44
1:K:126:LYS:C	1:K:128:GLY:H	2.21	0.44
1:K:119:PRO:HB3	1:K:209:PHE:CZ	2.52	0.44
2:L:193:THR:HG22	2:L:195:ILE:HD11	2.00	0.44
2:L:37:VAL:HG21	2:L:103:TRP:CH2	2.52	0.44
1:M:40:PRO:HD3	3:M:218:HOH:O	2.18	0.44
2:N:203:SER:O	2:N:205:THR:N	2.50	0.44
2:P:22:CYS:SG	2:P:22:CYS:O	2.74	0.44
2:P:29:PHE:CZ	2:P:52(A):PRO:HB3	2.52	0.44
1:C:201:LEU:HD13	1:C:205:VAL:HG23	1.99	0.44
2:D:2:VAL:O	2:D:2:VAL:HG13	2.18	0.44
2:F:140:CYS:O	2:F:179:SER:CA	2.63	0.44
2:F:212:GLU:HA	2:F:213:PRO:HD3	1.77	0.44
2:H:184:VAL:HG21	2:H:194:TYR:CE1	2.53	0.44
2:H:199:ASN:ND2	2:H:200:HIS:O	2.50	0.44
2:J:199:ASN:C	2:J:199:ASN:ND2	2.68	0.44
2:J:30:SER:CA	2:J:52(A):PRO:HB2	2.44	0.44
2:J:64:GLN:HG2	2:L:204:ASN:OD1	2.18	0.44
1:K:116:PHE:CD2	2:L:130:SER:HA	2.52	0.44
2:N:90:TYR:O	2:N:106:GLY:HA2	2.18	0.44
1:A:70:ASP:C	1:A:71:PHE:CD1	2.91	0.44
2:B:150:VAL:O	2:B:150:VAL:CG1	2.65	0.44
1:C:93:SER:OG	1:C:94:THR:N	2.50	0.44
1:E:150:VAL:C	1:E:152:ASN:N	2.70	0.44
1:G:150:VAL:O	1:G:151:ASP:HB2	2.16	0.44
1:G:138:ASN:CA	1:G:172:THR:HB	2.47	0.44
1:G:206:THR:CG2	1:G:207:LYS:N	2.79	0.44
2:H:128:SER:O	2:H:130:SER:N	2.44	0.44
2:H:70:THR:O	2:H:78:THR:HA	2.17	0.44
1:I:12:SER:O	1:I:13:ALA:CB	2.63	0.44
1:I:61:ARG:HH21	1:I:82:ASP:CG	2.19	0.44
2:J:62:LYS:C	2:J:64:GLN:N	2.70	0.44
1:K:210:ASN:ND2	1:K:210:ASN:H	2.09	0.44
2:L:11:VAL:HG13	2:L:110:THR:HB	1.99	0.44
2:P:72:ASP:OD2	2:P:74:ALA:HB2	2.17	0.44
1:A:145:LYS:HB3	1:A:197:THR:HG23	1.98	0.44
1:A:28:SER:HA	1:A:69:THR:CG2	2.45	0.44
1:E:124:GLN:HG2	1:E:129:THR:O	2.17	0.44
1:E:19:VAL:HG12	1:E:20:THR:N	2.33	0.44
1:E:207:LYS:O	1:E:208:SER:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:184:VAL:HB	2:F:185:PRO:HD2	1.99	0.44
2:F:188:SER:C	2:F:190:GLY:H	2.21	0.44
1:G:148:TRP:HD1	1:G:159:SER:HG	1.62	0.44
1:G:32:TYR:HD1	1:G:32:TYR:N	2.16	0.44
1:G:31:SER:O	1:G:50:ALA:HA	2.18	0.44
2:H:112:ALA:C	2:H:114:ALA:N	2.70	0.44
2:J:12:LYS:CD	2:J:18:VAL:HB	2.44	0.44
2:J:64:GLN:HB3	2:L:204:ASN:CG	2.38	0.44
1:K:48:ILE:HD12	1:K:73:LEU:CD1	2.47	0.44
2:L:7:SER:HB2	2:L:10:GLU:OE2	2.16	0.44
1:M:179:LEU:HD12	1:M:179:LEU:C	2.38	0.44
2:N:96:GLY:HA2	2:N:101:ASP:HB2	2.00	0.44
2:N:94:LYS:HE2	2:N:95:GLY:O	2.17	0.44
2:P:69:ILE:HG12	2:P:80:MET:HG2	1.99	0.44
1:C:61:ARG:HG3	1:C:62:PHE:CE1	2.53	0.44
2:D:138:LEU:HD12	2:D:138:LEU:O	2.18	0.44
2:D:119:PRO:HB3	2:D:145:TYR:HD2	1.82	0.44
2:D:210:LYS:CE	2:D:212:GLU:OE2	2.66	0.44
1:E:138:ASN:HA	1:E:173:TYR:O	2.17	0.44
1:E:149:LYS:HG2	1:E:154:LEU:HD13	2.00	0.44
1:G:136:LEU:HD22	1:G:175:LEU:HD22	2.00	0.44
2:H:76:SER:O	2:H:76:SER:OG	2.29	0.44
1:I:91:SER:O	1:I:93:SER:O	2.35	0.44
1:K:55:GLN:CG	1:K:56:SER:N	2.80	0.44
1:K:90:GLN:NE2	1:K:97:THR:OG1	2.51	0.44
2:L:51:ILE:HG12	2:L:52:ILE:N	2.32	0.44
2:L:6:GLN:NE2	2:L:106:GLY:HA2	2.33	0.44
1:M:150:VAL:HG11	1:M:189:HIS:HD2	1.82	0.44
1:M:40:PRO:C	1:M:42:LYS:H	2.21	0.44
2:P:100(L):MET:HE2	2:P:100(L):MET:N	2.32	0.44
2:B:126:PRO:CG	2:B:138:LEU:HB3	2.41	0.44
2:B:141:LEU:HG	2:B:141:LEU:O	2.18	0.44
2:D:139:GLY:O	2:D:140:CYS:SG	2.76	0.44
2:D:47:TRP:CZ3	2:D:49:GLY:HA2	2.53	0.44
2:D:51:ILE:CG1	2:D:52:ILE:N	2.77	0.44
1:E:124:GLN:HE22	1:E:131:SER:CB	2.31	0.44
1:E:183:LYS:O	1:E:187:GLU:HG2	2.18	0.44
2:F:17:SER:HB2	2:F:82:LEU:O	2.17	0.44
2:H:154:TRP:CZ3	2:H:196:CYS:HB3	2.53	0.44
1:I:48:ILE:HD13	1:I:64:GLY:CA	2.48	0.44
1:M:155:GLN:O	1:M:156:SER:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:33:LEU:C	1:M:33:LEU:HD22	2.37	0.44
1:O:107:LYS:HA	1:O:140:TYR:OH	2.17	0.44
2:P:178:LEU:HD12	2:P:178:LEU:C	2.38	0.44
2:P:37:VAL:HA	2:P:46:GLU:O	2.18	0.44
2:B:22:CYS:O	2:B:22:CYS:SG	2.76	0.44
2:B:23:LYS:NZ	2:B:75:THR:O	2.50	0.44
2:D:29:PHE:C	2:D:31:SER:H	2.21	0.44
1:E:96:HIS:CD2	1:E:96:HIS:N	2.86	0.44
1:G:106:ILE:HD12	1:G:166:GLN:OE1	2.17	0.44
2:H:195:ILE:O	2:H:196:CYS:C	2.56	0.44
2:J:36:TRP:CG	2:J:80:MET:HG2	2.52	0.44
1:K:55:GLN:HG3	1:K:56:SER:N	2.32	0.44
2:L:55:GLY:O	2:L:56:SER:HB3	2.16	0.44
2:L:66:ARG:CG	2:L:67:VAL:H	2.31	0.44
1:M:77:SER:O	1:M:78:LEU:C	2.55	0.44
2:N:100(J):HIS:CG	2:N:100(K):GLY:N	2.85	0.44
1:A:158:ASN:ND2	1:A:158:ASN:N	2.39	0.44
2:B:135:THR:O	2:B:135:THR:HG22	2.16	0.44
2:D:84:SER:C	2:D:86:ASP:H	2.22	0.44
1:E:96:HIS:CD2	1:E:96:HIS:H	2.35	0.44
2:F:34:ILE:HA	2:F:94:LYS:HB2	1.99	0.44
2:F:62:LYS:O	2:F:64:GLN:N	2.44	0.44
1:G:180:THR:HG21	2:H:143:LYS:HE3	1.99	0.44
2:H:6:GLN:NE2	2:H:107:THR:OG1	2.48	0.44
2:J:101:ASP:OD1	2:J:101:ASP:C	2.55	0.44
2:J:36:TRP:CE2	2:J:80:MET:HB2	2.53	0.44
1:K:126:LYS:O	1:K:128:GLY:N	2.50	0.44
1:K:164:THR:HG23	1:K:164:THR:O	2.18	0.44
2:L:36:TRP:HE1	2:L:78:THR:CG2	2.29	0.44
2:L:6:GLN:CD	2:L:106:GLY:HA2	2.38	0.44
1:A:147:GLN:HE22	1:M:11:LEU:HD22	1.82	0.44
1:O:51:ALA:HB1	1:O:71:PHE:HD2	1.82	0.44
1:O:90:GLN:NE2	1:O:95:SER:O	2.50	0.44
2:P:168:ALA:HA	2:P:178:LEU:HB3	1.99	0.44
2:P:169:VAL:HG22	2:P:177:SER:O	2.17	0.44
1:A:167:ASP:OD2	1:A:169:LYS:HE2	2.17	0.43
1:A:49:TYR:O	1:A:50:ALA:HB3	2.18	0.43
1:C:193:ALA:CB	1:C:208:SER:HB3	2.48	0.43
1:C:36:TYR:HA	1:C:45:LYS:O	2.18	0.43
2:D:35:SER:HB2	2:D:49:GLY:O	2.18	0.43
2:D:70:THR:O	2:D:78:THR:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:113:PRO:HA	1:E:137:ASN:O	2.18	0.43
1:G:210:ASN:HD22	1:G:210:ASN:HA	1.65	0.43
2:H:142:VAL:O	2:H:145:TYR:HD2	2.01	0.43
1:I:129:THR:HA	1:I:182:SER:HA	2.00	0.43
1:I:142:ARG:CZ	1:I:163:VAL:HG21	2.48	0.43
1:I:141:PRO:HD2	1:I:199:GLN:HB3	2.00	0.43
2:L:185:PRO:O	2:L:188:SER:OG	2.31	0.43
