



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 09:34 PM EDT

PDB ID : 2EXY
Title : Crystal structure of the E148Q Mutant of EcCIC, Fab complexed in absence of bound ions
Authors : Lobet, S.; Dutzler, R.
Deposited on : 2005-11-09
Resolution : 3.10 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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 : 2.35
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) : 2.35

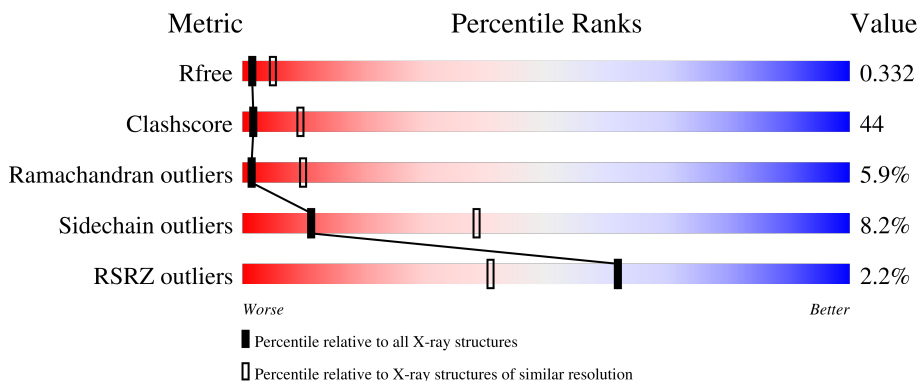
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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.



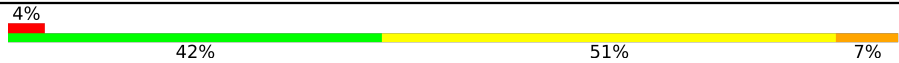
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	473	 4% 34% 51% 8% 6%
1	B	473	 4% 33% 51% 9% 7%
2	C	222	 4% 46% 45% 8%
2	E	222	 4% 45% 44% 10%
3	D	211	 4% 49% 45% 5%

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Mol	Chain	Length	Quality of chain
3	F	211	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a small red segment on the left labeled '4%', a large green segment labeled '42%', a large yellow segment labeled '51%', and a small orange segment on the right labeled '7%'.</p>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13223 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 H(+)/Cl(-) exchange transporter clcA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	444	3333	2190	561	562	20	0	0	0
1	B	441	3304	2174	554	556	20	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	148	GLN	GLU	engineered mutation	UNP P37019
B	148	GLN	GLU	engineered mutation	UNP P37019

- Molecule 2 is a protein called Fab Fragment (Heavy Chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	221	1672	1077	274	315	6	0	0	0
2	E	221	1672	1077	274	315	6	0	0	0

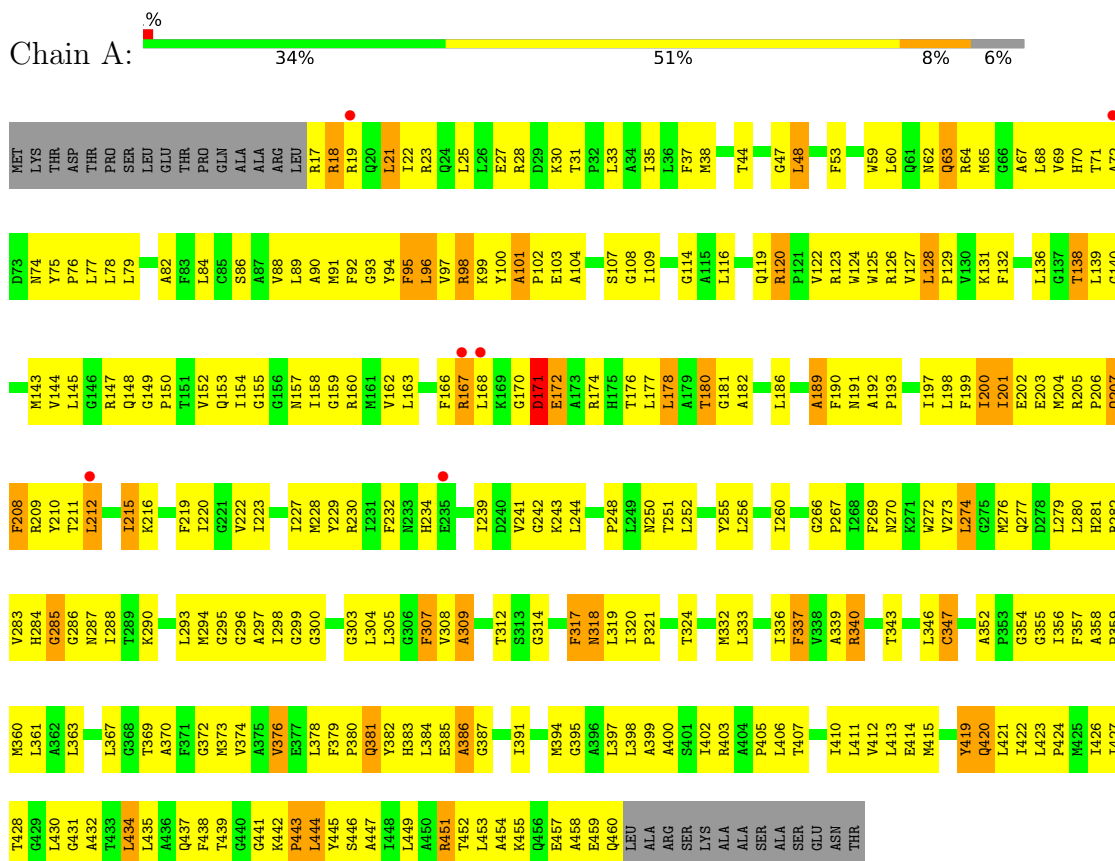
- Molecule 3 is a protein called Fab Fragment (Light Chain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	211	1621	1008	271	334	8	0	0	0
3	F	211	1621	1008	271	334	8	0	0	0

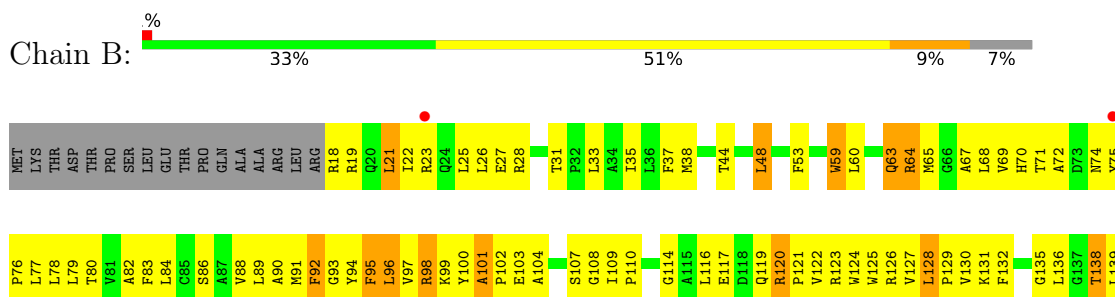
3 Residue-property plots i

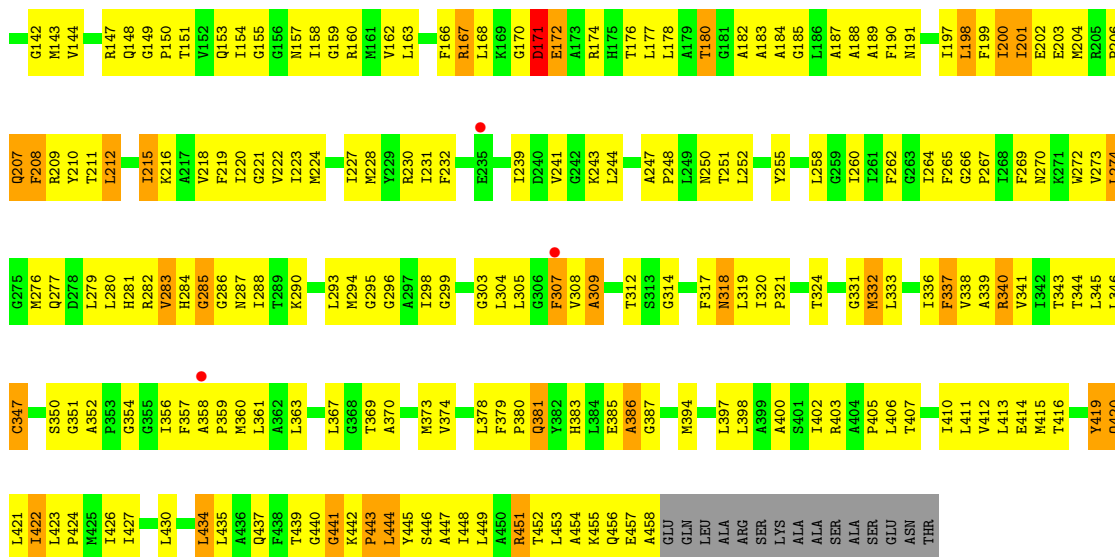
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: H(+)/Cl(-) exchange transporter clcA



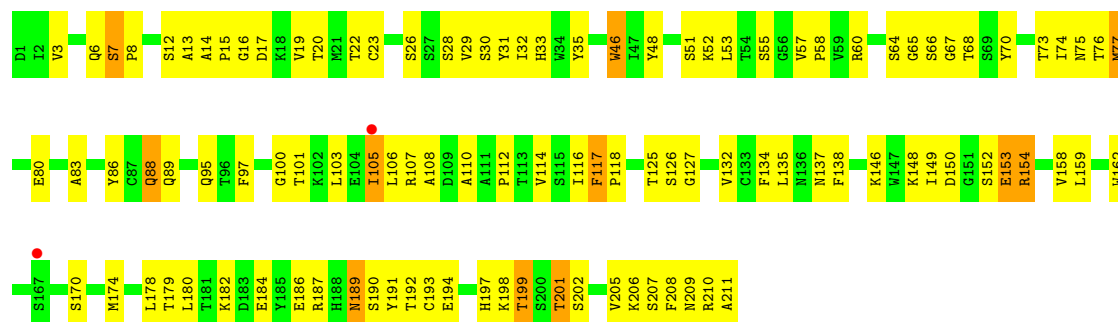
- Molecule 1: H(+)/Cl(-) exchange transporter clcA



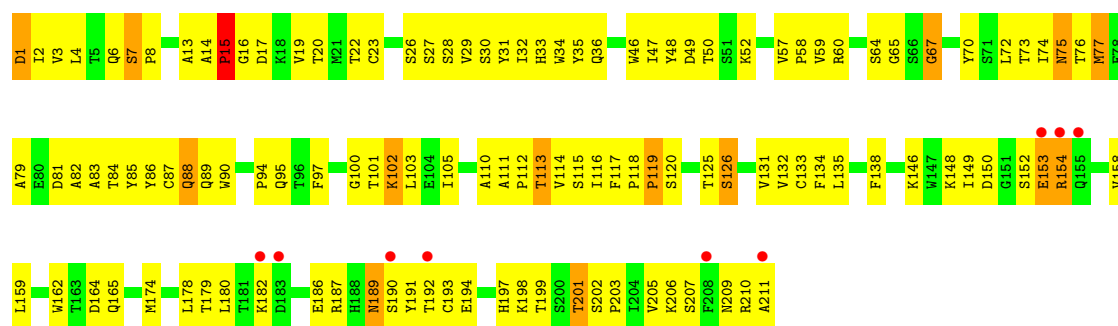




- Molecule 3: Fab Fragment (Light Chain)



- Molecule 3: Fab Fragment (Light Chain)



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	219.64Å 119.79Å 151.30Å 90.00° 128.09° 90.00°	Depositor
Resolution (Å)	19.97 – 3.10 49.45 – 3.10	Depositor EDS
% Data completeness (in resolution range)	95.6 (19.97-3.10) 95.5 (49.45-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 3.12Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.328 , 0.352 0.309 , 0.332	Depositor DCC
R_{free} test set	2595 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	82.6	Xtrriage
Anisotropy	0.573	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	13223	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.50	0/3405	0.68	0/4621
1	B	0.51	0/3376	0.69	0/4583
2	C	0.77	1/1721 (0.1%)	0.88	1/2355 (0.0%)
2	E	0.77	4/1721 (0.2%)	0.86	0/2355
3	D	0.62	0/1660	0.77	1/2257 (0.0%)
3	F	0.74	1/1660 (0.1%)	0.83	0/2257
All	All	0.63	6/13543 (0.0%)	0.77	2/18428 (0.0%)

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	B	0	1
2	E	0	1
3	F	0	1
All	All	0	3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	61	THR	CB-CG2	-7.07	1.29	1.52
2	E	121	SER	C-N	-6.33	1.19	1.34
2	E	121	SER	C-O	5.50	1.33	1.23
2	E	121	SER	CA-C	5.16	1.66	1.52
3	F	201	THR	CB-CG2	-5.14	1.35	1.52
2	E	61	THR	CB-CG2	-5.04	1.35	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	61	THR	OG1-CB-CG2	-9.16	88.94	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	201	THR	OG1-CB-CG2	-5.44	97.48	110.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	419	TYR	Sidechain
2	E	95	TYR	Sidechain
3	F	31	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	3333	0	3486	388	0
1	B	3304	0	3459	372	0
2	C	1672	0	1654	119	0
2	E	1672	0	1654	127	0
3	D	1621	0	1546	94	0
3	F	1621	0	1546	130	0
All	All	13223	0	13345	1156	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 44.