1:O:61:ARG:C	1:O:62:PHE:HD1	2.21	0.43
2:P:61:GLN:HA	2:P:64:GLN:CD	2.38	0.43
1:E:124:GLN:CB	3:E:216:HOH:O	2.64	0.43
1:E:167:ASP:HB3	1:E:170:ASP:OD2	2.18	0.43
2:F:210:LYS:HG2	2:F:212:GLU:HG2	2.00	0.43
1:G:113:PRO:HD3	1:G:198:HIS:CG	2.53	0.43
1:G:33:LEU:HA	1:G:89:GLN:O	2.18	0.43
2:H:66:ARG:NH2	2:H:86:ASP:OD1	2.51	0.43
2:J:10:GLU:HB2	2:J:109:VAL:HG22	2.00	0.43
1:K:198:HIS:ND1	1:K:199:GLN:N	2.65	0.43
2:L:119:PRO:CG	2:L:145:TYR:HB3	2.48	0.43
2:L:71:ALA:O	2:L:72:ASP:CB	2.66	0.43
2:P:100(L):MET:O	2:P:103:TRP:NE1	2.51	0.43
2:B:51:ILE:HB	2:B:57:ALA:CB	2.47	0.43
2:B:59:TYR:CD2	2:B:67:VAL:CG1	3.02	0.43
2:D:108:THR:CG2	2:D:108:THR:O	2.66	0.43
2:D:5:LEU:O	2:D:23:LYS:N	2.39	0.43
1:E:157:GLY:HA3	1:I:22:THR:HG23	2.01	0.43
2:F:171:GLN:HG3	2:F:175:LEU:O	2.18	0.43
2:F:30:SER:HA	2:F:52(A):PRO:HG2	2.00	0.43
1:G:69:THR:O	1:G:71:PHE:CD1	2.70	0.43
2:H:127:SER:O	2:H:128:SER:C	2.56	0.43
2:J:29:PHE:HA	2:J:32:TYR:HD1	1.83	0.43
2:J:64:GLN:CG	2:L:204:ASN:OD1	2.67	0.43
2:J:82(A):SER:O	2:J:82(B):SER:O	2.36	0.43
1:K:140:TYR:CD1	1:K:140:TYR:C	2.92	0.43
1:K:186:TYR:O	1:K:192:TYR:OH	2.34	0.43
1:K:112:ALA:HB1	1:K:201:LEU:HG	2.00	0.43
1:K:54:LEU:HD11	1:K:58:VAL:HG11	2.00	0.43
1:M:95:SER:HA	2:N:47:TRP:CH2	2.53	0.43
2:N:52:ILE:C	2:N:52(A):PRO:O	2.51	0.43
2:P:72:ASP:C	2:P:74:ALA:H	2.20	0.43
1:A:132:VAL:HG12	1:A:148:TRP:CH2	2.54	0.43
2:D:14:PRO:HD3	2:D:112:ALA:C	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:2:VAL:HG21	2:D:27:GLY:N	2.34	0.43
2:F:146:PHE:CD1	2:F:147:PRO:HA	2.54	0.43
1:G:117:ILE:HG12	1:G:117:ILE:O	2.17	0.43
1:G:14:SER:HB2	1:G:17:ASP:OD2	2.18	0.43
2:H:82:LEU:HD23	2:H:82(C):LEU:HD21	2.00	0.43
1:I:121:SER:O	1:I:122:ASP:C	2.55	0.43
2:J:171:GLN:HB2	2:J:173:SER:OG	2.18	0.43
2:J:201:LYS:C	2:J:203:SER:N	2.72	0.43
1:K:26:SER:HB2	1:K:27:GLN:HE22	1.83	0.43
1:K:96:HIS:O	2:L:47:TRP:CB	2.64	0.43
1:K:43:VAL:CG1	2:L:103:TRP:HB2	2.48	0.43
2:L:4:LEU:HA	2:L:23:LYS:O	2.18	0.43
1:M:175:LEU:HD23	1:M:176:SER:H	1.77	0.43
1:M:97:THR:HG22	1:M:98:PHE:N	2.34	0.43
2:N:203:SER:C	2:N:205:THR:H	2.22	0.43
1:O:190:LYS:HE2	1:O:210:ASN:OD1	2.17	0.43
1:A:210:ASN:O	1:A:211:ARG:C	2.57	0.43
2:B:205:THR:O	2:B:206:LYS:HG3	2.18	0.43
2:D:153:SER:OG	2:D:197:ASN:HB2	2.18	0.43
1:G:149:LYS:HB2	1:G:193:ALA:HB3	2.00	0.43
1:G:47:LEU:HD23	1:G:48:ILE:CG1	2.36	0.43
2:H:119:PRO:HB2	2:H:142:VAL:HG13	2.01	0.43
2:H:142:VAL:HG22	2:H:198:VAL:HG11	1.99	0.43
1:I:65:SER:HB2	1:I:72:THR:CG2	2.45	0.43
1:M:186:TYR:CE1	1:M:192:TYR:CZ	3.06	0.43
1:M:81:GLU:CD	1:M:81:GLU:H	2.21	0.43
1:O:148:TRP:HE3	1:O:193:ALA:O	2.00	0.43
1:O:80:PRO:HA	1:O:83:PHE:CE1	2.53	0.43
2:B:182:VAL:HG13	2:B:182:VAL:O	2.19	0.43
1:C:199:GLN:HA	1:O:199:GLN:HE22	1.84	0.43
2:D:75:THR:O	2:D:76:SER:HB2	2.19	0.43
2:D:85:GLU:CD	2:D:85:GLU:N	2.70	0.43
1:E:142:ARG:HB2	1:E:173:TYR:CE2	2.54	0.43
1:E:25:ALA:O	1:E:26:SER:C	2.57	0.43
2:H:121:VAL:O	2:H:121:VAL:HG12	2.18	0.43
1:I:2:ILE:HD12	1:I:93:SER:HB2	1.92	0.43
2:J:29:PHE:CG	2:J:29:PHE:O	2.72	0.43
2:J:53:VAL:O	2:J:54:PHE:CG	2.72	0.43
2:J:73:GLU:O	2:J:74:ALA:C	2.56	0.43
1:K:196:VAL:O	1:K:204:PRO:HA	2.18	0.43
2:L:23:LYS:O	2:L:24:ALA:O	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:30:SER:CB	2:N:53:VAL:HG23	2.49	0.43
1:O:199:GLN:HA	1:O:199:GLN:HE21	1.83	0.43
2:P:141:LEU:HD13	2:P:179:SER:HB3	2.00	0.43
2:B:120:SER:O	2:B:121:VAL:HG23	2.19	0.43
2:B:142:VAL:HG22	2:B:198:VAL:HG21	1.99	0.43
2:B:203:SER:O	2:B:204:ASN:C	2.56	0.43
2:F:117:LYS:HG2	2:F:118:GLY:O	2.18	0.43
2:F:56:SER:O	2:F:57:ALA:C	2.55	0.43
2:J:199:ASN:ND2	2:J:200:HIS:N	2.66	0.43
2:J:6:GLN:OE1	2:J:106:GLY:N	2.50	0.43
2:J:70:THR:O	2:J:79:TYR:N	2.38	0.43
2:L:195:ILE:HG21	2:L:208:ASP:HB3	2.01	0.43
1:M:42:LYS:HB3	3:M:227:HOH:O	2.18	0.43
1:O:40:PRO:O	1:O:41:GLY:C	2.57	0.43
2:P:145:TYR:HB2	2:P:200:HIS:CE1	2.54	0.43
2:P:154:TRP:HB2	2:P:159:LEU:HB3	2.00	0.43
2:P:141:LEU:HA	2:P:179:SER:HB2	2.00	0.43
1:A:154:LEU:HA	1:A:154:LEU:HD13	1.64	0.43
1:A:58:VAL:HA	1:A:59:PRO:HD3	1.88	0.43
2:B:105:GLN:HB2	3:B:232:HOH:O	2.19	0.43
2:B:138:LEU:HB2	2:B:211:VAL:HG11	2.00	0.43
2:B:38:ARG:NH1	2:B:86:ASP:HA	2.34	0.43
1:C:62:PHE:H	1:C:62:PHE:HD1	1.67	0.43
1:C:116:PHE:CD2	2:D:137:ALA:CB	3.01	0.43
2:D:32:TYR:HB2	2:D:34:ILE:HD11	2.00	0.43
2:H:146:PHE:HA	2:H:147:PRO:HA	1.80	0.43
1:I:49:TYR:C	1:I:51:ALA:H	2.20	0.43
2:J:48:MET:O	2:J:60:ALA:N	2.52	0.43
2:J:84:SER:HA	2:J:111:VAL:O	2.19	0.43
2:L:34:ILE:CD1	2:L:34:ILE:H	2.32	0.43
2:L:37:VAL:CG1	2:L:38:ARG:N	2.82	0.43
1:O:148:TRP:CZ3	1:O:194:CYS:HB3	2.54	0.43
1:O:50:ALA:O	1:O:52:SER:N	2.52	0.43
2:B:4:LEU:HB2	2:B:104:GLY:HA2	2.01	0.43
1:C:117:ILE:O	1:C:117:ILE:HG22	2.18	0.43
1:C:198:HIS:CE1	1:C:200:GLY:H	2.37	0.43
1:C:59:PRO:HG2	1:C:61:ARG:NH2	2.34	0.43
1:C:75:ILE:HG21	1:C:78:LEU:HD12	1.98	0.43
1:E:116:PHE:HD2	2:F:130:SER:HB2	1.83	0.43
1:G:186:TYR:CE2	1:G:211:ARG:HD3	2.54	0.43
1:G:112:ALA:HA	1:G:198:HIS:ND1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:26:SER:HA	2:L:172:SER:O	2.19	0.43
2:J:29:PHE:HA	2:J:32:TYR:CD1	2.54	0.43
2:F:62:LYS:HA	2:J:83:ARG:HH12	1.84	0.43
2:L:8:GLY:O	2:L:10:GLU:HG3	2.18	0.43
1:K:94:THR:O	2:L:47:TRP:CH2	2.72	0.43
1:K:98:PHE:CE1	2:L:47:TRP:HB2	2.41	0.43
2:N:55:GLY:O	2:N:56:SER:CB	2.65	0.43
1:O:43:VAL:HG13	2:P:103:TRP:HB2	1.99	0.43
1:O:55:GLN:HE21	1:O:56:SER:H	1.65	0.43
2:B:116:THR:HA	2:B:146:PHE:O	2.19	0.43
1:C:173:TYR:CD2	1:C:173:TYR:N	2.87	0.43
1:C:61:ARG:CZ	1:C:79:GLN:HG3	2.49	0.43