All (1156) 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)
3:D:16:GLY:HA2	3:D:76:THR:HG23	1.28	1.06
1:A:381:GLN:H	1:A:381:GLN:NE2	1.54	1.06
1:B:381:GLN:H	1:B:381:GLN:NE2	1.53	1.05
3:F:192:THR:HA	3:F:207:SER:HB3	1.37	1.05
1:A:223:ILE:HD11	1:B:426:ILE:HG22	1.39	1.04
1:A:28:ARG:HD2	1:B:207:GLN:HG2	1.40	1.03
2:C:45:LEU:HD12	2:C:45:LEU:H	1.24	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:GLN:HE21	1:B:381:GLN:N	1.57	1.01
1:A:207:GLN:HG2	1:B:28:ARG:HD2	1.43	1.00
3:F:194:GLU:HG2	3:F:205:VAL:HG12	1.42	0.99
3:D:194:GLU:HG2	3:D:205:VAL:HG12	1.44	0.99
1:A:381:GLN:HE21	1:A:381:GLN:N	1.60	0.98
1:A:98:ARG:HH11	1:A:98:ARG:HB3	1.29	0.98
2:E:45:LEU:HD12	2:E:45:LEU:H	1.26	0.98
3:F:7:SER:HB3	3:F:8:PRO:HD3	1.46	0.97
1:B:287:ASN:ND2	1:B:290:LYS:H	1.62	0.96
1:B:120:ARG:HB3	1:B:120:ARG:HH11	1.28	0.95
3:F:16:GLY:HA2	3:F:76:THR:HG23	1.45	0.94
1:A:252:LEU:HD22	1:A:427:ILE:HD12	1.49	0.94
3:D:192:THR:HA	3:D:207:SER:HB3	1.49	0.94
3:D:7:SER:HB3	3:D:8:PRO:HD3	1.49	0.93
1:B:98:ARG:HH11	1:B:98:ARG:HB3	1.34	0.92
1:B:154:ILE:O	1:B:158:ILE:HG12	1.69	0.92
1:A:426:ILE:HG22	1:B:223:ILE:HD11	1.52	0.91
1:A:287:ASN:ND2	1:A:290:LYS:H	1.69	0.91
1:A:75:TYR:HB3	1:A:76:PRO:HD3	1.51	0.90
2:C:127:PRO:HB3	2:C:153:TYR:HB3	1.53	0.90
1:A:220:ILE:HG12	1:B:430:LEU:HD21	1.55	0.89
1:A:274:LEU:HA	1:A:277:GLN:HE21	1.37	0.88
1:A:124:TRP:HA	1:A:157:ASN:HD22	1.38	0.88
1:A:274:LEU:O	1:A:277:GLN:HG2	1.73	0.88
1:A:154:ILE:O	1:A:158:ILE:HG12	1.74	0.88
1:A:430:LEU:HD21	1:B:220:ILE:HG12	1.55	0.88
1:A:305:LEU:HA	1:A:308:VAL:HG22	1.55	0.88
1:B:75:TYR:HB3	1:B:76:PRO:HD3	1.54	0.88
1:B:124:TRP:HA	1:B:157:ASN:HD22	1.39	0.87
1:B:305:LEU:HA	1:B:308:VAL:HG22	1.58	0.86
1:B:68:LEU:HD21	1:B:82:ALA:HB2	1.58	0.86
3:F:110:ALA:O	3:F:138:PHE:HA	1.76	0.86
1:B:274:LEU:O	1:B:277:GLN:HG2	1.75	0.85
3:F:14:ALA:O	3:F:17:ASP:HB2	1.76	0.85
1:B:109:ILE:HD12	1:B:445:TYR:HE2	1.40	0.85
1:B:287:ASN:HD22	1:B:290:LYS:H	1.17	0.85
1:B:198:LEU:HG	1:B:410:ILE:HD12	1.59	0.84
1:A:198:LEU:HG	1:A:410:ILE:HD12	1.57	0.84
1:A:274:LEU:HA	1:A:277:GLN:NE2	1.93	0.84
1:A:381:GLN:H	1:A:381:GLN:HE21	0.84	0.83
3:F:82:ALA:HB2	3:F:105:ILE:HD11	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:LEU:HD12	1:A:277:GLN:HE22	1.42	0.83
1:A:241:VAL:HG11	1:A:324:THR:HG21	1.61	0.83
2:E:107:TYR:HB3	3:F:33:HIS:CD2	2.13	0.83
1:A:18:ARG:NH1	1:B:457:GLU:HB3	1.96	0.81
2:C:132:LEU:HB2	2:C:147:GLY:O	1.78	0.81
3:D:95:GLN:OE1	3:D:95:GLN:N	2.14	0.81
2:E:204:ASN:HB3	2:E:215:ASP:OD1	1.80	0.81
1:A:279:LEU:HA	1:A:282:ARG:HH11	1.46	0.81
1:B:120:ARG:HD3	1:B:453:LEU:CD1	2.11	0.81
1:A:223:ILE:HD11	1:B:426:ILE:CG2	2.09	0.81
2:E:127:PRO:HB3	2:E:153:TYR:HB3	1.63	0.80
1:B:120:ARG:HB3	1:B:120:ARG:NH1	1.95	0.80
2:C:207:HIS:CE1	2:C:209:ALA:HB3	2.16	0.80
1:A:123:ARG:HA	1:A:125:TRP:CH2	2.17	0.80
2:C:172:HIS:HB2	2:C:188:SER:HB3	1.61	0.80
3:D:150:ASP:HA	3:D:190:SER:HB3	1.62	0.80
1:A:109:ILE:HD12	1:A:445:TYR:HE2	1.46	0.79
1:B:449:LEU:O	1:B:453:LEU:HB2	1.82	0.79
1:B:241:VAL:HG11	1:B:324:THR:HG21	1.65	0.79
3:D:30:SER:HA	3:D:70:TYR:OH	1.83	0.79
1:B:200:ILE:HG22	1:B:201:ILE:N	1.97	0.79
1:B:201:ILE:HG21	1:B:215:ILE:HD11	1.63	0.78
3:F:111:ALA:N	3:F:199:THR:HG21	1.98	0.78
1:A:120:ARG:HH11	1:A:120:ARG:HB3	1.48	0.78
1:A:44:THR:O	1:A:48:LEU:HD22	1.83	0.78
1:B:120:ARG:HH11	1:B:120:ARG:CB	1.95	0.78
1:A:449:LEU:O	1:A:453:LEU:HB2	1.83	0.78
1:B:451:ARG:HH11	1:B:451:ARG:CB	1.96	0.78
1:A:274:LEU:HD12	1:A:277:GLN:NE2	1.97	0.78
2:E:72:ARG:NH1	2:E:74:ASN:OD1	2.16	0.78
1:A:287:ASN:HD22	1:A:290:LYS:H	1.27	0.78
3:F:95:GLN:N	3:F:95:GLN:OE1	2.16	0.78
1:A:200:ILE:HG22	1:A:201:ILE:N	1.97	0.78
1:A:98:ARG:HB3	1:A:98:ARG:NH1	1.99	0.77
1:B:260:ILE:HG23	1:B:435:LEU:HG	1.64	0.77
2:C:107:TYR:HB3	3:D:33:HIS:CD2	2.20	0.77
1:B:279:LEU:HA	1:B:282:ARG:HH11	1.49	0.77
1:A:200:ILE:HD12	1:A:204:MET:HG3	1.64	0.77
1:A:281:HIS:HA	1:A:284:HIS:CE1	2.20	0.77
1:B:44:THR:O	1:B:48:LEU:HD22	1.85	0.76
3:F:192:THR:CA	3:F:207:SER:HB3	2.13	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:LEU:O	1:B:424:PRO:HD2	1.84	0.76
1:A:68:LEU:HD21	1:A:82:ALA:HB2	1.66	0.76
1:B:65:MET:C	1:B:67:ALA:H	1.89	0.76
1:A:201:ILE:HG21	1:A:215:ILE:HD11	1.66	0.76
3:D:189:ASN:HD21	3:D:211:ALA:H	1.31	0.76
1:B:150:PRO:O	1:B:154:ILE:HG13	1.85	0.76
1:B:374:VAL:HG12	1:B:378:LEU:CD1	2.16	0.76
2:E:45:LEU:HD12	2:E:45:LEU:N	2.00	0.76
1:A:374:VAL:HG12	1:A:378:LEU:CD1	2.16	0.75
1:A:423:LEU:HB3	1:A:424:PRO:HD3	1.69	0.75
2:C:126:PRO:HB3	2:C:210:SER:OG	1.86	0.75
1:B:281:HIS:HA	1:B:284:HIS:CE1	2.21	0.75
1:A:119:GLN:HB3	1:A:453:LEU:HD11	1.67	0.75
2:E:221:ARG:HH22	3:F:120:SER:HA	1.51	0.75
3:F:189:ASN:HD21	3:F:211:ALA:H	1.35	0.75
1:A:65:MET:C	1:A:67:ALA:H	1.90	0.74
1:B:274:LEU:HA	1:B:277:GLN:HE21	1.50	0.74
1:B:109:ILE:HD12	1:B:445:TYR:CE2	2.23	0.74
2:C:207:HIS:HE1	2:C:209:ALA:HB3	1.49	0.74
1:B:252:LEU:HD22	1:B:427:ILE:HD12	1.68	0.74
3:D:14:ALA:O	3:D:17:ASP:HB2	1.87	0.74
2:E:45:LEU:HD11	3:F:86:TYR:CD1	2.23	0.74
1:A:150:PRO:O	1:A:154:ILE:HG13	1.88	0.74
1:A:287:ASN:HD22	1:A:290:LYS:HG3	1.53	0.73
1:B:123:ARG:HH21	1:B:126:ARG:HH11	1.35	0.73
2:C:18:LEU:HD23	2:C:18:LEU:H	1.53	0.73
3:F:150:ASP:HA	3:F:190:SER:HB3	1.69	0.73
1:A:120:ARG:HD3	1:A:453:LEU:HD13	1.70	0.73
1:A:18:ARG:O	1:A:18:ARG:HG2	1.86	0.73
3:F:148:LYS:HB2	3:F:192:THR:OG1	1.89	0.72
1:A:120:ARG:HD3	1:A:453:LEU:CD1	2.19	0.72
2:C:51:ILE:HD11	2:C:55:SER:HB3	1.70	0.72
2:C:189:VAL:HG13	2:C:189:VAL:O	1.90	0.72
3:F:7:SER:HB3	3:F:8:PRO:CD	2.18	0.72
1:B:287:ASN:HD22	1:B:290:LYS:N	1.87	0.72
1:B:380:PRO:HD2	1:B:381:GLN:HE22	1.53	0.72
3:F:1:ASP:HB3	3:F:94:PRO:HD2	1.69	0.72
1:A:28:ARG:HD2	1:B:207:GLN:CG	2.17	0.72
2:E:41:PRO:HD3	2:E:92:ALA:HA	1.72	0.72
2:E:132:LEU:HD21	3:F:132:VAL:HG21	1.72	0.72
2:C:2:VAL:HA	2:C:26:GLY:HA3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:126:PRO:HB3	2:E:210:SER:OG	1.90	0.71
3:F:30:SER:HA	3:F:70:TYR:OH	1.90	0.71
1:B:119:GLN:HB3	1:B:453:LEU:HD11	1.72	0.71
2:C:124:THR:HG22	2:C:125:THR:N	2.06	0.71
1:A:260:ILE:HG23	1:A:435:LEU:HG	1.73	0.71
1:B:120:ARG:HD3	1:B:453:LEU:HD13	1.70	0.71
1:B:166:PHE:HB2	1:B:168:LEU:HD11	1.73	0.71
1:B:287:ASN:ND2	1:B:290:LYS:N	2.38	0.71
3:D:20:THR:HG23	3:D:73:THR:OG1	1.90	0.71
1:B:320:ILE:HG21	1:B:394:MET:CE	2.21	0.71
1:A:18:ARG:NH2	1:B:456:GLN:NE2	2.38	0.71
1:B:168:LEU:HD12	1:B:168:LEU:H	1.56	0.70
2:C:72:ARG:NH1	2:C:74:ASN:OD1	2.24	0.70
1:A:451:ARG:CB	1:A:451:ARG:HH11	2.04	0.70
1:B:206:PRO:HG2	1:B:211:THR:OG1	1.91	0.70
2:C:45:LEU:HD12	2:C:45:LEU:N	2.03	0.70
1:A:108:GLY:HA2	1:A:153:GLN:NE2	2.06	0.70
1:B:144:VAL:HG21	1:B:343:THR:HB	1.73	0.70
2:C:12:VAL:HG23	2:C:119:VAL:HG22	1.72	0.70
1:A:216:LYS:HD3	1:B:434:LEU:CD2	2.22	0.70
3:F:2:ILE:HD11	3:F:27:SER:HB2	1.74	0.70
1:A:144:VAL:HG21	1:A:343:THR:HB	1.73	0.69
1:B:182:ALA:HB1	1:B:204:MET:CE	2.22	0.69
1:B:381:GLN:H	1:B:381:GLN:HE21	0.80	0.69
1:A:22:ILE:HD13	1:B:454:ALA:HB2	1.73	0.69
1:A:123:ARG:HH21	1:A:126:ARG:HH11	1.36	0.69
1:B:274:LEU:HA	1:B:277:GLN:NE2	2.07	0.69
2:E:39:GLN:O	2:E:92:ALA:HB1	1.92	0.69
3:D:65:GLY:HA3	3:D:70:TYR:HA	1.75	0.69
1:A:18:ARG:NH2	1:B:456:GLN:HE21	1.90	0.69
1:A:109:ILE:HD12	1:A:445:TYR:CE2	2.28	0.69
3:D:148:LYS:HB2	3:D:192:THR:OG1	1.92	0.69
2:E:91:THR:OG1	2:E:119:VAL:HG23	1.91	0.69
1:A:79:LEU:H	1:A:79:LEU:CD2	2.06	0.69
1:A:426:ILE:CG2	1:B:223:ILE:HD11	2.22	0.69
1:B:197:ILE:HD13	1:B:219:PHE:CE1	2.28	0.69
1:A:207:GLN:CG	1:B:28:ARG:HD2	2.21	0.69
1:B:200:ILE:HD12	1:B:204:MET:HG3	1.74	0.69
2:C:39:GLN:O	2:C:92:ALA:HB1	1.93	0.69
3:F:7:SER:HB2	3:F:22:THR:HB	1.75	0.69
1:B:274:LEU:HD12	1:B:277:GLN:NE2	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:ALA:O	1:B:361:LEU:HB2	1.91	0.68
2:E:18:LEU:HD23	2:E:18:LEU:H	1.57	0.68
3:F:88:GLN:HB2	3:F:97:PHE:CD1	2.27	0.68
2:C:129:VAL:HG21	2:C:214:VAL:CG2	2.23	0.68
3:F:111:ALA:HB2	3:F:199:THR:HB	1.75	0.68
1:A:163:LEU:HD21	1:A:174:ARG:HG3	1.74	0.68
1:B:98:ARG:HB3	1:B:98:ARG:NH1	2.05	0.68
1:A:79:LEU:H	1:A:79:LEU:HD22	1.58	0.68
1:B:274:LEU:HD12	1:B:277:GLN:HE22	1.59	0.68
1:B:282:ARG:O	1:B:284:HIS:N	2.26	0.68
1:B:79:LEU:H	1:B:79:LEU:HD22	1.57	0.68
3:F:192:THR:HA	3:F:207:SER:CB	2.19	0.68
1:B:284:HIS:HA	1:B:290:LYS:HB3	1.75	0.68
3:D:7:SER:HB3	3:D:8:PRO:CD	2.23	0.68
1:A:182:ALA:HB1	1:A:204:MET:CE	2.24	0.68
1:A:17:ARG:HD2	1:A:17:ARG:C	2.14	0.68
1:A:380:PRO:HD2	1:A:381:GLN:HE22	1.59	0.67
1:A:458:ALA:N	1:A:460:GLN:HE22	1.91	0.67
1:B:172:GLU:O	1:B:176:THR:HB	1.93	0.67
2:C:204:ASN:HB3	2:C:215:ASP:OD1	1.93	0.67
1:B:79:LEU:H	1:B:79:LEU:CD2	2.07	0.67
1:B:374:VAL:HG12	1:B:378:LEU:HD11	1.77	0.67
1:A:120:ARG:HB3	1:A:120:ARG:NH1	2.09	0.67
1:A:421:LEU:O	1:A:424:PRO:HD2	1.95	0.67
1:A:199:PHE:HA	1:A:407:THR:OG1	1.95	0.67
1:B:451:ARG:HH11	1:B:451:ARG:HB3	1.59	0.66
2:E:129:VAL:HG21	2:E:214:VAL:CG2	2.25	0.66
3:F:7:SER:CB	3:F:8:PRO:HD3	2.22	0.66
1:A:458:ALA:H	1:A:460:GLN:HE22	1.43	0.66
3:D:13:ALA:HB3	3:D:77:MET:CE	2.25	0.66
1:A:97:VAL:HG22	1:A:104:ALA:HB3	1.76	0.66
1:A:434:LEU:CD2	1:B:216:LYS:HD3	2.25	0.66
1:A:403:ARG:NH2	1:A:437:GLN:HB2	2.10	0.66
2:C:18:LEU:HD23	2:C:18:LEU:N	2.08	0.66
2:C:41:PRO:HD3	2:C:92:ALA:HA	1.78	0.66
3:F:148:LYS:HA	3:F:152:SER:O	1.96	0.66
1:A:172:GLU:O	1:A:176:THR:HB	1.95	0.66
3:D:148:LYS:HA	3:D:152:SER:O	1.95	0.66
2:E:192:PRO:O	2:E:195:SER:HB3	1.95	0.66
2:E:189:VAL:HG13	2:E:189:VAL:O	1.95	0.66
1:A:403:ARG:HH22	1:A:437:GLN:HB2	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:GLY:HA3	1:A:400:ALA:HB1	1.78	0.66
3:D:192:THR:CA	3:D:207:SER:HB3	2.25	0.66
1:A:282:ARG:O	1:A:284:HIS:N	2.29	0.65
1:A:332:MET:O	1:A:336:ILE:HG13	1.95	0.65
1:A:403:ARG:HH22	1:A:437:GLN:CB	2.09	0.65
2:C:45:LEU:HD11	3:D:86:TYR:CD1	2.31	0.65
1:A:122:VAL:HG11	1:A:160:ARG:CB	2.26	0.65
1:A:166:PHE:HB2	1:A:168:LEU:HD11	1.77	0.65
1:A:374:VAL:HG12	1:A:378:LEU:HD11	1.79	0.65
2:C:129:VAL:HG21	2:C:214:VAL:HG21	1.78	0.65
2:E:6:GLU:HA	2:E:22:CYS:HA	1.78	0.65
2:E:172:HIS:HB2	2:E:188:SER:HB3	1.77	0.65
1:A:411:LEU:O	1:A:414:GLU:HB2	1.97	0.65
2:E:207:HIS:ND1	2:E:210:SER:HB3	2.12	0.65
1:A:197:ILE:HD13	1:A:219:PHE:CE1	2.32	0.65
1:B:108:GLY:HA2	1:B:153:GLN:NE2	2.12	0.65
1:B:423:LEU:HB3	1:B:424:PRO:HD3	1.79	0.65
3:F:22:THR:HG22	3:F:23:CYS:N	2.12	0.65
1:A:374:VAL:HG12	1:A:378:LEU:HD12	1.79	0.65
3:D:22:THR:HG22	3:D:23:CYS:N	2.12	0.65
1:A:250:ASN:OD1	1:A:251:THR:HG23	1.96	0.65
1:B:23:ARG:O	1:B:27:GLU:HB2	1.97	0.65
1:B:114:GLY:HA2	1:B:449:LEU:HD21	1.79	0.65
2:E:35:SER:HB2	2:E:49:GLY:O	1.97	0.65
1:A:114:GLY:HA2	1:A:449:LEU:HD21	1.79	0.64
1:A:168:LEU:HD12	1:A:168:LEU:H	1.61	0.64
1:A:357:PHE:CE1	1:A:398:LEU:HD22	2.31	0.64
3:F:134:PHE:O	3:F:135:LEU:HD23	1.97	0.64
3:D:182:LYS:HG2	3:D:186:GLU:OE1	1.97	0.64
2:E:34:MET:HB3	2:E:79:LEU:HD22	1.78	0.64
1:A:37:PHE:HD2	1:A:38:MET:HE2	1.62	0.64
1:A:318:ASN:N	1:A:318:ASN:HD22	1.95	0.64
2:E:2:VAL:HG23	2:E:2:VAL:O	1.96	0.64
2:E:146:LEU:HD12	2:E:201:VAL:HG11	1.79	0.64
1:A:220:ILE:CG1	1:B:430:LEU:HD21	2.26	0.64
1:B:119:GLN:O	1:B:120:ARG:HD2	1.98	0.64
1:B:410:ILE:O	1:B:414:GLU:HG2	1.98	0.64
1:A:18:ARG:HH11	1:B:457:GLU:HB3	1.62	0.64
1:B:250:ASN:OD1	1:B:251:THR:HG23	1.97	0.64
1:B:270:ASN:ND2	1:B:444:LEU:HD23	2.12	0.64
1:A:120:ARG:HH11	1:A:120:ARG:CB	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ARG:HG3	1:A:147:ARG:HH11	1.63	0.63
3:D:205:VAL:O	3:D:206:LYS:HG2	1.98	0.63
2:E:24:ALA:HB1	2:E:27:PHE:HE1	1.63	0.63
2:E:132:LEU:HB2	2:E:147:GLY:O	1.99	0.63
1:A:443:PRO:HB2	1:A:446:SER:HB2	1.80	0.63
3:F:65:GLY:HA3	3:F:70:TYR:HA	1.80	0.63
1:A:454:ALA:HB2	1:B:22:ILE:HD13	1.79	0.63
1:B:166:PHE:HB2	1:B:168:LEU:CD1	2.29	0.63
2:C:192:PRO:O	2:C:195:SER:HB3	1.98	0.63
3:D:179:THR:O	3:D:180:LEU:HD23	1.97	0.63
2:E:207:HIS:CE1	2:E:209:ALA:HB3	2.34	0.63
3:D:114:VAL:O	3:D:206:LYS:HD2	1.98	0.63
2:C:51:ILE:CD1	2:C:72:ARG:HD2	2.29	0.63
1:A:138:THR:HG22	1:A:143:MET:SD	2.38	0.63
1:B:163:LEU:HD21	1:B:174:ARG:HG3	1.81	0.63
1:A:269:PHE:O	1:A:273:VAL:HG12	1.99	0.62
1:A:320:ILE:HG21	1:A:394:MET:CE	2.29	0.62
1:B:266:GLY:HA3	1:B:400:ALA:HB1	1.81	0.62
2:E:45:LEU:H	2:E:45:LEU:CD1	2.09	0.62
3:F:20:THR:HG23	3:F:73:THR:OG1	1.99	0.62
3:F:190:SER:HA	3:F:209:ASN:OD1	1.99	0.62
1:A:287:ASN:ND2	1:A:290:LYS:HG3	2.14	0.62
1:B:374:VAL:HG12	1:B:378:LEU:HD12	1.81	0.62
1:A:86:SER:OG	1:A:303:GLY:HA3	1.99	0.62
3:D:7:SER:CB	3:D:8:PRO:HD3	2.25	0.62
1:A:71:THR:HB	1:A:77:LEU:HD23	1.81	0.62
1:A:410:ILE:O	1:A:414:GLU:HG2	1.99	0.62
3:F:111:ALA:HB2	3:F:199:THR:CB	2.30	0.62
1:B:199:PHE:HA	1:B:407:THR:OG1	2.00	0.61
1:B:279:LEU:O	1:B:279:LEU:HD23	1.98	0.61
3:F:13:ALA:HB3	3:F:77:MET:CE	2.29	0.61
1:A:437:GLN:NE2	1:B:31:THR:H	1.99	0.61
1:A:31:THR:H	1:B:437:GLN:NE2	1.97	0.61
3:F:7:SER:CB	3:F:22:THR:HB	2.30	0.61
1:A:23:ARG:O	1:A:27:GLU:HB2	2.00	0.61
1:A:75:TYR:HB3	1:A:76:PRO:CD	2.29	0.61
1:A:357:PHE:CE1	1:A:398:LEU:HD13	2.35	0.61
1:A:358:ALA:O	1:A:361:LEU:HB2	1.99	0.61
1:B:243:LYS:HE2	1:B:420:GLN:OE1	2.00	0.61
1:A:216:LYS:HD3	1:B:434:LEU:HD22	1.82	0.61
1:A:287:ASN:ND2	1:A:290:LYS:N	2.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:18:LEU:HD23	2:E:18:LEU:N	2.15	0.61
1:A:99:LYS:HB2	1:A:288:ILE:HD11	1.83	0.61
2:C:30:SER:C	2:C:32:TYR:H	2.04	0.61
1:B:147:ARG:HG3	1:B:147:ARG:HH11	1.65	0.61
2:C:129:VAL:CG2	2:C:214:VAL:HG21	2.30	0.61
1:B:443:PRO:HB2	1:B:446:SER:HB2	1.83	0.61
1:A:148:GLN:HE22	1:A:189:ALA:HB1	1.66	0.61
1:A:166:PHE:HB2	1:A:168:LEU:CD1	2.30	0.61
1:B:72:ALA:HA	1:B:78:LEU:HD21	1.81	0.61
1:B:320:ILE:HG21	1:B:394:MET:HE3	1.82	0.61
1:A:72:ALA:HA	1:A:78:LEU:HD21	1.83	0.61
1:A:413:LEU:HD11	1:A:419:TYR:HD1	1.65	0.60
1:A:298:ILE:CG2	1:A:346:LEU:HG	2.31	0.60
1:B:176:THR:O	1:B:180:THR:HG23	2.01	0.60
1:B:403:ARG:NH2	1:B:437:GLN:HB2	2.15	0.60
3:F:182:LYS:HG2	3:F:186:GLU:OE1	2.00	0.60
1:B:287:ASN:HD22	1:B:290:LYS:HG3	1.66	0.60
3:F:77:MET:SD	3:F:103:LEU:HD21	2.41	0.60
3:F:114:VAL:HG22	3:F:135:LEU:HD22	1.83	0.60
3:F:194:GLU:CG	3:F:205:VAL:HG12	2.24	0.60
2:C:185:LEU:O	2:C:185:LEU:HD12	2.00	0.60
1:A:284:HIS:HA	1:A:290:LYS:HB3	1.84	0.60
1:B:182:ALA:HB1	1:B:204:MET:HE3	1.84	0.60
2:C:6:GLU:HA	2:C:22:CYS:HA	1.82	0.60
1:A:190:PHE:CE2	1:A:411:LEU:HD21	2.37	0.60
3:F:95:GLN:H	3:F:95:GLN:CD	2.05	0.60
1:A:148:GLN:NE2	1:A:189:ALA:HB1	2.16	0.60
1:A:243:LYS:HE2	1:A:420:GLN:OE1	2.01	0.60
3:F:179:THR:O	3:F:180:LEU:HD23	2.01	0.60
1:A:53:PHE:HE2	1:A:147:ARG:HB2	1.66	0.59
1:A:255:TYR:CD2	1:A:424:PRO:HB3	2.36	0.59
2:E:207:HIS:HE1	2:E:209:ALA:HB3	1.67	0.59
1:B:357:PHE:CE1	1:B:398:LEU:HD13	2.36	0.59
2:E:129:VAL:CG2	2:E:214:VAL:HG21	2.32	0.59
3:F:34:TRP:CZ3	3:F:87:CYS:HB3	2.37	0.59
3:F:114:VAL:HG12	3:F:115:SER:N	2.17	0.59
3:F:116:ILE:HD13	3:F:193:CYS:HB2	1.84	0.59
2:C:51:ILE:HD13	2:C:72:ARG:HD2	1.84	0.59
1:B:318:ASN:HD22	1:B:319:LEU:H	1.49	0.59
1:A:122:VAL:HG11	1:A:160:ARG:HB3	1.84	0.59
1:A:434:LEU:HD22	1:B:216:LYS:HD3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:SER:OG	1:B:303:GLY:HA3	2.03	0.59
1:B:122:VAL:HG12	1:B:122:VAL:O	2.03	0.59
1:A:198:LEU:HG	1:A:410:ILE:CD1	2.32	0.59
1:B:71:THR:HB	1:B:77:LEU:HD23	1.85	0.59
1:A:212:LEU:HD12	1:A:212:LEU:H	1.67	0.59
3:D:153:GLU:HG3	3:D:154:ARG:H	1.67	0.59
2:E:49:GLY:HA3	2:E:70:ILE:CD1	2.33	0.59
2:E:185:LEU:HD12	2:E:185:LEU:O	2.03	0.59
3:F:15:PRO:HD3	3:F:105:ILE:HG22	1.83	0.59
1:A:451:ARG:HH11	1:A:451:ARG:HB3	1.66	0.59
1:B:97:VAL:HG22	1:B:104:ALA:HB3	1.85	0.59
1:B:171:ASP:HB2	1:B:212:LEU:HD22	1.83	0.59
2:E:121:SER:O	2:E:122:ALA:O	2.21	0.59
3:F:58:PRO:C	3:F:60:ARG:H	2.05	0.59
1:A:23:ARG:HG3	1:A:23:ARG:HH11	1.66	0.59
1:A:60:LEU:O	1:A:64:ARG:HG3	2.02	0.59
1:B:287:ASN:ND2	1:B:290:LYS:HG3	2.18	0.59
2:C:35:SER:HB2	2:C:49:GLY:O	2.02	0.59
1:A:17:ARG:HD2	1:A:17:ARG:O	2.02	0.58
1:A:385:GLU:O	1:A:387:GLY:N	2.36	0.58
1:A:270:ASN:ND2	1:A:444:LEU:HD23	2.16	0.58
1:A:356:ILE:O	1:A:360:MET:HG3	2.03	0.58
1:B:252:LEU:HD11	1:B:423:LEU:HD23	1.84	0.58
1:B:267:PRO:O	1:B:270:ASN:HB2	2.02	0.58
1:B:413:LEU:HD11	1:B:419:TYR:HD1	1.69	0.58
2:C:127:PRO:HB3	2:C:153:TYR:CB	2.31	0.58
2:C:146:LEU:HD12	2:C:201:VAL:HG11	1.86	0.58
1:A:266:GLY:N	1:A:267:PRO:HD2	2.18	0.58
1:B:457:GLU:O	1:B:458:ALA:HB3	2.04	0.58
2:C:132:LEU:HD21	3:D:132:VAL:HG21	1.86	0.58
3:D:95:GLN:H	3:D:95:GLN:CD	2.06	0.58
2:E:129:VAL:HG21	2:E:214:VAL:HG21	1.83	0.58
1:A:98:ARG:NH1	1:A:98:ARG:CB	2.67	0.58
1:A:122:VAL:HG12	1:A:122:VAL:O	2.03	0.58
1:B:336:ILE:O	1:B:340:ARG:HG3	2.03	0.58
3:D:158:VAL:O	3:D:159:LEU:HD23	2.03	0.58
3:F:72:LEU:C	3:F:72:LEU:HD23	2.24	0.58
3:F:153:GLU:HG3	3:F:154:ARG:H	1.68	0.58
1:B:403:ARG:HH22	1:B:437:GLN:CB	2.16	0.58
2:E:40:ALA:HA	2:E:92:ALA:CB	2.33	0.58
1:A:403:ARG:HH22	1:A:437:GLN:CA	2.17	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:GLN:HG3	1:B:190:PHE:CZ	2.39	0.58
1:B:227:ILE:O	1:B:231:ILE:HG12	2.03	0.58
2:E:30:SER:C	2:E:32:TYR:H	2.07	0.58
2:E:61:THR:HB	2:E:62:PRO:CD	2.34	0.58
3:F:111:ALA:H	3:F:199:THR:HG21	1.69	0.58
1:B:122:VAL:HG11	1:B:160:ARG:CB	2.33	0.58
3:D:117:PHE:CD1	3:D:117:PHE:N	2.72	0.58
3:D:189:ASN:ND2	3:D:211:ALA:H	2.01	0.58
1:B:19:ARG:HG2	1:B:19:ARG:HH11	1.69	0.58
1:B:239:ILE:HD13	1:B:394:MET:HE2	1.83	0.58
2:C:100:TYR:HB3	2:C:107:TYR:CE1	2.39	0.58
1:A:305:LEU:HA	1:A:308:VAL:CG2	2.32	0.57
1:A:336:ILE:O	1:A:340:ARG:HG3	2.04	0.57
1:A:402:ILE:HD12	1:A:445:TYR:CE1	2.39	0.57
1:B:63:GLN:C	1:B:65:MET:H	2.08	0.57
1:B:99:LYS:HB2	1:B:288:ILE:HD11	1.86	0.57
1:B:127:VAL:HB	1:B:157:ASN:ND2	2.18	0.57
1:A:79:LEU:HD22	1:A:79:LEU:N	2.19	0.57
1:B:403:ARG:HH22	1:B:437:GLN:HB2	1.69	0.57
2:C:124:THR:HG22	2:C:125:THR:H	1.68	0.57
1:A:23:ARG:HG3	1:A:23:ARG:NH1	2.19	0.57
1:A:252:LEU:HD22	1:A:427:ILE:CD1	2.31	0.57
1:B:75:TYR:O	1:B:79:LEU:HD23	2.04	0.57
1:B:90:ALA:O	1:B:94:TYR:HD1	1.87	0.57
3:D:134:PHE:O	3:D:135:LEU:HD23	2.04	0.57
1:A:31:THR:H	1:B:437:GLN:HE22	1.52	0.57
1:B:37:PHE:HD2	1:B:38:MET:HE2	1.69	0.57
2:C:178:LEU:HB2	2:C:183:TYR:CE2	2.40	0.57
1:A:148:GLN:HB3	1:A:190:PHE:HE1	1.68	0.57
1:A:287:ASN:HD22	1:A:290:LYS:N	1.99	0.57
1:A:170:GLY:O	1:A:172:GLU:N	2.37	0.57
2:C:185:LEU:HD12	2:C:185:LEU:C	2.24	0.57
2:E:91:THR:HG23	2:E:118:THR:HA	1.86	0.57
2:C:196:TRP:O	2:C:197:PRO:C	2.40	0.57
2:C:200:THR:HG22	2:C:200:THR:O	2.05	0.57
1:B:266:GLY:N	1:B:267:PRO:HD2	2.20	0.57
3:D:114:VAL:HG22	3:D:135:LEU:CD2	2.34	0.57
1:A:186:LEU:O	1:A:186:LEU:HG	2.05	0.56
1:B:318:ASN:HD22	1:B:318:ASN:N	2.02	0.56
1:A:206:PRO:HG2	1:A:211:THR:OG1	2.04	0.56
2:E:49:GLY:HA3	2:E:70:ILE:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:GLN:HG3	1:A:190:PHE:CZ	2.40	0.56
1:A:252:LEU:HD11	1:A:423:LEU:HD23	1.87	0.56
1:A:437:GLN:HE22	1:B:31:THR:H	1.51	0.56
1:B:320:ILE:HB	1:B:321:PRO:HD3	1.88	0.56
3:D:190:SER:HA	3:D:209:ASN:OD1	2.06	0.56
1:A:419:TYR:CE1	1:B:414:GLU:OE1	2.59	0.56
1:B:298:ILE:CG2	1:B:346:LEU:HG	2.35	0.56
1:B:357:PHE:CE1	1:B:398:LEU:HD22	2.40	0.56
3:D:125:THR:HG22	3:D:125:THR:O	2.03	0.56
1:A:200:ILE:CG2	1:A:201:ILE:N	2.67	0.56
2:C:40:ALA:HA	2:C:92:ALA:HB2	1.86	0.56
2:E:196:TRP:HB3	2:E:197:PRO:HD3	1.88	0.56
1:A:239:ILE:HD13	1:A:394:MET:HE2	1.88	0.56
1:B:170:GLY:O	1:B:172:GLU:N	2.39	0.56
2:E:98:ARG:NH1	2:E:109:ASP:OD2	2.29	0.56
1:A:75:TYR:O	1:A:79:LEU:HD23	2.05	0.56
1:A:333:LEU:HD11	1:A:373:MET:HE1	1.88	0.56
1:B:79:LEU:HD22	1:B:79:LEU:N	2.21	0.56
1:B:190:PHE:CE2	1:B:411:LEU:HD21	2.40	0.56
3:F:82:ALA:HB2	3:F:105:ILE:CD1	2.32	0.56
1:A:101:ALA:C	1:A:103:GLU:H	2.09	0.56
1:B:356:ILE:O	1:B:360:MET:HG3	2.06	0.56
2:E:40:ALA:HA	2:E:92:ALA:HB2	1.86	0.56
2:E:107:TYR:HB3	3:F:33:HIS:NE2	2.21	0.56
2:E:146:LEU:HD13	2:E:218:ILE:HG21	1.87	0.56
3:D:32:ILE:HG22	3:D:33:HIS:N	2.22	0.55
1:A:18:ARG:HH21	1:B:456:GLN:NE2	2.03	0.55
1:B:64:ARG:NH1	1:B:64:ARG:HB3	2.21	0.55
2:E:127:PRO:HB3	2:E:153:TYR:CB	2.35	0.55
3:F:114:VAL:HG22	3:F:135:LEU:CD2	2.35	0.55
3:D:114:VAL:HG22	3:D:135:LEU:HD22	1.87	0.55
3:D:192:THR:HA	3:D:207:SER:CB	2.30	0.55
1:A:35:ILE:CG2	1:A:176:THR:HG21	2.36	0.55
1:A:212:LEU:HD12	1:A:212:LEU:N	2.22	0.55
1:A:452:THR:HG22	1:A:452:THR:O	2.07	0.55
1:B:200:ILE:CG2	1:B:201:ILE:N	2.69	0.55
1:B:269:PHE:O	1:B:273:VAL:HG12	2.06	0.55
1:B:318:ASN:HD22	1:B:319:LEU:N	2.04	0.55
3:F:119:PRO:HD3	3:F:131:VAL:HG22	1.89	0.55
1:A:318:ASN:HD22	1:A:319:LEU:H	1.55	0.55
1:B:243:LYS:HE2	1:B:420:GLN:CG	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:111:ALA:CA	3:F:199:THR:HG21	2.36	0.55
2:C:109:ASP:OD2	2:C:110:VAL:HG23	2.07	0.55
2:C:156:GLU:HG2	2:C:183:TYR:CE1	2.41	0.55
1:B:294:MET:HG2	1:B:294:MET:O	2.06	0.55
2:E:100:TYR:HB3	2:E:107:TYR:CE1	2.42	0.55
1:A:17:ARG:HH21	1:B:119:GLN:NE2	2.03	0.55
1:B:123:ARG:HA	1:B:125:TRP:CH2	2.42	0.55
1:A:59:TRP:CZ3	1:A:60:LEU:HD23	2.42	0.55
1:A:199:PHE:CD1	1:A:407:THR:HG21	2.42	0.55
1:B:398:LEU:O	1:B:402:ILE:HG23	2.06	0.54
2:C:127:PRO:CB	2:C:153:TYR:HB3	2.32	0.54
2:E:132:LEU:HD21	3:F:132:VAL:CG2	2.35	0.54
1:B:65:MET:C	1:B:67:ALA:N	2.60	0.54
3:D:105:ILE:HB	3:D:170:SER:OG	2.07	0.54
1:B:380:PRO:HD2	1:B:381:GLN:NE2	2.20	0.54
1:A:92:PHE:O	1:A:96:LEU:HD23	2.07	0.54
1:A:457:GLU:HB3	1:B:18:ARG:NH1	2.22	0.54
3:F:29:VAL:CG2	3:F:32:ILE:HD11	2.37	0.54
1:A:255:TYR:CG	1:A:424:PRO:HB3	2.43	0.54
1:A:267:PRO:O	1:A:270:ASN:HB2	2.06	0.54
1:B:332:MET:O	1:B:336:ILE:HG13	2.08	0.54
3:F:29:VAL:O	3:F:67:GLY:HA2	2.08	0.54
1:A:243:LYS:HE2	1:A:420:GLN:CG	2.38	0.54
2:E:196:TRP:O	2:E:197:PRO:C	2.46	0.54
1:B:212:LEU:HD12	1:B:212:LEU:N	2.23	0.54
2:C:24:ALA:HB1	2:C:27:PHE:HE1	1.72	0.54
2:E:10:GLY:N	2:E:116:THR:O	2.41	0.54
1:A:65:MET:C	1:A:67:ALA:N	2.60	0.54
1:A:90:ALA:O	1:A:94:TYR:HD1	1.91	0.54
1:A:457:GLU:O	1:A:458:ALA:HB3	2.08	0.54
1:B:176:THR:HG22	1:B:177:LEU:N	2.22	0.54
1:B:197:ILE:HG13	1:B:222:VAL:HG21	1.89	0.54
1:B:273:VAL:HA	1:B:345:LEU:HD22	1.89	0.54
3:F:197:HIS:ND1	3:F:198:LYS:N	2.56	0.54
1:A:63:GLN:C	1:A:65:MET:H	2.11	0.53
1:A:101:ALA:O	1:A:103:GLU:N	2.41	0.53
3:D:12:SER:HB3	3:D:106:LEU:HB2	1.90	0.53
3:D:197:HIS:ND1	3:D:198:LYS:N	2.55	0.53
2:E:51:ILE:HD11	2:E:55:SER:HB3	1.89	0.53
2:C:18:LEU:N	2:C:18:LEU:CD2	2.71	0.53
2:C:40:ALA:HA	2:C:92:ALA:CB	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:LEU:HD11	1:B:117:GLU:OE1	2.09	0.53
3:D:48:TYR:CE1	3:D:52:LYS:HD2	2.43	0.53
3:F:210:ARG:HH11	3:F:210:ARG:HG2	1.73	0.53
1:A:318:ASN:N	1:A:318:ASN:ND2	2.55	0.53
1:B:92:PHE:O	1:B:96:LEU:HD23	2.07	0.53
1:B:108:GLY:O	1:B:153:GLN:HB2	2.09	0.53
1:A:99:LYS:O	1:A:99:LYS:HG3	2.08	0.53
1:A:443:PRO:O	1:A:446:SER:N	2.28	0.53
1:B:59:TRP:CE3	1:B:60:LEU:HD23	2.43	0.53
2:C:149:LEU:HD12	2:C:150:VAL:N	2.24	0.53
3:D:8:PRO:O	3:D:101:THR:HG23	2.09	0.53
1:A:62:ASN:O	1:A:65:MET:N	2.41	0.53
1:B:98:ARG:NH1	1:B:98:ARG:CB	2.72	0.53
2:C:91:THR:HG23	2:C:118:THR:HA	1.91	0.53
2:C:150:VAL:HG22	2:C:205:VAL:HG21	1.89	0.53
1:B:198:LEU:HD12	1:B:406:LEU:HG	1.90	0.53
3:D:3:VAL:HB	3:D:26:SER:HB3	1.90	0.53
3:F:32:ILE:HG22	3:F:33:HIS:N	2.24	0.53
1:A:108:GLY:O	1:A:153:GLN:HB2	2.08	0.53
1:B:136:LEU:HD12	1:B:136:LEU:H	1.73	0.53
1:B:187:ALA:O	1:B:189:ALA:N	2.42	0.53
1:B:443:PRO:O	1:B:445:TYR:N	2.41	0.53
3:D:22:THR:HG22	3:D:23:CYS:H	1.72	0.53
2:E:39:GLN:C	2:E:92:ALA:HB1	2.29	0.53
1:A:38:MET:HG3	1:A:168:LEU:HD21	1.91	0.53
1:B:202:GLU:O	1:B:202:GLU:HG2	2.09	0.53
2:C:30:SER:O	2:C:32:TYR:N	2.42	0.53
2:C:39:GLN:C	2:C:92:ALA:HB1	2.29	0.53
3:D:153:GLU:HG3	3:D:154:ARG:N	2.23	0.53
1:A:131:LYS:HE2	1:A:150:PRO:HA	1.91	0.52
1:B:75:TYR:HB3	1:B:76:PRO:CD	2.33	0.52
1:B:122:VAL:HG11	1:B:160:ARG:HB3	1.91	0.52
1:B:148:GLN:NE2	1:B:189:ALA:HB1	2.24	0.52
3:F:79:ALA:HA	3:F:105:ILE:HD13	1.90	0.52
1:B:74:ASN:CG	1:B:77:LEU:HB2	2.29	0.52
1:B:272:TRP:O	1:B:276:MET:HB2	2.09	0.52
2:E:72:ARG:HG3	2:E:74:ASN:OD1	2.09	0.52
1:A:248:PRO:HG2	1:A:251:THR:HG23	1.92	0.52
1:A:343:THR:O	1:A:347:CYS:HB2	2.10	0.52
3:D:58:PRO:C	3:D:60:ARG:H	2.12	0.52
1:B:171:ASP:CB	1:B:212:LEU:HD22	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ASN:CG	1:A:77:LEU:HB2	2.30	0.52
2:E:127:PRO:CB	2:E:153:TYR:HB3	2.37	0.52
1:B:109:ILE:CD1	1:B:445:TYR:HE2	2.17	0.52
1:A:109:ILE:CD1	1:A:445:TYR:HE2	2.21	0.52
1:A:192:ALA:HB1	1:A:414:GLU:HG3	1.92	0.52
1:B:101:ALA:O	1:B:103:GLU:N	2.43	0.52
3:D:88:GLN:HB2	3:D:97:PHE:CD1	2.44	0.52
3:F:115:SER:HB3	3:F:117:PHE:CE1	2.44	0.52
2:C:49:GLY:HA3	2:C:70:ILE:CD1	2.40	0.52
2:E:67:LYS:HE2	2:E:85:LYS:O	2.10	0.52
1:B:159:GLY:O	1:B:162:VAL:HG22	2.10	0.52
1:B:442:LYS:O	1:B:444:LEU:N	2.43	0.52
3:D:107:ARG:NE	3:D:108:ALA:O	2.41	0.51
1:B:101:ALA:C	1:B:103:GLU:H	2.14	0.51
3:F:75:ASN:O	3:F:76:THR:HB	2.11	0.51
1:B:333:LEU:HD11	1:B:373:MET:HE1	1.92	0.51
2:C:120:SER:OG	2:C:121:SER:N	2.43	0.51
3:F:153:GLU:HG3	3:F:154:ARG:N	2.25	0.51
3:F:158:VAL:O	3:F:159:LEU:HD23	2.11	0.51
1:A:18:ARG:HB2	1:B:119:GLN:OE1	2.10	0.51
1:A:65:MET:O	1:A:67:ALA:N	2.42	0.51
1:A:201:ILE:O	1:A:201:ILE:HG13	2.10	0.51
1:B:91:MET:O	1:B:93:GLY:N	2.44	0.51
1:B:370:ALA:O	1:B:374:VAL:HG23	2.11	0.51
1:B:411:LEU:O	1:B:414:GLU:HB2	2.11	0.51
2:C:32:TYR:CE2	2:C:98:ARG:HD3	2.45	0.51
2:E:171:VAL:C	2:E:172:HIS:HD1	2.14	0.51
1:A:119:GLN:O	1:A:120:ARG:HD2	2.11	0.51
1:A:198:LEU:HD12	1:A:406:LEU:HG	1.91	0.51
2:C:163:ASN:ND2	2:C:167:LEU:HD23	2.26	0.51
2:E:38:ARG:HE	2:E:46:LYS:NZ	2.07	0.51
1:A:59:TRP:CE3	1:A:60:LEU:HD23	2.44	0.51
1:A:64:ARG:HB3	1:A:64:ARG:NH1	2.25	0.51
1:B:21:LEU:HD22	1:B:25:LEU:HG	1.93	0.51
2:C:30:SER:C	2:C:32:TYR:N	2.64	0.51
3:F:29:VAL:HG21	3:F:32:ILE:HD11	1.93	0.51
1:A:28:ARG:CD	1:B:207:GLN:HG2	2.28	0.51
1:A:128:LEU:HB2	1:A:129:PRO:CD	2.41	0.51
1:A:220:ILE:HG12	1:B:430:LEU:CD2	2.36	0.51