1:E:136:LEU:HD22	1:E:175:LEU:HD22	2.00	0.43
1:E:161:GLU:HA	1:E:176:SER:O	2.18	0.43
2:F:126:PRO:CB	2:F:189:LEU:HD13	2.48	0.43
2:F:210:LYS:HE2	2:F:212:GLU:OE1	2.19	0.43
2:F:50:GLY:O	2:F:57:ALA:HA	2.19	0.43
1:G:49:TYR:O	1:G:50:ALA:HB3	2.19	0.43
1:G:54:LEU:HD11	1:G:62:PHE:O	2.19	0.43
2:H:48:MET:CE	2:H:90:TYR:HE2	2.31	0.43
2:J:136:ALA:N	2:J:184:VAL:O	2.51	0.43
2:J:60:ALA:O	2:J:61:GLN:C	2.57	0.43
1:K:122:ASP:C	1:K:124:GLN:H	2.22	0.43
2:L:10:GLU:HG3	3:L:218:HOH:O	2.19	0.43
2:N:150:VAL:HG22	2:N:151:THR:N	2.33	0.43
2:N:206:LYS:C	2:N:207:VAL:HG23	2.39	0.43
1:A:132:VAL:O	1:A:132:VAL:HG12	2.19	0.42
1:A:198:HIS:C	1:A:200:GLY:N	2.72	0.42
1:A:29:ILE:O	1:A:30:SER:CB	2.61	0.42
1:A:75:ILE:CD1	1:A:78:LEU:HD23	2.49	0.42
1:C:193:ALA:HB2	1:C:208:SER:HB2	2.01	0.42
2:D:6:GLN:HE21	2:D:6:GLN:HB3	1.66	0.42
1:G:179:LEU:HG	1:G:181:LEU:CD1	2.45	0.42
2:H:116:THR:O	2:H:117:LYS:HB2	2.19	0.42
1:I:120:PRO:HG3	1:I:186:TYR:CE1	2.54	0.42
2:J:103:TRP:CD1	2:J:103:TRP:N	2.87	0.42
2:J:198:VAL:HG12	2:J:199:ASN:N	2.34	0.42
1:K:49:TYR:O	1:K:50:ALA:HB3	2.18	0.42
2:L:136:ALA:HB3	2:L:184:VAL:O	2.18	0.42
2:L:75:THR:O	2:L:76:SER:HB2	2.19	0.42
2:P:12:LYS:HE3	2:P:18:VAL:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:203:SER:C	2:P:205:THR:H	2.22	0.42
1:A:189:HIS:O	1:A:211:ARG:CD	2.60	0.42
2:B:13:LYS:O	2:B:15:GLY:N	2.53	0.42
1:E:26:SER:HB2	1:E:27:GLN:CD	2.39	0.42
2:H:207:VAL:HG12	2:H:208:ASP:H	1.84	0.42
1:I:54:LEU:HD11	1:I:58:VAL:CG1	2.48	0.42
2:J:160:THR:HA	2:J:163:VAL:HG21	2.01	0.42
2:J:34:ILE:HA	2:J:93:ALA:O	2.19	0.42
2:L:94:LYS:HB3	2:L:102:VAL:CG1	2.37	0.42
1:M:165:GLU:O	1:M:166:GLN:C	2.57	0.42
1:M:129:THR:HA	1:M:182:SER:HA	2.01	0.42
1:M:136:LEU:HD21	1:M:196:VAL:CG2	2.49	0.42
1:M:187:GLU:CG	1:M:211:ARG:HD2	2.49	0.42
1:M:39:LYS:O	1:M:42:LYS:HB2	2.19	0.42
1:M:4:MET:HB3	1:M:99:GLY:CA	2.46	0.42
1:O:8:PRO:HD2	1:O:10:SER:H	1.80	0.42
2:P:100(L):MET:CE	2:P:100(L):MET:N	2.82	0.42
2:P:84:SER:C	2:P:86:ASP:H	2.22	0.42
1:A:124:GLN:HG2	1:A:129:THR:O	2.19	0.42
1:A:33:LEU:C	1:A:33:LEU:CD1	2.84	0.42
2:B:51:ILE:HD12	2:B:57:ALA:HB2	2.00	0.42
2:B:85:GLU:HG3	2:B:85:GLU:H	1.58	0.42
2:F:124:LEU:HD21	2:F:141:LEU:HB2	2.01	0.42
1:G:37:GLN:HG2	1:G:84:ALA:CB	2.49	0.42
1:G:55:GLN:CD	1:G:56:SER:H	2.22	0.42
1:G:61:ARG:HB3	3:G:226:HOH:O	2.20	0.42
2:H:4:LEU:O	2:H:104:GLY:HA2	2.20	0.42
1:I:184:ALA:HB1	1:I:188:LYS:NZ	2.34	0.42
1:I:91:SER:HA	1:I:96:HIS:CD2	2.54	0.42
1:K:165:GLU:O	1:K:166:GLN:C	2.58	0.42
1:K:26:SER:HB2	1:K:27:GLN:NE2	2.34	0.42
2:L:90:TYR:O	2:L:106:GLY:HA2	2.18	0.42
2:L:38:ARG:HH21	2:L:86:ASP:HA	1.71	0.42
1:O:103:LYS:C	1:O:104:LEU:HD23	2.40	0.42
1:O:195:GLU:CG	1:O:204:PRO:HB3	2.49	0.42
2:P:197:ASN:CA	2:P:208:ASP:OD2	2.58	0.42
2:P:73:GLU:HA	2:P:76:SER:HA	2.01	0.42
1:A:33:LEU:HD11	1:A:35:TRP:CD1	2.53	0.42
2:B:138:LEU:CD2	2:B:182:VAL:HG13	2.50	0.42
2:H:139:GLY:O	2:H:211:VAL:HG21	2.20	0.42
1:I:135:LEU:HD13	2:J:181:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:136:LEU:CD2	1:K:196:VAL:HG11	2.50	0.42
2:L:12:LYS:N	2:L:110:THR:O	2.46	0.42
1:O:108:ARG:C	1:O:108:ARG:HE	2.23	0.42
2:P:18:VAL:HG13	2:P:18:VAL:O	2.20	0.42
2:P:49:GLY:HA3	2:P:58:ASN:O	2.19	0.42
1:C:43:VAL:CG1	1:C:44:PRO:HD2	2.50	0.42
1:C:50:ALA:HB3	1:C:53:SER:CB	2.38	0.42
2:D:4:LEU:HB2	2:D:104:GLY:HA2	2.02	0.42
2:F:40:ALA:HA	2:F:88:ALA:CB	2.50	0.42
1:G:27:GLN:HB3	3:G:228:HOH:O	2.20	0.42
2:H:201:LYS:O	2:H:204:ASN:N	2.46	0.42
2:H:201:LYS:C	2:H:204:ASN:H	2.20	0.42
2:L:150:VAL:HG23	2:L:200:HIS:HB2	2.00	0.42
1:O:186:TYR:CE2	1:O:211:ARG:HD2	2.54	0.42
1:A:116:PHE:HB2	1:A:135:LEU:HB3	2.01	0.42
1:A:144:ALA:HB2	1:A:198:HIS:HD2	1.83	0.42
1:C:134:CYS:HB2	1:C:148:TRP:CZ2	2.54	0.42
1:C:49:TYR:HD1	2:D:100(J):HIS:O	2.02	0.42
2:D:52:ILE:O	2:D:52(A):PRO:C	2.58	0.42
2:H:151:THR:O	2:H:198:VAL:HA	2.19	0.42
1:I:33:LEU:HG	1:I:71:PHE:CG	2.54	0.42
2:J:123:PRO:HG3	2:J:209:LYS:NZ	2.34	0.42
2:J:192:GLN:NE2	2:J:193:THR:N	2.67	0.42
2:J:47:TRP:CZ3	2:J:49:GLY:HA2	2.55	0.42
2:J:67:VAL:CG2	2:J:68:THR:H	2.27	0.42
1:K:79:GLN:H	1:K:82:ASP:HB2	1.84	0.42
2:L:194:TYR:O	2:L:210:LYS:HA	2.20	0.42
1:M:186:TYR:O	1:M:192:TYR:OH	2.36	0.42
1:M:3:GLN:CB	1:M:26:SER:CB	2.97	0.42
2:P:170:LEU:HD12	2:P:171:GLN:H	1.85	0.42
2:P:23:LYS:HG2	2:P:24:ALA:N	2.34	0.42
1:A:6:GLN:NE2	1:A:101:GLY:CA	2.83	0.42
1:C:145:LYS:HZ1	1:C:147:GLN:HE21	1.68	0.42
1:C:64:GLY:HA2	1:C:72:THR:O	2.19	0.42
2:D:126:PRO:HG3	2:D:138:LEU:CB	2.39	0.42
2:D:71:ALA:CA	2:D:77:THR:O	2.67	0.42
2:D:87:THR:O	2:D:88:ALA:HB2	2.18	0.42
1:E:193:ALA:HB2	1:E:208:SER:HB2	2.02	0.42
2:F:100(J):HIS:HB3	2:F:100(K):GLY:H	1.65	0.42
2:F:131:THR:HG22	2:F:136:ALA:CA	2.49	0.42
1:G:28:SER:OG	1:G:68:GLY:HA2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:32:TYR:CD1	2:H:94:LYS:HG3	2.54	0.42
1:I:97:THR:HG22	1:I:98:PHE:N	2.33	0.42
2:J:125:ALA:HA	2:J:126:PRO:HD3	1.76	0.42
1:K:189:HIS:O	1:K:211:ARG:NH2	2.53	0.42
2:N:204:ASN:OD1	2:P:64:GLN:HB3	2.19	0.42
1:O:163:VAL:HG22	1:O:175:LEU:HD12	2.02	0.42
1:O:50:ALA:C	1:O:52:SER:H	2.23	0.42
1:C:145:LYS:HD3	1:C:197:THR:HG21	2.02	0.42
1:C:164:THR:O	1:C:164:THR:HG22	2.20	0.42
2:D:23:LYS:HD3	2:D:24:ALA:O	2.20	0.42
2:D:46:GLU:O	2:D:47:TRP:C	2.58	0.42
2:F:2:VAL:O	2:F:2:VAL:HG13	2.20	0.42
2:F:64:GLN:C	2:F:66:ARG:H	2.23	0.42
1:G:32:TYR:CD2	1:G:92:TYR:HA	2.55	0.42
2:H:3:GLN:CD	2:H:5:LEU:HD21	2.40	0.42
2:J:151:THR:O	2:J:152:VAL:CG2	2.64	0.42
2:J:72:ASP:O	2:J:76:SER:CA	2.67	0.42
1:K:135:LEU:HD12	1:K:136:LEU:N	2.35	0.42
1:K:212:GLY:O	1:K:213:GLU:HG3	2.19	0.42
1:K:85:THR:OG1	1:K:103:LYS:HB2	2.19	0.42
1:K:89:GLN:HE21	1:K:89:GLN:HB3	1.50	0.42
2:L:14:PRO:C	2:L:16:SER:H	2.23	0.42
1:M:58:VAL:O	1:M:59:PRO:C	2.57	0.42
1:O:72:THR:HG22	1:O:73:LEU:N	2.34	0.42
2:P:19:LYS:HB2	2:P:81:GLU:HB2	2.00	0.42
1:A:198:HIS:ND1	1:A:199:GLN:N	2.67	0.42
2:B:138:LEU:HD21	2:B:182:VAL:HG13	2.02	0.42
2:D:53:VAL:HG12	2:D:54:PHE:N	2.34	0.42
2:F:56:SER:O	2:F:57:ALA:O	2.38	0.42
1:G:79:GLN:O	1:G:80:PRO:C	2.58	0.42
2:H:34:ILE:N	2:H:34:ILE:HD12	2.34	0.42
1:I:83:PHE:CD1	1:I:106:ILE:HG12	2.54	0.42
1:I:122:ASP:O	1:I:123:GLU:C	2.57	0.42
2:J:4:LEU:HA	2:J:24:ALA:CA	2.41	0.42
2:L:24:ALA:O	2:L:25:SER:HB2	2.20	0.42
2:L:30:SER:C	2:L:53:VAL:HG23	2.40	0.42
2:N:204:ASN:OD1	2:P:64:GLN:HB2	2.19	0.42
1:O:175:LEU:HD23	1:O:176:SER:N	2.34	0.42
1:A:117:ILE:CG2	2:B:129:LYS:HB3	2.49	0.42
2:B:100(J):HIS:N	3:B:230:HOH:O	2.53	0.42
1:E:113:PRO:HB3	1:E:139:PHE:CG	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:146:PHE:CE1	2:F:147:PRO:HB3	2.55	0.42
2:H:72:ASP:O	2:H:76:SER:HA	2.20	0.42
1:I:140:TYR:C	1:I:198:HIS:HE1	2.23	0.42
1:K:48:ILE:CG2	1:K:52:SER:O	2.68	0.42
2:P:29:PHE:HE2	2:P:78:THR:HG1	1.68	0.42
2:P:82(C):LEU:HB3	2:P:111:VAL:HG11	2.01	0.42
1:A:149:LYS:HG3	1:A:154:LEU:HD13	2.02	0.41
2:B:170:LEU:HD13	2:B:176:TYR:CD1	2.55	0.41
2:B:37:VAL:HG13	2:B:46:GLU:C	2.40	0.41
1:G:154:LEU:H	1:G:154:LEU:CD2	2.32	0.41
1:G:39:LYS:CD	1:G:84:ALA:HB2	2.44	0.41
2:H:140:CYS:SG	2:H:211:VAL:HG21	2.60	0.41
2:H:51:ILE:CD1	2:H:57:ALA:HB2	2.49	0.41
1:I:12:SER:HA	1:I:105:GLU:HG2	2.02	0.41
1:I:144:ALA:CB	1:I:175:LEU:HD13	2.50	0.41
1:I:95:SER:O	1:I:96:HIS:CD2	2.72	0.41
2:L:90:TYR:CE1	2:L:109:VAL:HB	2.54	0.41
2:L:6:GLN:OE1	2:L:92:CYS:N	2.52	0.41
1:M:19:VAL:CG2	1:M:78:LEU:HD21	2.50	0.41
1:E:179:LEU:HD12	1:E:180:THR:N	2.35	0.41
2:F:39:GLN:HG3	2:F:43:GLN:O	2.20	0.41
1:G:132:VAL:CG1	1:G:148:TRP:CH2	3.02	0.41
1:I:182:SER:C	1:I:184:ALA:N	2.71	0.41
2:J:67:VAL:HB	2:J:82:LEU:HD12	2.02	0.41
2:J:93:ALA:HB1	2:J:100(L):MET:HB3	2.02	0.41
1:K:48:ILE:HG23	1:K:52:SER:O	2.20	0.41
1:M:102:THR:HG22	1:M:102:THR:O	2.20	0.41
1:M:63:SER:O	1:M:73:LEU:HD12	2.20	0.41
1:A:33:LEU:CD1	1:A:35:TRP:NE1	2.75	0.41
2:D:47:TRP:CH2	2:D:49:GLY:HA2	2.55	0.41
1:E:30:SER:O	1:E:71:PHE:HZ	2.04	0.41
2:H:152:VAL:HG11	2:H:180:SER:HB3	2.01	0.41
1:I:193:ALA:CA	1:I:208:SER:HB3	2.50	0.41
2:J:189:LEU:HD23	2:J:194:TYR:HE2	1.85	0.41
2:J:155:ASN:OD1	2:J:193:THR:O	2.38	0.41
2:J:17:SER:HB3	2:J:82(A):SER:OG	2.20	0.41
2:L:150:VAL:HG22	2:L:151:THR:H	1.84	0.41
1:O:193:ALA:HB1	1:O:206:THR:HG22	2.02	0.41
2:P:103:TRP:N	2:P:103:TRP:CD1	2.87	0.41
2:D:152:VAL:CG1	2:D:153:SER:N	2.83	0.41
2:F:2:VAL:HA	2:F:26:GLY:CA	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:94:LYS:HE2	2:F:95:GLY:N	2.36	0.41
2:H:155:ASN:HD22	2:H:159:LEU:HB3	1.85	0.41
2:H:72:ASP:O	2:H:76:SER:CA	2.68	0.41
2:J:52:ILE:O	2:J:53:VAL:N	2.40	0.41
1:K:195:GLU:CB	1:K:206:THR:HG23	2.44	0.41
1:K:6:GLN:HB2	1:K:100:GLN:HE21	1.85	0.41
2:L:116:THR:HG23	2:L:202:PRO:O	2.20	0.41
2:L:55:GLY:O	2:L:56:SER:OG	2.35	0.41
1:M:49:TYR:O	1:M:50:ALA:HB3	2.20	0.41
2:N:188:SER:O	2:N:189:LEU:C	2.59	0.41
2:N:29:PHE:HB2	2:N:76:SER:HB2	2.03	0.41
2:N:52:ILE:HG21	2:N:54:PHE:CZ	2.54	0.41
1:O:132:VAL:HG12	1:O:133:VAL:N	2.35	0.41
1:O:203:SER:C	1:O:204:PRO:O	2.59	0.41
1:O:80:PRO:HA	1:O:83:PHE:HE1	1.85	0.41
1:O:89:GLN:HE22	2:P:100(L):MET:HE1	1.85	0.41
2:P:40:ALA:HB3	2:P:43:GLN:HG3	2.02	0.41
1:A:11:LEU:HD22	1:A:104:LEU:HD23	1.86	0.41
2:B:145:TYR:O	2:B:175:LEU:HB3	2.20	0.41
2:B:52:ILE:HG22	2:B:53:VAL:HG23	2.03	0.41
1:C:70:ASP:OD2	1:C:70:ASP:N	2.52	0.41
1:C:36:TYR:HE1	1:C:89:GLN:NE2	2.19	0.41
2:H:124:LEU:CG	2:H:141:LEU:H	2.28	0.41
2:H:28:THR:O	2:H:29:PHE:O	2.38	0.41
1:I:33:LEU:HB3	1:I:51:ALA:HB2	2.02	0.41
2:J:203:SER:O	2:J:204:ASN:C	2.59	0.41
2:L:170:LEU:CD1	2:L:174:GLY:O	2.68	0.41
2:L:39:GLN:O	2:L:89:VAL:HG23	2.20	0.41
1:M:136:LEU:CG	1:M:196:VAL:HG21	2.48	0.41
1:M:43:VAL:HG13	1:M:44:PRO:HD2	2.02	0.41
1:M:48:ILE:HD12	1:M:73:LEU:HD13	2.02	0.41
2:N:72:ASP:O	2:N:76:SER:N	2.52	0.41
2:B:120:SER:C	2:B:121:VAL:HG23	2.40	0.41
2:B:123:PRO:C	2:B:125:ALA:H	2.23	0.41
2:B:124:LEU:HB2	2:B:139:GLY:O	2.21	0.41
2:B:211:VAL:O	2:B:212:GLU:HG2	2.20	0.41
2:B:21:SER:O	2:B:22:CYS:CB	2.68	0.41
1:C:195:GLU:HB2	1:C:206:THR:OG1	2.19	0.41
2:D:29:PHE:CE1	2:D:73:GLU:HA	2.55	0.41
2:D:36:TRP:HZ2	2:D:78:THR:O	2.03	0.41
1:E:136:LEU:HD11	1:E:146:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:169:LYS:HG3	1:G:170:ASP:OD1	2.20	0.41
1:G:182:SER:C	1:G:184:ALA:N	2.72	0.41
1:G:148:TRP:CZ3	1:G:194:CYS:HB3	2.55	0.41
1:G:39:LYS:HZ1	1:G:81:GLU:C	2.24	0.41
1:G:47:LEU:O	1:G:48:ILE:HG12	2.21	0.41
2:H:169:VAL:HG12	2:H:169:VAL:O	2.20	0.41
1:E:147:GLN:NE2	1:I:11:LEU:CD2	2.68	0.41
1:I:118:PHE:CE1	2:J:124:LEU:O	2.73	0.41
1:K:108:ARG:HD3	1:K:171:SER:O	2.20	0.41
1:K:67:SER:HA	1:K:71:PHE:CZ	2.55	0.41
1:O:49:TYR:CE1	1:O:53:SER:HB3	2.55	0.41
2:P:192:GLN:NE2	2:P:193:THR:H	2.03	0.41
1:A:113:PRO:HB3	1:A:139:PHE:HB3	2.02	0.41
2:B:39:GLN:C	2:B:88:ALA:HB1	2.41	0.41
1:C:33:LEU:HD21	1:C:88:CYS:HB2	2.03	0.41
2:D:51:ILE:O	2:D:52:ILE:HG12	2.20	0.41
1:E:198:HIS:ND1	1:E:200:GLY:N	2.67	0.41
2:F:2:VAL:HB	2:F:27:GLY:N	2.36	0.41
1:G:186:TYR:CE1	1:G:192:TYR:CE2	3.04	0.41
1:G:95:SER:O	1:G:96:HIS:C	2.58	0.41
2:H:150:VAL:HG22	2:H:151:THR:O	2.20	0.41