2:C:156:GLU:OE2	2:C:176:ALA:HB3	2.11	0.51
2:E:24:ALA:HB1	2:E:27:PHE:CE1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:LEU:HB2	1:B:129:PRO:CD	2.41	0.51
2:C:67:LYS:HE2	2:C:85:LYS:O	2.10	0.51
3:D:7:SER:CB	3:D:8:PRO:CD	2.88	0.51
1:A:18:ARG:NH1	1:B:457:GLU:CB	2.71	0.51
1:A:357:PHE:CZ	1:A:398:LEU:HD13	2.46	0.51
1:B:255:TYR:CD2	1:B:424:PRO:HB3	2.46	0.51
3:D:210:ARG:HG2	3:D:210:ARG:HH11	1.74	0.51
1:A:191:ASN:O	1:A:191:ASN:ND2	2.44	0.50
1:A:459:GLU:O	1:A:459:GLU:HG2	2.10	0.50
1:A:123:ARG:HD2	1:A:125:TRP:CZ2	2.46	0.50
1:B:95:PHE:O	1:B:97:VAL:N	2.44	0.50
3:F:205:VAL:O	3:F:206:LYS:HG2	2.11	0.50
1:A:197:ILE:HG13	1:A:222:VAL:HG21	1.92	0.50
1:A:430:LEU:C	1:A:432:ALA:N	2.64	0.50
1:B:284:HIS:HA	1:B:290:LYS:CB	2.40	0.50
3:D:86:TYR:CE2	3:D:100:GLY:HA3	2.46	0.50
3:F:116:ILE:CD1	3:F:193:CYS:HB2	2.41	0.50
3:F:114:VAL:HG13	3:F:135:LEU:HD23	1.92	0.50
3:F:116:ILE:HD13	3:F:193:CYS:CB	2.42	0.50
3:D:7:SER:HB2	3:D:22:THR:HB	1.92	0.50
1:A:298:ILE:HG21	1:A:346:LEU:HG	1.92	0.50
1:B:53:PHE:HE2	1:B:147:ARG:HB2	1.77	0.50
1:B:413:LEU:CD1	1:B:422:ILE:HD13	2.41	0.50
2:C:34:MET:HB3	2:C:79:LEU:HD22	1.93	0.50
1:A:139:LEU:HD13	1:A:147:ARG:HB3	1.93	0.50
1:B:358:ALA:N	1:B:359:PRO:HD2	2.27	0.50
2:C:12:VAL:CG2	2:C:119:VAL:HG22	2.40	0.50
2:E:200:THR:HG22	2:E:200:THR:O	2.11	0.50
1:B:65:MET:O	1:B:67:ALA:N	2.44	0.50
1:B:197:ILE:HD13	1:B:219:PHE:CD1	2.46	0.50
1:B:212:LEU:HD12	1:B:212:LEU:H	1.77	0.50
3:D:110:ALA:C	3:D:199:THR:HG21	2.33	0.50
1:A:123:ARG:HA	1:A:125:TRP:CZ3	2.47	0.49
1:A:138:THR:O	1:A:143:MET:HG3	2.13	0.49
1:A:190:PHE:HD1	1:A:190:PHE:H	1.59	0.49
1:A:255:TYR:HB3	1:A:428:THR:OG1	2.12	0.49
1:A:320:ILE:HB	1:A:321:PRO:HD3	1.94	0.49
1:A:361:LEU:HD23	1:A:394:MET:O	2.13	0.49
1:B:35:ILE:CG2	1:B:176:THR:HG21	2.42	0.49
1:B:412:VAL:O	1:B:416:THR:HG23	2.12	0.49
1:A:33:LEU:C	1:A:33:LEU:HD23	2.32	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:THR:HG22	1:A:177:LEU:N	2.27	0.49
2:C:111:TRP:N	2:C:111:TRP:CD1	2.80	0.49
2:E:132:LEU:CD2	3:F:132:VAL:HG21	2.40	0.49
1:A:17:ARG:C	1:A:19:ARG:H	2.16	0.49
1:A:274:LEU:CA	1:A:277:GLN:HE21	2.18	0.49
1:A:356:ILE:O	1:A:356:ILE:HG12	2.13	0.49
1:B:241:VAL:HG12	1:B:244:LEU:HD21	1.95	0.49
2:E:207:HIS:CE1	2:E:210:SER:H	2.30	0.49
3:D:77:MET:SD	3:D:103:LEU:HD21	2.52	0.49
3:D:107:ARG:NH2	3:D:108:ALA:O	2.43	0.49
3:D:194:GLU:CG	3:D:205:VAL:HG12	2.29	0.49
2:E:30:SER:O	2:E:32:TYR:N	2.46	0.49
2:E:79:LEU:HD23	2:E:96:CYS:HB2	1.94	0.49
2:E:108:PHE:CD1	3:F:88:GLN:NE2	2.79	0.49
1:B:144:VAL:HG11	1:B:344:THR:OG1	2.12	0.49
1:B:148:GLN:HE22	1:B:189:ALA:HB1	1.77	0.49
1:B:223:ILE:O	1:B:227:ILE:HD13	2.12	0.49
1:B:357:PHE:CZ	1:B:398:LEU:HD13	2.47	0.49
2:C:124:THR:CG2	2:C:125:THR:N	2.74	0.49
3:D:19:VAL:HG12	3:D:74:ILE:HB	1.94	0.49
1:A:176:THR:O	1:A:180:THR:HG23	2.11	0.49
2:C:196:TRP:O	2:C:199:GLU:N	2.45	0.49
1:A:284:HIS:HA	1:A:290:LYS:CB	2.43	0.49
1:B:318:ASN:N	1:B:318:ASN:ND2	2.60	0.49
1:B:403:ARG:HH22	1:B:437:GLN:CA	2.26	0.49
2:C:29:TYR:OH	2:C:34:MET:HG3	2.13	0.49
2:E:72:ARG:HG3	2:E:72:ARG:HH11	1.78	0.49
2:E:178:LEU:HD12	2:E:182:LEU:O	2.12	0.49
1:A:84:LEU:O	1:A:88:VAL:HG23	2.12	0.49
1:A:171:ASP:HB2	1:A:212:LEU:HD22	1.94	0.49
1:A:380:PRO:HD2	1:A:381:GLN:NE2	2.26	0.49
3:D:29:VAL:CG2	3:D:32:ILE:HD11	2.43	0.49
1:A:241:VAL:HG12	1:A:244:LEU:HD21	1.95	0.49
1:A:294:MET:O	1:A:298:ILE:HG13	2.13	0.49
1:B:59:TRP:CZ3	1:B:60:LEU:HD23	2.48	0.49
1:B:148:GLN:HB3	1:B:190:PHE:HE1	1.77	0.49
1:B:320:ILE:HD13	1:B:394:MET:HE2	1.94	0.49
1:B:385:GLU:O	1:B:386:ALA:C	2.51	0.49
2:C:24:ALA:HB1	2:C:27:PHE:CE1	2.46	0.49
2:C:126:PRO:HB3	2:C:210:SER:HG	1.75	0.49
1:A:18:ARG:CZ	1:B:456:GLN:HE21	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:PHE:CE1	1:A:363:LEU:HD12	2.48	0.48
1:A:383:HIS:HD2	2:C:33:TRP:CE3	2.31	0.48
1:A:402:ILE:HD12	1:A:445:TYR:CD1	2.48	0.48
1:B:100:TYR:O	1:B:101:ALA:HB2	2.12	0.48
1:B:183:ALA:O	1:B:184:ALA:C	2.51	0.48
1:B:220:ILE:O	1:B:224:MET:HG2	2.12	0.48
2:C:72:ARG:O	2:C:72:ARG:HG2	2.12	0.48
2:E:163:ASN:ND2	2:E:167:LEU:HD23	2.28	0.48
3:F:153:GLU:O	3:F:154:ARG:HB2	2.12	0.48
1:B:23:ARG:HG3	1:B:23:ARG:HH11	1.78	0.48
2:E:98:ARG:O	2:E:109:ASP:HB3	2.13	0.48
1:A:202:GLU:HG2	1:A:202:GLU:O	2.13	0.48
1:A:270:ASN:HA	1:A:273:VAL:CG1	2.43	0.48
3:F:8:PRO:O	3:F:101:THR:HG23	2.13	0.48
3:F:189:ASN:ND2	3:F:211:ALA:H	2.05	0.48
1:A:109:ILE:HG21	1:A:445:TYR:CD2	2.48	0.48
1:B:262:PHE:CZ	1:B:367:LEU:HD23	2.48	0.48
2:C:107:TYR:HB3	3:D:33:HIS:NE2	2.29	0.48
3:D:153:GLU:O	3:D:154:ARG:HB2	2.12	0.48
3:D:178:LEU:HD12	3:D:179:THR:N	2.29	0.48
1:B:33:LEU:HD23	1:B:33:LEU:C	2.34	0.48
1:B:78:LEU:HD13	1:B:307:PHE:CZ	2.49	0.48
2:C:37:VAL:HG22	2:C:47:TRP:HA	1.96	0.48
2:E:16:GLY:O	2:E:86:VAL:HG13	2.14	0.48
1:A:320:ILE:HG21	1:A:394:MET:HE3	1.95	0.48
1:B:131:LYS:HE2	1:B:150:PRO:HA	1.95	0.48
2:E:144:VAL:O	2:E:144:VAL:HG13	2.14	0.48
3:F:79:ALA:O	3:F:105:ILE:HD11	2.14	0.48
1:A:128:LEU:CB	1:A:129:PRO:CD	2.91	0.48
1:A:228:MET:O	1:A:232:PHE:HD1	1.97	0.48
1:A:414:GLU:OE1	1:B:419:TYR:CE1	2.67	0.48
1:B:250:ASN:ND2	2:E:105:TYR:CD1	2.80	0.48
1:B:305:LEU:C	1:B:307:PHE:H	2.16	0.48
2:E:69:ILE:HG22	2:E:69:ILE:O	2.14	0.48
1:B:124:TRP:HA	1:B:157:ASN:ND2	2.19	0.48
1:B:270:ASN:ND2	1:B:444:LEU:CD2	2.77	0.48
2:C:38:ARG:HE	2:C:46:LYS:NZ	2.12	0.48
1:A:100:TYR:O	1:A:101:ALA:HB2	2.14	0.48
1:B:74:ASN:HB3	1:B:77:LEU:HB3	1.96	0.48
1:B:402:ILE:HD12	1:B:445:TYR:CD1	2.49	0.48
2:E:30:SER:C	2:E:32:TYR:N	2.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:106:TRP:HD1	2:E:106:TRP:H	1.61	0.48
1:A:35:ILE:HG23	1:A:176:THR:HG21	1.96	0.47
1:A:91:MET:C	1:A:93:GLY:N	2.67	0.47
1:B:84:LEU:O	1:B:88:VAL:HG23	2.13	0.47
1:B:312:THR:HG22	1:B:339:ALA:HB3	1.96	0.47
2:C:49:GLY:HA3	2:C:70:ILE:HD12	1.96	0.47
2:C:196:TRP:HB3	2:C:197:PRO:HD3	1.95	0.47
3:D:6:GLN:OE1	3:D:86:TYR:HA	2.14	0.47
1:A:279:LEU:HA	1:A:282:ARG:NH1	2.22	0.47
1:A:308:VAL:O	1:A:309:ALA:HB2	2.14	0.47
1:B:23:ARG:HG3	1:B:23:ARG:NH1	2.29	0.47
1:B:99:LYS:HG3	1:B:99:LYS:O	2.13	0.47
1:B:402:ILE:HD12	1:B:445:TYR:CE1	2.49	0.47
1:B:441:GLY:O	1:B:442:LYS:HG3	2.14	0.47
3:F:164:ASP:O	3:F:165:GLN:C	2.52	0.47
1:A:127:VAL:HB	1:A:157:ASN:ND2	2.29	0.47
1:A:293:LEU:C	1:A:295:GLY:N	2.67	0.47
1:B:25:LEU:C	1:B:27:GLU:H	2.18	0.47
1:B:128:LEU:CB	1:B:129:PRO:CD	2.92	0.47
2:C:6:GLU:CD	2:C:114:GLY:HA2	2.35	0.47
2:E:5:LEU:HD13	2:E:5:LEU:C	2.34	0.47
1:B:294:MET:O	1:B:298:ILE:HG13	2.15	0.47
2:C:22:CYS:O	2:C:78:THR:HG23	2.13	0.47
2:E:87:ARG:HG3	2:E:89:GLU:OE2	2.15	0.47
1:B:38:MET:HG3	1:B:168:LEU:HD21	1.95	0.47
1:B:241:VAL:HG12	1:B:241:VAL:O	2.13	0.47
2:C:63:SER:HG	2:C:68:PHE:HE1	1.61	0.47
2:E:185:LEU:HD12	2:E:185:LEU:C	2.35	0.47
1:A:370:ALA:O	1:A:374:VAL:HG23	2.15	0.47
2:C:126:PRO:CB	2:C:210:SER:OG	2.59	0.47
2:C:221:ARG:CZ	3:D:118:PRO:HG2	2.44	0.47
2:E:18:LEU:N	2:E:18:LEU:CD2	2.78	0.47
1:A:200:ILE:HA	1:A:204:MET:HB2	1.95	0.47
1:A:241:VAL:HG12	1:A:241:VAL:O	2.14	0.47
1:B:138:THR:HG21	1:B:352:ALA:HB1	1.96	0.47
1:B:385:GLU:O	1:B:387:GLY:N	2.48	0.47
1:A:122:VAL:HG21	1:A:178:LEU:HD11	1.96	0.47
1:A:150:PRO:CG	1:A:354:GLY:HA2	2.45	0.47
1:A:422:ILE:HG23	1:A:423:LEU:N	2.29	0.47
2:E:36:TRP:CE2	2:E:81:LEU:HB2	2.50	0.47
3:F:34:TRP:CE2	3:F:72:LEU:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ARG:HD3	1:A:163:LEU:HD23	1.97	0.47
3:F:3:VAL:HB	3:F:26:SER:HB3	1.97	0.47
2:C:12:VAL:O	2:C:119:VAL:HA	2.14	0.47
3:F:73:THR:HG22	3:F:74:ILE:N	2.29	0.47
1:A:284:HIS:C	1:A:286:GLY:H	2.19	0.46
1:A:109:ILE:HG21	1:A:445:TYR:HD2	1.80	0.46
1:A:451:ARG:O	1:A:455:LYS:HB2	2.16	0.46
2:C:103:TYR:HD2	3:D:31:TYR:CE2	2.33	0.46
3:D:106:LEU:HD23	3:D:107:ARG:N	2.30	0.46
3:F:36:GLN:HG3	3:F:85:TYR:CE2	2.50	0.46
1:A:22:ILE:HD13	1:B:454:ALA:CB	2.44	0.46
1:A:144:VAL:O	1:A:145:LEU:HD23	2.15	0.46
1:A:150:PRO:HG2	1:A:354:GLY:HA2	1.97	0.46
1:B:318:ASN:ND2	1:B:319:LEU:N	2.64	0.46
1:A:28:ARG:NH2	1:B:443:PRO:HB3	2.31	0.46
1:A:293:LEU:C	1:A:295:GLY:H	2.18	0.46
1:B:94:TYR:CZ	1:B:352:ALA:HB2	2.50	0.46
2:C:144:VAL:O	2:C:144:VAL:HG13	2.15	0.46
3:F:88:GLN:HB2	3:F:97:PHE:HD1	1.78	0.46
1:A:109:ILE:HG12	1:A:152:VAL:HG11	1.97	0.46
1:A:270:ASN:ND2	1:A:444:LEU:HG	2.31	0.46
1:A:437:GLN:C	1:A:439:THR:H	2.18	0.46
1:B:91:MET:C	1:B:93:GLY:N	2.66	0.46
1:B:198:LEU:HG	1:B:410:ILE:CD1	2.38	0.46
1:B:331:GLY:O	1:B:333:LEU:N	2.48	0.46
2:C:4:LEU:HD12	2:C:4:LEU:HA	1.72	0.46
3:F:49:ASP:O	3:F:50:THR:HB	2.16	0.46
1:A:25:LEU:C	1:A:27:GLU:H	2.19	0.46
1:A:248:PRO:HG2	1:A:251:THR:CG2	2.46	0.46
1:A:272:TRP:O	1:A:276:MET:HB2	2.15	0.46
1:A:444:LEU:O	1:A:444:LEU:HD13	2.16	0.46
1:B:452:THR:HG22	1:B:452:THR:O	2.15	0.46
2:C:38:ARG:HH21	2:C:46:LYS:HZ2	1.63	0.46
3:D:46:TRP:HA	3:D:46:TRP:CE3	2.51	0.46
3:D:73:THR:HG22	3:D:74:ILE:N	2.30	0.46
3:F:7:SER:CB	3:F:8:PRO:CD	2.85	0.46
3:F:116:ILE:HD12	3:F:133:CYS:HB2	1.98	0.46
1:A:287:ASN:HD22	1:A:290:LYS:CG	2.25	0.46
1:B:138:THR:HG22	1:B:143:MET:SD	2.54	0.46
1:B:282:ARG:O	1:B:285:GLY:N	2.49	0.46
2:E:72:ARG:O	2:E:72:ARG:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:ILE:HG23	1:B:176:THR:HG21	1.97	0.46
1:B:440:GLY:O	1:B:441:GLY:O	2.34	0.46
2:C:189:VAL:O	2:C:189:VAL:CG1	2.59	0.46
2:C:210:SER:O	2:C:212:THR:HG23	2.15	0.46
2:E:162:TRP:CZ3	2:E:203:CYS:HB3	2.51	0.46
1:A:358:ALA:N	1:A:359:PRO:HD2	2.30	0.46
1:B:99:LYS:C	1:B:100:TYR:CD1	2.90	0.46
2:E:48:ILE:HG22	2:E:49:GLY:N	2.31	0.46
2:E:66:ASP:O	2:E:67:LYS:C	2.54	0.46
3:F:29:VAL:HG23	3:F:70:TYR:CE1	2.50	0.46
1:A:136:LEU:HD12	1:A:136:LEU:N	2.31	0.46
1:A:294:MET:O	1:A:294:MET:HG2	2.16	0.46
1:A:358:ALA:HB3	1:A:359:PRO:CD	2.46	0.46
1:B:139:LEU:HD13	1:B:147:ARG:HB3	1.97	0.46
3:D:105:ILE:HD12	3:D:170:SER:OG	2.16	0.46
3:F:82:ALA:HB2	3:F:105:ILE:CG1	2.45	0.46
1:A:203:GLU:CD	1:B:28:ARG:HH22	2.20	0.45
1:B:94:TYR:HE2	1:B:350:SER:O	1.99	0.45
1:B:305:LEU:HA	1:B:308:VAL:CG2	2.37	0.45
1:B:312:THR:HG22	1:B:339:ALA:CB	2.46	0.45
2:E:4:LEU:HD12	2:E:4:LEU:HA	1.73	0.45
3:F:64:SER:OG	3:F:65:GLY:N	2.49	0.45
3:F:79:ALA:CA	3:F:105:ILE:HD13	2.46	0.45
1:A:359:PRO:O	1:A:363:LEU:HD23	2.17	0.45
1:B:109:ILE:HB	1:B:445:TYR:CE2	2.51	0.45
2:C:196:TRP:HD1	2:C:201:VAL:HG23	1.81	0.45
3:D:29:VAL:HG23	3:D:70:TYR:CE1	2.50	0.45
1:A:74:ASN:HB3	1:A:77:LEU:HB3	1.97	0.45
1:A:97:VAL:HG12	1:A:98:ARG:N	2.31	0.45
1:A:430:LEU:HD21	1:B:220:ILE:CG1	2.38	0.45
3:F:19:VAL:HG12	3:F:74:ILE:HB	1.99	0.45
1:A:192:ALA:HB1	1:A:414:GLU:CG	2.46	0.45
1:A:270:ASN:HA	1:A:273:VAL:HG12	1.97	0.45
2:C:45:LEU:H	2:C:45:LEU:CD1	2.07	0.45
2:C:196:TRP:CG	2:C:197:PRO:N	2.84	0.45
3:D:22:THR:CG2	3:D:23:CYS:N	2.77	0.45
2:E:196:TRP:CG	2:E:197:PRO:N	2.85	0.45
3:F:90:TRP:CZ2	3:F:95:GLN:NE2	2.84	0.45
1:A:200:ILE:HG22	1:A:201:ILE:H	1.80	0.45
1:A:318:ASN:HD22	1:A:319:LEU:N	2.13	0.45
1:A:385:GLU:O	1:A:386:ALA:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:LEU:HD12	1:B:136:LEU:N	2.31	0.45
1:B:287:ASN:HD22	1:B:290:LYS:CG	2.30	0.45
2:C:109:ASP:CG	2:C:110:VAL:HG23	2.37	0.45
3:D:65:GLY:CA	3:D:70:TYR:HA	2.44	0.45
1:A:94:TYR:CZ	1:A:352:ALA:HB2	2.51	0.45
1:A:413:LEU:CD1	1:A:422:ILE:HD13	2.46	0.45
1:B:270:ASN:ND2	1:B:444:LEU:CG	2.79	0.45
2:C:64:LEU:N	2:C:64:LEU:HD23	2.32	0.45
2:E:64:LEU:O	2:E:65:LYS:C	2.55	0.45
2:E:207:HIS:ND1	2:E:210:SER:CB	2.79	0.45
3:F:22:THR:CG2	3:F:23:CYS:N	2.78	0.45
1:B:116:LEU:HD23	1:B:178:LEU:HD23	1.99	0.45
1:B:402:ILE:HG12	1:B:402:ILE:O	2.16	0.45
2:E:45:LEU:HD11	3:F:86:TYR:CE1	2.51	0.45
1:A:123:ARG:HD2	1:A:125:TRP:HZ2	1.82	0.45
1:A:298:ILE:HG23	1:A:346:LEU:HG	1.98	0.45
1:A:423:LEU:HB3	1:A:424:PRO:CD	2.44	0.45
1:B:123:ARG:HD2	1:B:125:TRP:CZ2	2.52	0.45
1:B:270:ASN:ND2	1:B:444:LEU:HG	2.31	0.45
2:C:2:VAL:O	2:C:2:VAL:HG13	2.16	0.45
1:A:116:LEU:HD23	1:A:178:LEU:HD23	1.98	0.45
1:B:90:ALA:CB	1:B:299:GLY:HA3	2.46	0.45
1:B:183:ALA:C	1:B:185:GLY:N	2.68	0.45
1:B:298:ILE:HG21	1:B:346:LEU:HG	1.98	0.45
3:D:201:THR:CG2	3:D:202:SER:N	2.79	0.45
2:E:149:LEU:HD12	2:E:150:VAL:N	2.32	0.45
1:A:399:ALA:O	1:A:403:ARG:HA	2.17	0.45
1:A:420:GLN:H	1:A:420:GLN:HG3	1.49	0.45
1:B:343:THR:O	1:B:347:CYS:HB2	2.17	0.45
1:B:359:PRO:O	1:B:363:LEU:HD23	2.17	0.45
2:C:146:LEU:HD13	2:C:218:ILE:HG21	1.98	0.45
2:E:131:PRO:HB3	2:E:216:LYS:HG3	1.99	0.45
3:F:48:TYR:CE1	3:F:52:LYS:HD2	2.52	0.45
3:F:149:ILE:HG12	3:F:191:TYR:CE2	2.52	0.45
1:A:167:ARG:HG2	1:A:167:ARG:HH11	1.82	0.44
1:A:208:PHE:O	1:A:209:ARG:HB3	2.17	0.44
1:A:270:ASN:ND2	1:A:444:LEU:CD2	2.79	0.44
1:B:37:PHE:O	1:B:37:PHE:CD2	2.71	0.44
1:B:135:GLY:O	1:B:136:LEU:C	2.54	0.44
1:B:421:LEU:O	1:B:424:PRO:CD	2.59	0.44
2:C:99:LEU:HD21	2:C:108:PHE:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:32:ILE:HG12	3:D:70:TYR:CE2	2.52	0.44
1:A:219:PHE:HB3	1:B:430:LEU:HD13	1.99	0.44
1:A:357:PHE:HE1	1:A:398:LEU:HD22	1.78	0.44
1:B:182:ALA:HB3	1:B:200:ILE:HD11	1.98	0.44
1:B:437:GLN:C	1:B:439:THR:H	2.21	0.44
2:C:156:GLU:OE1	2:C:157:PRO:HA	2.17	0.44
2:E:162:TRP:CZ3	2:E:203:CYS:CB	3.00	0.44
1:A:210:TYR:CE1	1:B:208:PHE:HA	2.52	0.44
3:F:58:PRO:C	3:F:60:ARG:N	2.70	0.44
3:F:189:ASN:ND2	3:F:210:ARG:N	2.65	0.44
1:A:21:LEU:HD22	1:A:25:LEU:HG	1.99	0.44
1:B:63:GLN:C	1:B:65:MET:N	2.71	0.44
1:B:272:TRP:N	1:B:272:TRP:CD1	2.83	0.44
2:E:69:ILE:HB	2:E:82:GLN:HB2	1.99	0.44
2:E:167:LEU:HD21	2:E:191:VAL:HG11	1.97	0.44
2:E:178:LEU:HD12	2:E:179:GLN:H	1.82	0.44
3:F:187:ARG:HG3	3:F:187:ARG:O	2.17	0.44
1:A:160:ARG:CD	1:A:163:LEU:HD23	2.47	0.44
1:A:442:LYS:O	1:A:444:LEU:N	2.51	0.44
1:B:163:LEU:CD2	1:B:174:ARG:HA	2.47	0.44
1:B:218:VAL:O	1:B:221:GLY:N	2.50	0.44
1:B:411:LEU:O	1:B:415:MET:HG2	2.17	0.44
3:F:33:HIS:CE1	3:F:49:ASP:H	2.35	0.44
1:A:437:GLN:O	1:A:439:THR:N	2.51	0.44
1:B:383:HIS:HD2	2:E:33:TRP:CE3	2.36	0.44
2:C:29:TYR:CZ	2:C:34:MET:HG3	2.52	0.44
2:C:60:TYR:CD1	2:C:60:TYR:N	2.85	0.44
3:F:86:TYR:HE2	3:F:100:GLY:HA3	1.83	0.44
1:A:37:PHE:HD2	1:A:38:MET:CE	2.28	0.44
1:A:91:MET:HG3	1:A:296:GLY:HA3	1.99	0.44
1:A:382:TYR:HB3	1:A:384:LEU:HD21	1.99	0.44
3:F:35:TYR:CD1	3:F:35:TYR:N	2.85	0.44
3:F:119:PRO:CD	3:F:131:VAL:HG22	2.48	0.44
1:A:109:ILE:HB	1:A:445:TYR:CE2	2.53	0.44
1:A:150:PRO:HD3	1:A:355:GLY:N	2.33	0.44
1:B:369:THR:HG22	1:B:373:MET:HE3	2.00	0.44
3:D:7:SER:CB	3:D:22:THR:HB	2.47	0.44
3:D:53:LEU:HB3	3:D:57:VAL:HB	1.99	0.44
1:A:270:ASN:ND2	1:A:444:LEU:CG	2.81	0.44
1:B:148:GLN:O	1:B:149:GLY:C	2.56	0.44
1:B:248:PRO:HG2	1:B:251:THR:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:GLN:C	1:B:439:THR:N	2.71	0.44
2:C:67:LYS:HA	2:C:67:LYS:HD3	1.77	0.44
2:C:121:SER:O	2:C:122:ALA:C	2.56	0.44
3:D:162:TRP:CD1	3:D:174:MET:HB2	2.53	0.44
2:E:61:THR:HB	2:E:62:PRO:HD2	1.99	0.44
1:A:69:VAL:CG1	1:A:70:HIS:N	2.81	0.43
1:A:155:GLY:HA3	1:A:181:GLY:O	2.17	0.43
1:A:211:THR:HG22	1:A:212:LEU:N	2.33	0.43
1:A:280:LEU:O	1:A:284:HIS:CE1	2.71	0.43
1:A:307:PHE:O	1:A:307:PHE:CG	2.71	0.43
1:B:64:ARG:HB3	1:B:64:ARG:HH11	1.82	0.43
2:C:40:ALA:HB3	2:C:43:LYS:HB2	2.00	0.43
3:D:6:GLN:HG3	3:D:100:GLY:H	1.82	0.43
1:B:224:MET:O	1:B:228:MET:HG2	2.18	0.43
2:C:210:SER:OG	2:C:212:THR:HG23	2.17	0.43
2:E:38:ARG:HE	2:E:46:LYS:HZ1	1.64	0.43
3:F:60:ARG:NH1	3:F:81:ASP:OD1	2.51	0.43
1:A:138:THR:HG21	1:A:352:ALA:HB1	2.00	0.43
1:A:454:ALA:O	1:A:458:ALA:HB3	2.18	0.43
1:B:109:ILE:HG21	1:B:445:TYR:CD2	2.53	0.43
1:B:215:ILE:HG22	1:B:216:LYS:N	2.32	0.43
2:C:162:TRP:C	2:C:164:SER:N	2.71	0.43
2:E:67:LYS:HA	2:E:67:LYS:HD3	1.65	0.43
1:A:128:LEU:HB2	1:A:129:PRO:HD2	2.00	0.43
1:A:136:LEU:HD12	1:A:136:LEU:H	1.82	0.43
1:A:398:LEU:O	1:A:402:ILE:HG23	2.18	0.43
1:B:148:GLN:HG2	1:B:358:ALA:HB2	1.99	0.43
1:B:446:SER:O	1:B:449:LEU:N	2.51	0.43
2:C:185:LEU:C	2:C:185:LEU:CD1	2.87	0.43
1:A:250:ASN:ND2	2:C:105:TYR:CD1	2.82	0.43
1:A:266:GLY:HA3	1:A:400:ALA:CB	2.47	0.43
1:A:372:GLY:O	1:A:376:VAL:HG23	2.18	0.43
1:B:116:LEU:CD2	1:B:178:LEU:HD23	2.48	0.43
1:B:136:LEU:H	1:B:136:LEU:CD1	2.31	0.43
1:B:337:PHE:CE1	1:B:363:LEU:HD12	2.54	0.43
1:A:279:LEU:HD23	1:A:279:LEU:O	2.18	0.43
1:B:126:ARG:O	1:B:130:VAL:HG23	2.19	0.43
1:B:187:ALA:C	1:B:189:ALA:N	2.72	0.43
1:A:90:ALA:CB	1:A:299:GLY:HA3	2.49	0.43
1:A:136:LEU:O	1:A:140:GLY:N	2.51	0.43
1:A:148:GLN:HB3	1:A:190:PHE:CE1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ALA:HB1	1:A:204:MET:HE2	2.00	0.43
1:A:28:ARG:HH22	1:B:203:GLU:CD	2.22	0.43
1:A:99:LYS:C	1:A:100:TYR:CD1	2.91	0.43
1:A:305:LEU:C	1:A:307:PHE:H	2.22	0.43
1:B:21:LEU:CD2	1:B:25:LEU:HG	2.49	0.43
1:B:298:ILE:HG23	1:B:346:LEU:HG	1.99	0.43
1:B:457:GLU:O	1:B:458:ALA:CB	2.66	0.43
2:C:167:LEU:HD21	2:C:191:VAL:HG11	2.00	0.43
2:E:4:LEU:HB3	2:E:112:GLY:CA	2.48	0.43
3:F:82:ALA:CB	3:F:105:ILE:HD11	2.41	0.43
1:A:367:LEU:HD12	1:A:367:LEU:O	2.19	0.43
1:A:380:PRO:CD	1:A:381:GLN:HE22	2.30	0.43
1:B:223:ILE:HG22	1:B:227:ILE:HD13	2.01	0.43
1:B:250:ASN:HD22	2:E:105:TYR:HE1	1.62	0.43
1:B:264:ILE:HG13	1:B:265:PHE:N	2.33	0.43
2:C:16:GLY:O	2:C:86:VAL:HG13	2.18	0.43
2:E:125:THR:HA	2:E:126:PRO:HD2	1.94	0.43
3:F:79:ALA:O	3:F:105:ILE:CD1	2.66	0.43
1:B:78:LEU:HD13	1:B:307:PHE:CE2	2.54	0.43
1:B:92:PHE:CD1	1:B:92:PHE:C	2.93	0.43
1:B:284:HIS:C	1:B:286:GLY:H	2.21	0.43
1:B:308:VAL:O	1:B:309:ALA:HB2	2.19	0.43
2:E:178:LEU:HB2	2:E:183:TYR:CE2	2.54	0.43
1:A:210:TYR:N	1:B:210:TYR:HB2	2.34	0.42
1:A:210:TYR:HB2	1:B:210:TYR:N	2.33	0.42
1:A:430:LEU:O	1:A:432:ALA:N	2.52	0.42
1:B:208:PHE:O	1:B:209:ARG:HB3	2.19	0.42
1:B:293:LEU:C	1:B:295:GLY:H	2.22	0.42
1:B:307:PHE:O	1:B:307:PHE:CG	2.71	0.42
1:B:394:MET:O	1:B:394:MET:HG2	2.19	0.42
2:E:29:TYR:OH	2:E:34:MET:HG3	2.18	0.42
1:A:256:LEU:HD12	1:A:256:LEU:HA	1.86	0.42
1:A:295:GLY:C	1:A:297:ALA:N	2.73	0.42
2:C:131:PRO:HB3	2:C:216:LYS:HG3	2.01	0.42
2:E:51:ILE:CD1	2:E:72:ARG:HD2	2.49	0.42
1:A:78:LEU:HD13	1:A:307:PHE:CZ	2.55	0.42
1:B:89:LEU:HD23	1:B:89:LEU:HA	1.92	0.42
1:B:320:ILE:HD13	1:B:394:MET:CE	2.49	0.42
1:B:444:LEU:HD13	1:B:444:LEU:O	2.20	0.42
2:C:107:TYR:CD1	2:C:107:TYR:C	2.93	0.42
1:A:282:ARG:O	1:A:285:GLY:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:27:PHE:HE2	2:E:98:ARG:HG3	1.85	0.42
3:F:84:THR:OG1	3:F:102:LYS:HG3	2.19	0.42
1:A:17:ARG:C	1:A:19:ARG:N	2.73	0.42
1:A:190:PHE:HE2	1:A:361:LEU:HD11	1.84	0.42
1:A:234:HIS:NE2	3:F:52:LYS:NZ	2.67	0.42
1:A:317:PHE:HD2	1:A:317:PHE:HA	1.71	0.42
3:D:112:PRO:HB3	3:D:138:PHE:HB3	2.01	0.42
3:D:118:PRO:HB3	3:D:208:PHE:CE1	2.55	0.42
2:E:33:TRP:CE2	2:E:52:ASN:HB2	2.55	0.42
1:A:171:ASP:CB	1:A:212:LEU:HD22	2.49	0.42
1:B:128:LEU:HB2	1:B:129:PRO:HD2	2.02	0.42
1:B:207:GLN:HB3	1:B:208:PHE:CE1	2.54	0.42
1:B:276:MET:O	1:B:280:LEU:HB2	2.20	0.42
2:E:126:PRO:CB	2:E:210:SER:OG	2.62	0.42
1:A:434:LEU:HD22	1:A:434:LEU:HA	1.92	0.42
1:B:155:GLY:O	1:B:158:ILE:N	2.50	0.42
2:E:38:ARG:HH21	2:E:46:LYS:HZ2	1.66	0.42
3:F:90:TRP:CH2	3:F:95:GLN:NE2	2.88	0.42
3:F:162:TRP:CD2	3:F:174:MET:HG3	2.54	0.42
1:A:95:PHE:O	1:A:97:VAL:N	2.53	0.42
1:A:159:GLY:O	1:A:162:VAL:HG22	2.19	0.42
1:A:395:GLY:O	1:A:398:LEU:HB2	2.20	0.42
1:A:422:ILE:CG2	1:A:423:LEU:N	2.83	0.42
1:A:437:GLN:C	1:A:439:THR:N	2.73	0.42
3:D:89:GLN:CD	3:D:89:GLN:C	2.78	0.42
3:D:116:ILE:HD12	3:D:193:CYS:HB2	2.02	0.42
2:E:64:LEU:N	2:E:64:LEU:HD23	2.34	0.42
1:A:116:LEU:HD23	1:A:178:LEU:CD2	2.50	0.42
1:A:191:ASN:HB2	1:A:229:TYR:CE2	2.55	0.42
1:B:228:MET:O	1:B:232:PHE:HD1	2.03	0.42
3:F:82:ALA:O	3:F:83:ALA:HB2	2.19	0.42
3:F:114:VAL:CG1	3:F:115:SER:N	2.83	0.42
3:F:192:THR:CB	3:F:207:SER:HB3	2.48	0.42
1:A:91:MET:O	1:A:93:GLY:N	2.53	0.42
1:A:190:PHE:CD1	1:A:190:PHE:N	2.87	0.42
1:A:190:PHE:HD2	1:A:415:MET:SD	2.42	0.42
1:A:270:ASN:HA	1:A:270:ASN:HD22	1.58	0.42
1:A:276:MET:O	1:A:280:LEU:HB2	2.20	0.42
1:A:380:PRO:CD	1:A:381:GLN:NE2	2.83	0.42
1:B:69:VAL:CG1	1:B:70:HIS:N	2.83	0.42
1:B:80:THR:O	1:B:83:PHE:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:PHE:O	1:B:96:LEU:C	2.58	0.42
1:B:190:PHE:HE2	1:B:361:LEU:HD11	1.85	0.42
2:E:76:LYS:O	2:E:77:ASP:C	2.58	0.42
2:E:179:GLN:O	2:E:180:ALA:HB3	2.20	0.42
3:F:117:PHE:HA	3:F:118:PRO:HD3	1.79	0.42
1:B:98:ARG:HH11	1:B:98:ARG:CB	2.15	0.41
1:B:172:GLU:HG2	1:B:212:LEU:O	2.20	0.41
2:C:181:ALA:O	2:C:182:LEU:HD23	2.20	0.41
1:A:215:ILE:HG22	1:A:216:LYS:N	2.35	0.41
1:B:258:LEU:O	1:B:258:LEU:HG	2.20	0.41
1:B:283:VAL:HG12	1:B:283:VAL:O	2.19	0.41
2:C:29:TYR:CD2	2:C:77:ASP:HA	2.56	0.41
2:C:176:ALA:HA	2:C:185:LEU:HB3	2.02	0.41
3:D:35:TYR:HE1	3:D:88:GLN:HB3	1.86	0.41
2:E:99:LEU:HD21	2:E:108:PHE:CD2	2.55	0.41
2:E:131:PRO:HD3	2:E:216:LYS:HG2	2.01	0.41
3:F:6:GLN:HE21	3:F:6:GLN:HB3	1.64	0.41
1:A:337:PHE:HE1	1:A:363:LEU:HD12	1.84	0.41
1:A:427:ILE:O	1:A:427:ILE:HG22	2.20	0.41
1:B:255:TYR:CG	1:B:424:PRO:HB3	2.55	0.41
2:C:196:TRP:O	2:C:198:SER:N	2.52	0.41
2:E:32:TYR:O	2:E:72:ARG:NH2	2.53	0.41
2:E:107:TYR:CB	3:F:33:HIS:CD2	2.95	0.41
2:E:151:LYS:HB2	2:E:151:LYS:HE3	1.78	0.41
3:F:73:THR:CG2	3:F:74:ILE:N	2.83	0.41
1:A:78:LEU:O	1:A:79:LEU:C	2.59	0.41
1:A:223:ILE:CG2	1:A:227:ILE:HD13	2.51	0.41
1:B:167:ARG:HG2	1:B:167:ARG:HH11	1.85	0.41
1:B:218:VAL:O	1:B:219:PHE:C	2.58	0.41
2:C:66:ASP:O	2:C:67:LYS:C	2.58	0.41
2:C:132:LEU:HD21	3:D:132:VAL:CG2	2.50	0.41
3:D:22:THR:CG2	3:D:23:CYS:H	2.32	0.41
3:F:33:HIS:O	3:F:87:CYS:HA	2.20	0.41
3:F:47:ILE:HG22	3:F:48:TYR:N	2.35	0.41
3:F:115:SER:CB	3:F:117:PHE:HE1	2.34	0.41
1:A:443:PRO:O	1:A:445:TYR:N	2.54	0.41
1:B:110:PRO:HG2	1:B:448:ILE:HG21	2.02	0.41
1:B:198:LEU:CD1	1:B:406:LEU:HG	2.51	0.41
1:B:199:PHE:CD1	1:B:407:THR:HG21	2.55	0.41
2:E:38:ARG:NE	2:E:46:LYS:HZ1	2.18	0.41
2:E:72:ARG:NH1	2:E:72:ARG:HG3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:86:TYR:CE2	3:F:100:GLY:HA3	2.54	0.41
3:F:95:GLN:N	3:F:95:GLN:CD	2.71	0.41
1:A:30:LYS:NZ	1:B:442:LYS:HE2	2.35	0.41
1:A:96:LEU:O	1:A:100:TYR:HB2	2.20	0.41
1:A:148:GLN:O	1:A:149:GLY:C	2.59	0.41
1:A:250:ASN:ND2	2:C:105:TYR:HD1	2.17	0.41
1:A:369:THR:HG22	1:A:373:MET:HE3	2.01	0.41
1:A:430:LEU:O	1:A:431:GLY:C	2.57	0.41
1:B:148:GLN:HB3	1:B:190:PHE:CE1	2.56	0.41
1:B:420:GLN:HE21	1:B:420:GLN:HB2	1.62	0.41
3:D:189:ASN:ND2	3:D:210:ARG:N	2.68	0.41
3:F:4:LEU:HD11	3:F:89:GLN:HG3	2.03	0.41
1:A:250:ASN:HD22	2:C:105:TYR:HD1	1.61	0.41
1:B:293:LEU:C	1:B:295:GLY:N	2.72	0.41
1:B:380:PRO:CD	1:B:381:GLN:NE2	2.82	0.41
2:E:109:ASP:OD2	2:E:110:VAL:HG23	2.21	0.41
1:A:47:GLY:O	1:A:48:LEU:C	2.58	0.41
1:B:191:ASN:ND2	1:B:191:ASN:O	2.53	0.41
1:B:267:PRO:O	1:B:270:ASN:N	2.53	0.41
1:B:273:VAL:HG11	1:B:444:LEU:HD21	2.03	0.41
2:C:99:LEU:HD21	2:C:108:PHE:CE2	2.55	0.41
3:D:127:GLY:HA2	3:D:182:LYS:HB2	2.02	0.41
2:E:134:PRO:HD3	2:E:146:LEU:CD2	2.51	0.41
3:F:57:VAL:HA	3:F:58:PRO:HD3	1.95	0.41
1:A:63:GLN:N	1:A:63:GLN:OE1	2.53	0.41
1:A:86:SER:HB2	1:A:300:GLY:HA2	2.02	0.41
1:A:205:ARG:HA	1:A:206:PRO:HD2	1.92	0.41
1:A:394:MET:O	1:A:394:MET:HG2	2.21	0.41
1:B:91:MET:HG3	1:B:296:GLY:HA3	2.02	0.41
1:B:247:ALA:HA	1:B:248:PRO:HD2	1.76	0.41
1:B:402:ILE:O	1:B:402:ILE:CG1	2.69	0.41
2:C:124:THR:CG2	2:C:125:THR:H	2.32	0.41
3:D:86:TYR:HE2	3:D:100:GLY:HA3	1.83	0.41
2:E:18:LEU:HD11	2:E:117:VAL:CG1	2.51	0.41
2:E:38:ARG:HE	2:E:46:LYS:HE3	1.86	0.41
3:F:90:TRP:CG	3:F:95:GLN:HB3	2.56	0.41
3:F:202:SER:HA	3:F:203:PRO:HD2	1.92	0.41
1:A:21:LEU:CD2	1:A:25:LEU:HG	2.51	0.41
1:A:63:GLN:C	1:A:65:MET:N	2.74	0.41
1:A:75:TYR:CB	1:A:76:PRO:HD3	2.37	0.41
1:B:270:ASN:HA	1:B:273:VAL:CG1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:ASN:HB3	1:B:290:LYS:HB2	2.02	0.41
1:B:331:GLY:C	1:B:333:LEU:N	2.75	0.41
3:F:125:THR:O	3:F:125:THR:HG22	2.21	0.41
1:A:198:LEU:CD1	1:A:406:LEU:HG	2.51	0.40
1:B:150:PRO:CG	1:B:354:GLY:HA2	2.51	0.40
1:B:270:ASN:HA	1:B:273:VAL:HG12	2.02	0.40
1:B:337:PHE:O	1:B:341:VAL:HG23	2.21	0.40
3:D:66:SER:O	3:D:68:THR:N	2.54	0.40
3:D:149:ILE:HG12	3:D:191:TYR:CE2	2.56	0.40
2:E:33:TRP:CZ2	2:E:52:ASN:HB2	2.57	0.40
1:A:33:LEU:HD23	1:A:33:LEU:O	2.21	0.40
1:A:210:TYR:H	1:B:210:TYR:HB2	1.87	0.40
1:A:312:THR:HG22	1:A:339:ALA:HB3	2.02	0.40
1:B:166:PHE:C	1:B:167:ARG:HG2	2.42	0.40
1:B:211:THR:HG22	1:B:212:LEU:H	1.86	0.40
1:B:437:GLN:O	1:B:439:THR:N	2.54	0.40
2:C:103:TYR:CD2	3:D:31:TYR:CE2	3.09	0.40
3:D:58:PRO:C	3:D:60:ARG:N	2.74	0.40
2:E:174:PHE:HA	2:E:175:PRO:HD3	1.96	0.40
3:F:59:VAL:HG12	3:F:59:VAL:O	2.21	0.40
3:F:125:THR:O	3:F:126:SER:HB3	2.22	0.40
3:F:178:LEU:HD12	3:F:179:THR:N	2.36	0.40
1:A:193:PRO:HA	1:A:222:VAL:CG1	2.52	0.40
1:A:282:ARG:C	1:A:284:HIS:H	2.25	0.40
1:B:109:ILE:HG21	1:B:445:TYR:HD2	1.85	0.40
1:B:148:GLN:O	1:B:151:THR:N	2.51	0.40
1:B:279:LEU:HD23	1:B:279:LEU:C	2.41	0.40
3:D:74:ILE:CG2	3:D:77:MET:HA	2.51	0.40
3:D:184:GLU:O	3:D:187:ARG:HG2	2.22	0.40
2:E:51:ILE:HD13	2:E:72:ARG:HD2	2.02	0.40
3:F:113:THR:HG22	3:F:113:THR:O	2.21	0.40
1:A:223:ILE:HG22	1:A:227:ILE:HD13	2.02	0.40
1:B:197:ILE:CG1	1:B:222:VAL:HG21	2.51	0.40
1:B:250:ASN:ND2	2:E:105:TYR:HD1	2.19	0.40
1:B:270:ASN:HA	1:B:270:ASN:HD22	1.57	0.40
3:D:64:SER:OG	3:D:65:GLY:N	2.54	0.40
2:E:107:TYR:CD1	2:E:107:TYR:C	2.95	0.40
1:A:89:LEU:HD23	1:A:89:LEU:HA	1.86	0.40
1:A:109:ILE:CG2	1:A:445:TYR:HD2	2.34	0.40
1:A:136:LEU:H	1:A:136:LEU:CD1	2.34	0.40
1:B:139:LEU:O	1:B:142:GLY:N	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:ARG:O	1:B:455:LYS:HB2	2.21	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	442/473 (93%)	311 (70%)	103 (23%)	28 (6%)	1	8
1	B	439/473 (93%)	296 (67%)	111 (25%)	32 (7%)	1	6
2	C	219/222 (99%)	174 (80%)	35 (16%)	10 (5%)	2	15
2	E	219/222 (99%)	180 (82%)	28 (13%)	11 (5%)	2	13
3	D	209/211 (99%)	169 (81%)	27 (13%)	13 (6%)	1	9
3	F	209/211 (99%)	165 (79%)	36 (17%)	8 (4%)	3	19
All	All	1737/1812 (96%)	1295 (75%)	340 (20%)	102 (6%)	1	10