2:H:178:LEU:C	2:H:178:LEU:HD12	2.40	0.41
2:H:36:TRP:CD2	2:H:80:MET:HG3	2.54	0.41
1:I:37:GLN:HB2	1:I:47:LEU:HD11	2.01	0.41
2:J:6:GLN:HG3	2:J:104:GLY:HA3	2.03	0.41
1:K:124:GLN:C	1:K:126:LYS:N	2.73	0.41
1:K:66:GLY:HA3	1:K:70:ASP:O	2.21	0.41
1:M:136:LEU:CD1	1:M:136:LEU:N	2.84	0.41
2:N:87:THR:O	2:N:88:ALA:HB2	2.20	0.41
1:O:83:PHE:CD1	1:O:106:ILE:HD13	2.56	0.41
2:B:72:ASP:C	2:B:72:ASP:OD2	2.59	0.41
1:C:210:ASN:N	1:C:210:ASN:ND2	2.67	0.41
1:E:90:GLN:O	1:E:90:GLN:OE1	2.37	0.41
2:F:214:LYS:OXT	2:F:214:LYS:HG3	2.21	0.41
1:I:122:ASP:HA	1:I:125:LEU:HB2	2.03	0.41
2:J:154:TRP:HB3	2:J:159:LEU:HD23	2.03	0.41
1:K:195:GLU:HB2	1:K:206:THR:CG2	2.45	0.41
2:L:115:SER:O	2:L:146:PHE:HB3	2.19	0.41
2:P:146:PHE:C	2:P:146:PHE:HD2	2.23	0.41
2:B:72:ASP:OD2	2:B:74:ALA:HB3	2.21	0.41
1:E:115:VAL:HG21	1:E:205:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:202:SER:OG	1:E:203:SER:N	2.54	0.41
2:F:87:THR:CG2	2:F:110:THR:HA	2.28	0.41
1:G:139:PHE:HZ	1:G:175:LEU:H	1.69	0.41
1:G:73:LEU:C	1:G:73:LEU:CD2	2.82	0.41
1:I:159:SER:C	1:I:160:GLN:HG2	2.41	0.41
2:J:101:ASP:OD1	2:J:101:ASP:O	2.38	0.41
2:J:90:TYR:HD1	2:J:90:TYR:N	2.18	0.41
1:K:198:HIS:C	1:K:200:GLY:H	2.25	0.41
1:K:203:SER:O	1:K:204:PRO:C	2.59	0.41
2:N:117:LYS:HG2	2:N:118:GLY:O	2.21	0.41
1:O:164:THR:HG22	1:O:174:SER:H	1.85	0.41
1:O:37:GLN:CG	1:O:38:GLN:N	2.83	0.41
2:P:199:ASN:ND2	2:P:200:HIS:N	2.68	0.41
2:P:94:LYS:CD	2:P:94:LYS:C	2.89	0.41
1:A:55:GLN:O	1:A:58:VAL:HG23	2.21	0.41
1:C:120:PRO:HD3	1:C:132:VAL:HG22	2.03	0.41
1:G:148:TRP:O	1:G:155:GLN:N	2.53	0.41
1:G:158:ASN:HD22	1:K:22:THR:CG2	2.34	0.41
1:G:32:TYR:CB	1:G:92:TYR:H	2.34	0.41
1:I:182:SER:O	1:I:183:LYS:C	2.59	0.41
1:I:195:GLU:CG	1:I:196:VAL:N	2.84	0.41
1:I:89:GLN:HB2	1:I:98:PHE:HE2	1.85	0.41
2:J:161:SER:C	2:J:163:VAL:N	2.72	0.41
1:K:60:SER:C	1:K:62:PHE:H	2.23	0.41
2:L:115:SER:CB	2:L:117:LYS:HE2	2.48	0.41
2:L:195:ILE:N	2:L:195:ILE:HD12	2.36	0.41
2:L:35:SER:N	2:L:93:ALA:O	2.53	0.41
1:M:140:TYR:CA	1:M:141:PRO:O	2.67	0.41
1:M:96:HIS:O	2:N:47:TRP:CG	2.73	0.41
2:N:178:LEU:C	2:N:178:LEU:CD1	2.85	0.41
2:P:6:GLN:NE2	2:P:90:TYR:O	2.52	0.41
1:A:108:ARG:NH2	1:A:111:ALA:HB2	2.36	0.41
1:C:151:ASP:O	1:C:152:ASN:HB2	2.20	0.41
1:E:112:ALA:HB1	1:E:201:LEU:HD21	2.01	0.41
2:F:168:ALA:HB2	2:F:178:LEU:HD23	2.02	0.41
2:F:80:MET:O	2:F:80:MET:SD	2.79	0.41
2:H:172:SER:C	2:H:174:GLY:H	2.24	0.41
2:J:171:GLN:C	2:J:173:SER:N	2.72	0.41
2:J:2:VAL:HG11	2:J:94:LYS:NZ	2.36	0.41
2:J:28:THR:C	2:J:30:SER:H	2.23	0.41
1:K:149:LYS:HZ2	1:K:193:ALA:HB3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:85:GLU:N	2:L:85:GLU:OE2	2.54	0.41
1:M:140:TYR:CD1	1:M:141:PRO:N	2.89	0.41
2:N:184:VAL:CG2	2:N:194:TYR:OH	2.68	0.41
2:N:85:GLU:C	2:N:87:THR:H	2.24	0.41
1:O:117:ILE:HG22	2:P:129:LYS:HB3	2.03	0.41
1:O:20:THR:HG23	1:O:72:THR:HG23	2.03	0.41
2:B:195:ILE:HD11	2:B:210:LYS:HD2	2.03	0.40
1:A:95:SER:HA	2:B:47:TRP:CZ3	2.56	0.40
2:D:191:THR:O	2:D:192:GLN:C	2.59	0.40
1:E:121:SER:HB2	1:E:123:GLU:OE2	2.21	0.40
1:E:48:ILE:HD12	1:E:73:LEU:CD1	2.40	0.40
2:F:115:SER:O	2:F:116:THR:C	2.58	0.40
2:F:125:ALA:HA	2:F:126:PRO:HD3	1.81	0.40
2:F:20:VAL:O	2:F:21:SER:HB3	2.22	0.40
2:F:38:ARG:O	2:F:46:GLU:N	2.54	0.40
1:G:196:VAL:HG12	1:G:197:THR:N	2.36	0.40
2:H:172:SER:C	2:H:174:GLY:N	2.74	0.40
1:K:156:SER:C	1:K:158:ASN:N	2.74	0.40
1:K:33:LEU:HB3	1:K:71:PHE:CD2	2.56	0.40
1:M:136:LEU:O	1:M:139:PHE:CE1	2.74	0.40
1:O:108:ARG:NH1	1:O:172:THR:CG2	2.84	0.40
1:O:183:LYS:O	1:O:184:ALA:C	2.59	0.40
2:P:207:VAL:CG1	2:P:208:ASP:N	2.84	0.40
1:A:198:HIS:C	1:A:200:GLY:H	2.23	0.40
1:A:40:PRO:C	1:A:42:LYS:N	2.73	0.40
2:B:4:LEU:HD13	2:B:92:CYS:O	2.21	0.40
2:B:83:ARG:O	2:B:111:VAL:HG11	2.21	0.40
1:C:18:ARG:NH1	1:C:76:SER:O	2.54	0.40
1:C:61:ARG:HD3	1:C:79:GLN:NE2	2.36	0.40
2:D:32:TYR:HB2	2:D:34:ILE:HD12	2.03	0.40
2:D:73:GLU:C	2:D:75:THR:H	2.23	0.40
2:D:73:GLU:C	2:D:75:THR:N	2.74	0.40
1:E:164:THR:CG2	1:E:174:SER:HB2	2.51	0.40
1:E:26:SER:C	1:E:27:GLN:NE2	2.75	0.40
1:E:96:HIS:O	1:E:97:THR:HG23	2.21	0.40
2:F:142:VAL:HB	2:F:178:LEU:CD1	2.51	0.40
2:F:152:VAL:HG11	2:F:180:SER:CB	2.51	0.40
2:F:185:PRO:O	2:F:188:SER:OG	2.28	0.40
2:F:29:PHE:CB	2:F:76:SER:HB2	2.51	0.40
2:F:17:SER:HB2	2:F:82(A):SER:HA	1.99	0.40
1:G:184:ALA:O	1:G:185:ASP:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:189:LEU:C	2:J:191:THR:N	2.73	0.40
1:K:111:ALA:O	1:K:139:PHE:CA	2.66	0.40
1:K:125:LEU:O	1:K:128:GLY:N	2.48	0.40
2:L:39:GLN:C	2:L:88:ALA:HB1	2.42	0.40
2:N:36:TRP:CZ2	2:N:80:MET:HB2	2.57	0.40
1:O:154:LEU:HA	1:O:154:LEU:HD22	1.88	0.40
2:P:82(A):SER:O	2:P:82(C):LEU:N	2.54	0.40
1:A:117:ILE:HB	1:A:207:LYS:HG2	2.03	0.40
1:A:124:GLN:HE22	1:A:131:SER:CB	2.34	0.40
2:B:170:LEU:HD13	2:B:176:TYR:CZ	2.56	0.40
2:B:176:TYR:CD2	2:B:176:TYR:N	2.89	0.40
1:C:11:LEU:HD22	1:C:12:SER:N	2.37	0.40
1:C:34:ASN:OD1	1:C:49:TYR:HA	2.22	0.40
2:D:12:LYS:O	2:D:13:LYS:C	2.59	0.40
2:D:77:THR:CG2	2:D:78:THR:N	2.84	0.40
2:H:197:ASN:HA	2:H:208:ASP:OD2	2.21	0.40
2:J:51:ILE:HG23	2:J:52:ILE:N	2.37	0.40
2:J:62:LYS:HG3	2:J:63:PHE:N	2.36	0.40
1:K:210:ASN:O	1:K:211:ARG:C	2.60	0.40
2:L:128:SER:HA	2:L:131:THR:OG1	2.22	0.40
2:L:193:THR:HG22	2:L:195:ILE:CD1	2.51	0.40
2:L:20:VAL:C	3:L:215:HOH:O	2.60	0.40
2:L:8:GLY:C	2:L:107:THR:CG2	2.90	0.40
1:M:136:LEU:HD21	1:M:196:VAL:HG22	2.03	0.40
2:N:203:SER:C	2:N:205:THR:N	2.75	0.40
1:O:115:VAL:O	1:O:116:PHE:CD2	2.75	0.40
1:O:122:ASP:HA	1:O:125:LEU:HD12	2.03	0.40