All (102) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	PHE
1	A	171	ASP
1	A	201	ILE
1	A	283	VAL
1	A	307	PHE
1	A	309	ALA
1	A	386	ALA
1	B	132	PHE
1	B	171	ASP
1	B	201	ILE
1	B	283	VAL

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Mol	Chain	Res	Type
1	B	309	ALA
1	B	441	GLY
1	B	444	LEU
2	C	65	LYS
2	C	106	TRP
2	C	140	ALA
3	D	7	SER
3	D	67	GLY
3	D	126	SER
3	D	153	GLU
2	E	65	LYS
2	E	106	TRP
2	E	122	ALA
2	E	140	ALA
3	F	7	SER
3	F	67	GLY
3	F	112	PRO
3	F	126	SER
1	A	102	PRO
1	A	314	GLY
1	A	441	GLY
1	A	444	LEU
1	B	102	PRO
1	B	307	PHE
1	B	314	GLY
1	B	332	MET
1	B	351	GLY
1	B	386	ALA
1	B	443	PRO
2	C	9	GLY
3	D	105	ILE
2	E	9	GLY
3	F	153	GLU
1	A	96	LEU
1	A	189	ALA
1	A	337	PHE
1	A	438	PHE
1	A	443	PRO
1	A	447	ALA
1	B	92	PHE
1	B	96	LEU
1	B	188	ALA

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Mol	Chain	Res	Type
2	C	31	ARG
2	C	53	PRO
2	C	109	ASP
2	C	196	TRP
3	D	154	ARG
3	F	113	THR
3	F	154	ARG
1	A	107	SER
1	A	419	TYR
1	B	95	PHE
1	B	107	SER
1	B	128	LEU
1	B	447	ALA
2	C	157	PRO
3	D	15	PRO
3	D	55	SER
3	D	83	ALA
3	D	199	THR
2	E	31	ARG
2	E	64	LEU
1	A	95	PHE
1	A	128	LEU
1	B	26	LEU
1	B	64	ARG
1	B	285	GLY
1	B	337	PHE
1	B	405	PRO
3	D	51	SER
3	D	137	ASN
2	E	53	PRO
2	E	196	TRP
1	A	242	GLY
1	A	412	VAL
1	B	59	TRP
1	B	101	ALA
1	B	422	ILE
3	D	80	GLU
3	F	15	PRO
1	A	376	VAL
1	B	200	ILE
2	C	54	VAL
1	A	200	ILE

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Mol	Chain	Res	Type
1	B	121	PRO
1	A	101	ALA
1	A	285	GLY
2	E	14	PRO
1	A	405	PRO
1	B	338	VAL
2	E	157	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	335/358 (94%)	305 (91%)	30 (9%)	9	34
1	B	332/358 (93%)	304 (92%)	28 (8%)	11	38
2	C	181/182 (100%)	163 (90%)	18 (10%)	8	29
2	E	181/182 (100%)	162 (90%)	19 (10%)	7	26
3	D	185/185 (100%)	177 (96%)	8 (4%)	29	62
3	F	185/185 (100%)	173 (94%)	12 (6%)	17	47
All	All	1399/1450 (96%)	1284 (92%)	115 (8%)	11	38