1:O:175:LEU:HD23	1:O:175:LEU:C	2.42	0.40
2:P:6:GLN:N	2:P:105:GLN:OE1	2.52	0.40
1:A:141:PRO:HB2	1:A:143:GLU:OE2	2.21	0.40
1:A:143:GLU:CD	1:A:143:GLU:N	2.75	0.40
2:B:5:LEU:O	2:B:23:LYS:N	2.55	0.40
2:D:84:SER:O	2:D:86:ASP:N	2.49	0.40
2:F:11:VAL:HG11	2:F:146:PHE:CZ	2.57	0.40
2:F:48:MET:O	2:F:60:ALA:N	2.55	0.40
2:F:61:GLN:OE1	2:J:83:ARG:HD3	2.22	0.40
2:F:63:PHE:HD1	2:F:63:PHE:H	1.68	0.40
1:G:90:GLN:C	1:G:90:GLN:OE1	2.60	0.40
1:G:92:TYR:O	1:G:93:SER:C	2.60	0.40
2:H:131:THR:HA	2:H:135:THR:O	2.21	0.40
1:I:79:GLN:HB3	1:I:81:GLU:OE1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:166:PHE:HA	2:J:167:PRO:HD3	1.90	0.40
2:J:17:SER:HB3	2:J:82(A):SER:CB	2.51	0.40
1:K:121:SER:HB2	1:K:123:GLU:OE1	2.21	0.40
1:O:14:SER:O	1:O:17:ASP:OD1	2.39	0.40
2:P:7:SER:OG	2:P:10:GLU:OE2	2.36	0.40
1:A:48:ILE:CG2	1:A:49:TYR:H	2.34	0.40
1:A:28:SER:CA	1:A:69:THR:HG22	2.47	0.40
2:D:34:ILE:H	2:D:34:ILE:HD12	1.87	0.40
1:G:113:PRO:HA	1:G:137:ASN:O	2.22	0.40
1:G:60:SER:C	1:G:62:PHE:N	2.75	0.40
2:H:164:HIS:N	2:H:164:HIS:ND1	2.69	0.40
1:I:36:TYR:HE2	2:J:100(L):MET:O	2.05	0.40
1:I:6:GLN:OE1	1:I:101:GLY:N	2.44	0.40
2:L:50:GLY:O	2:L:57:ALA:CB	2.65	0.40
1:M:180:THR:C	1:M:181:LEU:HD12	2.42	0.40
1:M:141:PRO:HG2	1:M:198:HIS:HE2	1.86	0.40
1:O:134:CYS:HB3	1:O:177:SER:HB3	2.04	0.40
1:O:33:LEU:HD13	1:O:34:ASN:N	2.37	0.40
1:O:35:TRP:CB	1:O:73:LEU:HD13	2.52	0.40
2:P:184:VAL:HG11	2:P:194:TYR:CZ	2.56	0.40
2:P:75:THR:OG1	2:P:77:THR:OG1	2.35	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [\(i\)](#)

### 5.3.1 Protein backbone [\(i\)](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	209/212 (99%)	170 (81%)	29 (14%)	10 (5%)	<b>2</b>   <b>8</b>
1	C	210/212 (99%)	171 (81%)	24 (11%)	15 (7%)	<b>1</b>   <b>3</b>
1	E	209/212 (99%)	168 (80%)	32 (15%)	9 (4%)	<b>2</b>   <b>10</b>
1	G	209/212 (99%)	167 (80%)	28 (13%)	14 (7%)	<b>1</b>   <b>3</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	209/212 (99%)	160 (77%)	39 (19%)	10 (5%)	2	8
1	K	209/212 (99%)	160 (77%)	37 (18%)	12 (6%)	1	5
1	M	209/212 (99%)	166 (79%)	32 (15%)	11 (5%)	2	6
1	O	209/212 (99%)	164 (78%)	34 (16%)	11 (5%)	2	6
2	B	212/230 (92%)	153 (72%)	40 (19%)	19 (9%)	1	1
2	D	212/230 (92%)	152 (72%)	44 (21%)	16 (8%)	1	2
2	F	213/230 (93%)	153 (72%)	42 (20%)	18 (8%)	1	2
2	H	212/230 (92%)	146 (69%)	42 (20%)	24 (11%)	0	1
2	J	212/230 (92%)	151 (71%)	40 (19%)	21 (10%)	0	1
2	L	211/230 (92%)	152 (72%)	39 (18%)	20 (10%)	0	1
2	N	212/230 (92%)	164 (77%)	30 (14%)	18 (8%)	1	2
2	P	212/230 (92%)	152 (72%)	37 (18%)	23 (11%)	0	1
All	All	3369/3536 (95%)	2549 (76%)	569 (17%)	251 (8%)	1	2

All (251) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	211	ARG
2	B	22	CYS
2	B	30	SER
2	B	61	GLN
2	B	82(B)	SER
2	B	101	ASP
2	B	130	SER
1	C	7	SER
1	C	8	PRO
1	C	63	SER
1	C	78	LEU
1	C	184	ALA
2	D	53	VAL
2	D	100(L)	MET
1	E	8	PRO
1	E	67	SER
1	E	143	GLU
2	F	2	VAL
2	F	52(A)	PRO
2	F	53	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	F	57	ALA
2	F	61	GLN
2	F	158	ALA
2	F	182	VAL
2	F	213	PRO
1	G	8	PRO
1	G	117	ILE
1	G	143	GLU
2	H	29	PHE
2	H	30	SER
2	H	76	SER
2	H	149	PRO
2	H	189	LEU
1	I	8	PRO
1	I	92	TYR
1	I	184	ALA
2	J	63	PHE
2	J	74	ALA
2	J	87	THR
2	J	146	PHE
2	J	182	VAL
2	J	204	ASN
1	K	8	PRO
1	K	157	GLY
1	K	203	SER
2	L	7	SER
2	L	24	ALA
2	L	56	SER
2	L	72	ASP
2	L	182	VAL
2	L	203	SER
1	M	8	PRO
1	M	93	SER
2	N	9	ALA
2	N	32	TYR
2	N	56	SER
2	N	61	GLN
2	N	144	ASP
1	O	8	PRO
1	O	15	VAL
1	O	59	PRO
1	O	113	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	O	171	SER
1	O	183	LYS
1	O	204	PRO
2	P	7	SER
2	P	16	SER
2	P	22	CYS
2	P	61	GLN
2	P	146	PHE
2	P	204	ASN
1	A	41	GLY
1	A	68	GLY
1	A	121	SER
2	B	16	SER
2	B	53	VAL
2	B	125	ALA
2	B	188	SER
2	B	204	ASN
1	C	30	SER
1	C	32	TYR
1	C	54	LEU
1	C	185	ASP
2	D	28	THR
2	D	55	GLY
2	D	85	GLU
2	D	111	VAL
1	E	152	ASN
2	F	20	VAL
2	F	55	GLY
2	F	63	PHE
2	F	71	ALA
1	G	7	SER
1	G	92	TYR
1	G	96	HIS
1	G	187	GLU
2	H	82(C)	LEU
2	H	85	GLU
2	H	112	ALA
2	H	198	VAL
2	H	209	LYS
2	J	65	GLY
2	J	109	VAL
2	J	127	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	J	164	HIS
1	K	30	SER
1	K	53	SER
1	K	125	LEU
2	L	9	ALA
2	L	14	PRO
2	L	26	GLY
2	L	29	PHE
2	L	51	ILE
2	L	61	GLN
1	M	30	SER
1	M	152	ASN
1	M	156	SER
2	N	25	SER
2	N	53	VAL
2	N	82(B)	SER
2	N	86	ASP
2	N	189	LEU
1	O	138	ASN
2	P	2	VAL
2	P	18	VAL
2	P	29	PHE
2	P	32	TYR
2	P	127	SER
1	A	30	SER
1	A	40	PRO
1	A	138	ASN
1	A	156	SER
2	B	55	GLY
2	B	62	LYS
2	B	82(A)	SER
1	C	28	SER
1	C	67	SER
2	D	30	SER
2	D	116	THR
2	D	202	PRO
1	E	138	ASN
1	E	156	SER
2	F	82(C)	LEU
2	F	144	ASP
2	F	189	LEU
1	G	54	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	168	SER
1	G	186	TYR
2	H	3	GLN
2	H	16	SER
1	I	13	ALA
1	I	152	ASN
2	J	9	ALA
2	J	29	PHE
2	J	82(B)	SER
2	L	187	SER
1	M	78	LEU
2	N	6	GLN
2	N	127	SER
2	N	204	ASN
1	O	51	ALA
2	P	56	SER
2	P	82(B)	SER
2	P	100(L)	MET
2	P	177	SER
2	B	14	PRO
2	B	51	ILE
2	B	52(A)	PRO
1	C	186	TYR
2	D	3	GLN
2	D	52(A)	PRO
2	D	114	ALA
2	D	144	ASP
2	D	192	GLN
1	E	84	ALA
1	E	108	ARG
2	F	101	ASP
1	G	11	LEU
1	G	76	SER
1	G	184	ALA
2	H	88	ALA
2	H	113	SER
2	H	129	LYS
2	H	147	PRO
2	H	201	LYS
1	I	30	SER
1	I	111	ALA
1	I	138	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	I	142	ARG
2	J	73	GLU
2	J	126	PRO
1	K	166	GLN
2	L	25	SER
2	L	82(B)	SER
2	L	114	ALA
2	L	144	ASP
1	M	59	PRO
1	M	138	ASN
2	N	72	ASP
2	N	158	ALA
2	P	3	GLN
2	P	30	SER
2	P	52(A)	PRO
1	A	93	SER
1	C	156	SER
1	C	166	GLN
1	C	204	PRO
2	D	60	ALA
2	D	123	PRO
2	H	117	LYS
2	H	124	LEU
1	I	188	LYS
2	J	152	VAL
1	K	109	THR
2	L	74	ALA
2	L	201	LYS
1	M	123	GLU
2	N	31	SER
2	P	33	ALA
2	P	62	LYS
2	P	74	ALA
2	P	201	LYS
2	B	155	ASN
1	E	40	PRO
2	F	88	ALA
2	F	123	PRO
1	G	30	SER
2	H	61	GLN
2	J	18	VAL
2	J	202	PRO

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Mol	Chain	Res	Type
1	K	93	SER
2	L	177	SER
1	M	81	GLU
2	N	106	GLY
1	O	43	VAL
2	P	202	PRO
1	K	44	PRO
1	K	204	PRO
1	M	204	PRO
1	O	112	ALA
2	H	150	VAL
2	J	53	VAL
2	J	100(K)	GLY
2	H	152	VAL
2	H	185	PRO
2	H	195	ILE
2	J	52(A)	PRO
2	B	149	PRO
2	N	149	PRO
1	K	141	PRO

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	187/188 (100%)	159 (85%)	28 (15%)	3 9
1	C	188/188 (100%)	162 (86%)	26 (14%)	3 10
1	E	187/188 (100%)	161 (86%)	26 (14%)	3 10
1	G	187/188 (100%)	168 (90%)	19 (10%)	7 22
1	I	187/188 (100%)	166 (89%)	21 (11%)	6 18
1	K	187/188 (100%)	165 (88%)	22 (12%)	5 16
1	M	187/188 (100%)	163 (87%)	24 (13%)	4 13
1	O	187/188 (100%)	157 (84%)	30 (16%)	2 7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	176/189 (93%)	153 (87%)	23 (13%)	4	12
2	D	176/189 (93%)	164 (93%)	12 (7%)	16	42
2	F	177/189 (94%)	160 (90%)	17 (10%)	8	25
2	H	176/189 (93%)	158 (90%)	18 (10%)	7	22
2	J	176/189 (93%)	158 (90%)	18 (10%)	7	22
2	L	176/189 (93%)	158 (90%)	18 (10%)	7	22
2	N	176/189 (93%)	160 (91%)	16 (9%)	9	28
2	P	176/189 (93%)	153 (87%)	23 (13%)	4	12
All	All	2906/3016 (96%)	2565 (88%)	341 (12%)	5	16

All (341) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	8	PRO
1	A	11	LEU
1	A	18	ARG
1	A	19	VAL
1	A	20	THR
1	A	26	SER
1	A	27	GLN
1	A	28	SER
1	A	33	LEU
1	A	56	SER
1	A	65	SER
1	A	72	THR
1	A	74	THR
1	A	75	ILE
1	A	90	GLN
1	A	94	THR
1	A	102	THR
1	A	105	GLU
1	A	135	LEU
1	A	154	LEU
1	A	158	ASN
1	A	175	LEU
1	A	180	THR
1	A	181	LEU
1	A	185	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	195	GLU
1	A	211	ARG
2	B	5	LEU
2	B	17	SER
2	B	22	CYS
2	B	28	THR
2	B	30	SER
2	B	53	VAL
2	B	54	PHE
2	B	58	ASN
2	B	61	GLN
2	B	66	ARG
2	B	73	GLU
2	B	85	GLU
2	B	100(J)	HIS
2	B	101	ASP
2	B	135	THR
2	B	149	PRO
2	B	169	VAL
2	B	178	LEU
2	B	187	SER
2	B	191	THR
2	B	193	THR
2	B	199	ASN
2	B	208	ASP
1	C	3	GLN
1	C	5	THR
1	C	6	GLN
1	C	10	SER
1	C	11	LEU
1	C	23	CYS
1	C	49	TYR
1	C	62	PHE
1	C	70	ASP
1	C	72	THR
1	C	80	PRO
1	C	89	GLN
1	C	90	GLN
1	C	94	THR
1	C	104	LEU
1	C	105	GLU
1	C	117	ILE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	127	SER
1	C	129	THR
1	C	164	THR
1	C	176	SER
1	C	180	THR
1	C	185	ASP
1	C	195	GLU
1	C	197	THR
1	C	204	PRO
2	D	29	PHE
2	D	52(A)	PRO
2	D	59	TYR
2	D	61	GLN
2	D	66	ARG
2	D	101	ASP
2	D	138	LEU
2	D	151	THR
2	D	161	SER
2	D	182	VAL
2	D	193	THR
2	D	205	THR
1	E	22	THR
1	E	26	SER
1	E	40	PRO
1	E	47	LEU
1	E	49	TYR
1	E	63	SER
1	E	72	THR
1	E	76	SER
1	E	85	THR
1	E	90	GLN
1	E	93	SER
1	E	98	PHE
1	E	105	GLU
1	E	126	LYS
1	E	127	SER
1	E	129	THR
1	E	131	SER
1	E	143	GLU
1	E	152	ASN
1	E	154	LEU
1	E	158	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	161	GLU
1	E	165	GLU
1	E	180	THR
1	E	197	THR
1	E	210	ASN
2	F	21	SER
2	F	22	CYS
2	F	52(A)	PRO
2	F	54	PHE
2	F	78	THR
2	F	82(B)	SER
2	F	84	SER
2	F	103	TRP
2	F	108	THR
2	F	135	THR
2	F	145	TYR
2	F	147	PRO
2	F	172	SER
2	F	180	SER
2	F	193	THR
2	F	199	ASN
2	F	205	THR
1	G	2	ILE
1	G	17	ASP
1	G	22	THR
1	G	23	CYS
1	G	24	ARG
1	G	34	ASN
1	G	72	THR
1	G	78	LEU
1	G	79	GLN
1	G	89	GLN
1	G	90	GLN
1	G	106	ILE
1	G	137	ASN
1	G	158	ASN
1	G	166	GLN
1	G	175	LEU
1	G	180	THR
1	G	209	PHE
1	G	210	ASN
2	H	3	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	H	18	VAL
2	H	38	ARG
2	H	54	PHE
2	H	58	ASN
2	H	64	GLN
2	H	69	ILE
2	H	70	THR
2	H	76	SER
2	H	80	MET
2	H	82(B)	SER
2	H	101	ASP
2	H	110	THR
2	H	176	TYR
2	H	178	LEU
2	H	183	THR
2	H	191	THR
2	H	199	ASN
1	I	11	LEU
1	I	22	THR
1	I	33	LEU
1	I	34	ASN
1	I	43	VAL
1	I	52	SER
1	I	54	LEU
1	I	72	THR
1	I	73	LEU
1	I	77	SER
1	I	90	GLN
1	I	109	THR
1	I	126	LYS
1	I	127	SER
1	I	164	THR
1	I	169	LYS
1	I	174	SER
1	I	177	SER
1	I	181	LEU
1	I	207	LYS
1	I	210	ASN
2	J	17	SER
2	J	29	PHE
2	J	43	GLN
2	J	45	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	J	61	GLN
2	J	66	ARG
2	J	81	GLU
2	J	85	GLU
2	J	90	TYR
2	J	91	PHE
2	J	132	SER
2	J	135	THR
2	J	149	PRO
2	J	150	VAL
2	J	164	HIS
2	J	191	THR
2	J	199	ASN
2	J	208	ASP
1	K	18	ARG
1	K	32	TYR
1	K	44	PRO
1	K	70	ASP
1	K	77	SER
1	K	81	GLU
1	K	89	GLN
1	K	90	GLN
1	K	94	THR
1	K	100	GLN
1	K	105	GLU
1	K	108	ARG
1	K	110	VAL
1	K	126	LYS
1	K	152	ASN
1	K	161	GLU
1	K	165	GLU
1	K	179	LEU
1	K	195	GLU
1	K	204	PRO
1	K	206	THR
1	K	210	ASN
2	L	7	SER
2	L	17	SER
2	L	89	VAL
2	L	102	VAL
2	L	110	THR
2	L	119	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	L	140	CYS
2	L	141	LEU
2	L	149	PRO
2	L	159	LEU
2	L	165	THR
2	L	172	SER
2	L	175	LEU
2	L	182	VAL
2	L	196	CYS
2	L	197	ASN
2	L	207	VAL
2	L	208	ASP
1	M	18	ARG
1	M	22	THR
1	M	33	LEU
1	M	36	TYR
1	M	37	GLN
1	M	44	PRO
1	M	59	PRO
1	M	72	THR
1	M	77	SER
1	M	78	LEU
1	M	90	GLN
1	M	98	PHE
1	M	104	LEU
1	M	105	GLU
1	M	117	ILE
1	M	136	LEU
1	M	158	ASN
1	M	160	GLN
1	M	164	THR
1	M	165	GLU
1	M	179	LEU
1	M	180	THR
1	M	181	LEU
1	M	210	ASN
2	N	6	GLN
2	N	67	VAL
2	N	124	LEU
2	N	131	THR
2	N	140	CYS
2	N	147	PRO

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	N	149	PRO
2	N	178	LEU
2	N	181	VAL
2	N	182	VAL
2	N	184	VAL
2	N	186	SER
2	N	196	CYS
2	N	199	ASN
2	N	208	ASP
2	N	212	GLU
1	O	5	THR
1	O	11	LEU
1	O	20	THR
1	O	21	ILE
1	O	22	THR