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	21	LEU
1	A	48	LEU
1	A	63	GLN
1	A	98	ARG
1	A	120	ARG
1	A	138	THR
1	A	167	ARG
1	A	171	ASP
1	A	172	GLU
1	A	178	LEU

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Mol	Chain	Res	Type
1	A	180	THR
1	A	207	GLN
1	A	208	PHE
1	A	212	LEU
1	A	215	ILE
1	A	230	ARG
1	A	274	LEU
1	A	304	LEU
1	A	317	PHE
1	A	318	ASN
1	A	340	ARG
1	A	347	CYS
1	A	379	PHE
1	A	381	GLN
1	A	391	ILE
1	A	397	LEU
1	A	420	GLN
1	A	434	LEU
1	A	451	ARG
1	B	21	LEU
1	B	48	LEU
1	B	63	GLN
1	B	98	ARG
1	B	120	ARG
1	B	138	THR
1	B	167	ARG
1	B	171	ASP
1	B	172	GLU
1	B	180	THR
1	B	198	LEU
1	B	207	GLN
1	B	208	PHE
1	B	212	LEU
1	B	215	ILE
1	B	230	ARG
1	B	274	LEU
1	B	304	LEU
1	B	317	PHE
1	B	318	ASN
1	B	340	ARG
1	B	347	CYS
1	B	379	PHE

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Mol	Chain	Res	Type
1	B	381	GLN
1	B	397	LEU
1	B	420	GLN
1	B	434	LEU
1	B	451	ARG
2	C	4	LEU
2	C	18	LEU
2	C	27	PHE
2	C	41	PRO
2	C	45	LEU
2	C	61	THR
2	C	67	LYS
2	C	72	ARG
2	C	77	ASP
2	C	107	TYR
2	C	115	THR
2	C	157	PRO
2	C	172	HIS
2	C	185	LEU
2	C	200	THR
2	C	203	CYS
2	C	204	ASN
2	C	221	ARG
3	D	28	SER
3	D	46	TRP
3	D	75	ASN
3	D	77	MET
3	D	88	GLN
3	D	117	PHE
3	D	146	LYS
3	D	189	ASN
2	E	4	LEU
2	E	27	PHE
2	E	45	LEU
2	E	61	THR
2	E	67	LYS
2	E	72	ARG
2	E	77	ASP
2	E	98	ARG
2	E	107	TYR
2	E	124	THR
2	E	127	PRO

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Mol	Chain	Res	Type
2	E	157	PRO
2	E	167	LEU
2	E	172	HIS
2	E	185	LEU
2	E	186	SER
2	E	200	THR
2	E	203	CYS
2	E	204	ASN
3	F	1	ASP
3	F	15	PRO
3	F	28	SER
3	F	46	TRP
3	F	75	ASN
3	F	77	MET
3	F	88	GLN
3	F	102	LYS
3	F	119	PRO
3	F	146	LYS
3	F	189	ASN
3	F	201	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	148	GLN
1	A	157	ASN
1	A	207	GLN
1	A	270	ASN
1	A	277	GLN
1	A	287	ASN
1	A	318	ASN
1	A	327	ASN
1	A	381	GLN
1	A	383	HIS
1	A	437	GLN
1	A	456	GLN
1	A	460	GLN
1	B	62	ASN
1	B	119	GLN
1	B	148	GLN
1	B	157	ASN

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Mol	Chain	Res	Type
1	B	207	GLN
1	B	270	ASN
1	B	277	GLN
1	B	287	ASN
1	B	318	ASN
1	B	327	ASN
1	B	381	GLN
1	B	383	HIS
1	B	437	GLN
1	B	456	GLN
3	D	93	HIS
3	D	136	ASN
3	D	137	ASN
3	D	155	GLN
3	D	189	ASN
2	E	163	ASN
3	F	136	ASN
3	F	137	ASN
3	F	155	GLN
3	F	189	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	121:SER	C	122:ALA	N	1.19

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95th 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 ²)	Q<0.9
1	A	444/473 (93%)	-0.05	6 (1%) 75 56	50, 77, 100, 111	0
1	B	441/473 (93%)	-0.05	5 (1%) 80 64	46, 76, 103, 121	0
2	C	221/222 (99%)	0.11	9 (4%) 37 18	43, 74, 94, 125	0
2	E	221/222 (99%)	0.16	8 (3%) 42 22	40, 75, 95, 116	0
3	D	211/211 (100%)	0.23	2 (0%) 84 69	57, 85, 98, 103	0
3	F	211/211 (100%)	0.16	9 (4%) 35 17	40, 71, 99, 110	0
All	All	1749/1812 (96%)	0.06	39 (2%) 62 41	40, 77, 99, 125	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	72	ALA	5.0
2	C	136	SER	4.7
1	B	235	GLU	3.8
1	A	235	GLU	3.7
3	F	153	GLU	3.5
2	E	135	GLY	3.4
2	C	135	GLY	3.4
2	E	222	ALA	3.2
1	A	19	ARG	3.1
3	F	208	PHE	3.0
1	A	167	ARG	2.9
2	E	134	PRO	2.9
1	B	75	TYR	2.9
3	D	167	SER	2.8
3	D	105	ILE	2.7
3	F	154	ARG	2.6
2	C	142	SER	2.6
1	B	23	ARG	2.5
3	F	190	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	168	LEU	2.4
1	B	358	ALA	2.4
2	C	138	ALA	2.4
2	E	133	ALA	2.3
2	C	137	ALA	2.3
3	F	192	THR	2.3
3	F	183	ASP	2.3
2	C	29	TYR	2.2
3	F	155	GLN	2.2
2	C	103	TYR	2.2
2	E	179	GLN	2.1
3	F	182	LYS	2.1
3	F	211	ALA	2.1
2	C	77	ASP	2.1
1	A	212	LEU	2.0
2	E	136	SER	2.0
2	E	140	ALA	2.0
2	E	221	ARG	2.0
2	C	133	ALA	2.0
1	B	307	PHE	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 monosaccharides 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.