1	O	34	ASN
1	O	59	PRO
1	O	69	THR
1	O	77	SER
1	O	78	LEU
1	O	89	GLN
1	O	90	GLN
1	O	106	ILE
1	O	108	ARG
1	O	113	PRO
1	O	126	LYS
1	O	129	THR
1	O	131	SER
1	O	135	LEU
1	O	138	ASN
1	O	147	GLN
1	O	151	ASP
1	O	154	LEU
1	O	156	SER
1	O	158	ASN
1	O	164	THR
1	O	185	ASP
1	O	199	GLN
1	O	202	SER
1	O	209	PHE
2	P	7	SER
2	P	22	CYS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	P	100(L)	MET
2	P	101	ASP
2	P	116	THR
2	P	135	THR
2	P	138	LEU
2	P	140	CYS
2	P	146	PHE
2	P	148	GLU
2	P	150	VAL
2	P	159	LEU
2	P	160	THR
2	P	161	SER
2	P	170	LEU
2	P	172	SER
2	P	182	VAL
2	P	183	THR
2	P	196	CYS
2	P	197	ASN
2	P	199	ASN
2	P	202	PRO
2	P	212	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	27	GLN
1	A	55	GLN
1	A	89	GLN
1	A	124	GLN
1	A	137	ASN
1	A	138	ASN
1	A	158	ASN
2	B	43	GLN
2	B	64	GLN
2	B	164	HIS
2	B	192	GLN
2	B	199	ASN
1	C	3	GLN
1	C	27	GLN
1	C	79	GLN
1	C	89	GLN
1	C	90	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	147	GLN
1	C	189	HIS
1	C	199	GLN
1	C	210	ASN
2	D	64	GLN
2	D	171	GLN
1	E	27	GLN
1	E	37	GLN
1	E	96	HIS
1	E	137	ASN
1	E	138	ASN
1	E	147	GLN
1	E	189	HIS
1	E	210	ASN
2	F	6	GLN
2	F	43	GLN
2	F	164	HIS
2	F	199	ASN
1	G	34	ASN
1	G	79	GLN
1	G	137	ASN
1	G	138	ASN
1	G	155	GLN
1	G	210	ASN
2	H	1	GLN
2	H	43	GLN
2	H	100(J)	HIS
2	H	155	ASN
2	H	164	HIS
2	H	171	GLN
2	H	199	ASN
1	I	55	GLN
1	I	89	GLN
1	I	96	HIS
1	I	100	GLN
1	I	124	GLN
1	I	138	ASN
1	I	155	GLN
1	I	158	ASN
1	I	199	GLN
1	I	210	ASN
2	J	39	GLN

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Mol	Chain	Res	Type
2	J	61	GLN
2	J	164	HIS
2	J	171	GLN
2	J	199	ASN
1	K	89	GLN
1	K	100	GLN
1	K	138	ASN
1	K	152	ASN
1	K	210	ASN
2	L	1	GLN
2	L	64	GLN
2	L	164	HIS
1	M	37	GLN
1	M	38	GLN
1	M	55	GLN
1	M	96	HIS
1	M	138	ASN
1	M	198	HIS
1	M	210	ASN
2	N	39	GLN
2	N	199	ASN
1	O	89	GLN
1	O	124	GLN
1	O	137	ASN
1	O	138	ASN
1	O	199	GLN
2	P	39	GLN
2	P	164	HIS
2	P	192	GLN
2	P	199	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.



## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	211/212 (99%)	-0.52	0 <span style="border: 1px solid black; padding: 0 2px;">100</span> <span style="border: 1px solid black; padding: 0 2px;">100</span>	27, 49, 72, 79	0
1	C	212/212 (100%)	-0.57	1 (0%) <span style="border: 1px solid black; padding: 0 2px;">91</span> <span style="border: 1px solid black; padding: 0 2px;">91</span>	24, 45, 68, 75	0
1	E	211/212 (99%)	-0.59	0 <span style="border: 1px solid black; padding: 0 2px;">100</span> <span style="border: 1px solid black; padding: 0 2px;">100</span>	30, 49, 65, 76	0
1	G	211/212 (99%)	-0.45	0 <span style="border: 1px solid black; padding: 0 2px;">100</span> <span style="border: 1px solid black; padding: 0 2px;">100</span>	33, 53, 86, 100	0
1	I	211/212 (99%)	-0.55	0 <span style="border: 1px solid black; padding: 0 2px;">100</span> <span style="border: 1px solid black; padding: 0 2px;">100</span>	31, 50, 71, 82	0
1	K	211/212 (99%)	-0.57	0 <span style="border: 1px solid black; padding: 0 2px;">100</span> <span style="border: 1px solid black; padding: 0 2px;">100</span>	36, 52, 66, 76	0
1	M	211/212 (99%)	-0.60	0 <span style="border: 1px solid black; padding: 0 2px;">100</span> <span style="border: 1px solid black; padding: 0 2px;">100</span>	24, 45, 59, 75	0
1	O	211/212 (99%)	-0.58	0 <span style="border: 1px solid black; padding: 0 2px;">100</span> <span style="border: 1px solid black; padding: 0 2px;">100</span>	25, 44, 61, 67	0
2	B	216/230 (93%)	-0.49	0 <span style="border: 1px solid black; padding: 0 2px;">100</span> <span style="border: 1px solid black; padding: 0 2px;">100</span>	32, 58, 81, 89	0
2	D	216/230 (93%)	-0.34	3 (1%) <span style="border: 1px solid black; padding: 0 2px;">75</span> <span style="border: 1px solid black; padding: 0 2px;">75</span>	27, 58, 87, 99	0
2	F	217/230 (94%)	-0.37	0 <span style="border: 1px solid black; padding: 0 2px;">100</span> <span style="border: 1px solid black; padding: 0 2px;">100</span>	28, 64, 93, 105	0
2	H	216/230 (93%)	-0.24	1 (0%) <span style="border: 1px solid black; padding: 0 2px;">91</span> <span style="border: 1px solid black; padding: 0 2px;">91</span>	39, 71, 96, 99	0
2	J	216/230 (93%)	-0.42	1 (0%) <span style="border: 1px solid black; padding: 0 2px;">91</span> <span style="border: 1px solid black; padding: 0 2px;">91</span>	39, 65, 91, 96	0
2	L	215/230 (93%)	-0.37	1 (0%) <span style="border: 1px solid black; padding: 0 2px;">91</span> <span style="border: 1px solid black; padding: 0 2px;">91</span>	37, 63, 82, 100	0
2	N	216/230 (93%)	-0.49	0 <span style="border: 1px solid black; padding: 0 2px;">100</span> <span style="border: 1px solid black; padding: 0 2px;">100</span>	29, 54, 75, 87	0
2	P	216/230 (93%)	-0.46	1 (0%) <span style="border: 1px solid black; padding: 0 2px;">91</span> <span style="border: 1px solid black; padding: 0 2px;">91</span>	28, 52, 86, 92	0
All	All	3417/3536 (96%)	-0.47	8 (0%) <span style="border: 1px solid black; padding: 0 2px;">95</span> <span style="border: 1px solid black; padding: 0 2px;">95</span>	24, 53, 84, 105	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	130	SER	4.0
2	J	55	GLY	3.3
2	H	203	SER	2.8
1	C	212	GLY	2.8
2	D	128	SER	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	27	GLY	2.5
2	D	131	THR	2.1
2	P	4	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.