



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 04:31 PM EDT

PDB ID : 2HU0
Title : N1 neuraminidase in complex with oseltamivir 1
Authors : Russell, R.J.; Haire, L.F.; Stevens, D.J.; Collins, P.J.; Lin, Y.P.; Blackburn, G.M.; Hay, A.J.; Gamblin, S.J.; Skehel, J.J.
Deposited on : 2006-07-26
Resolution : 2.95 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
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) : 2.23.2

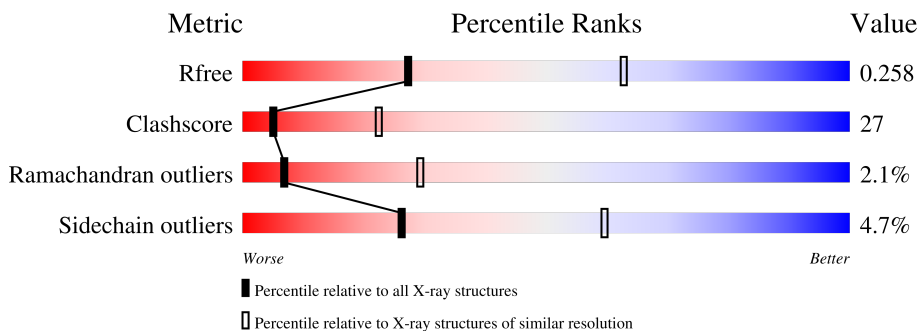
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	387	
1	B	387	
1	C	387	
1	D	387	
1	E	387	
1	F	387	
1	G	387	

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Mol	Chain	Length	Quality of chain
1	H	387	 57% 36% 5% **

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 23716 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.

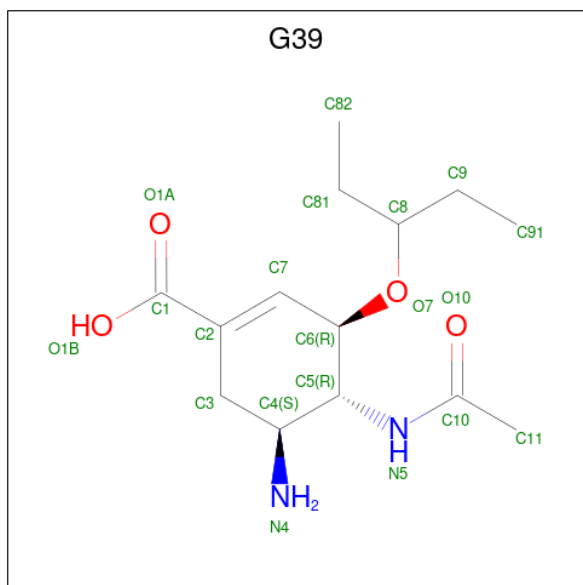
- Molecule 1 is a protein called Neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	385	2962	1858	510	573	21	0	0	0
1	B	385	2962	1858	510	573	21	0	0	0
1	C	385	2962	1858	510	573	21	0	0	0
1	D	385	2962	1858	510	573	21	0	0	0
1	E	385	2962	1858	510	573	21	0	0	0
1	F	385	2962	1858	510	573	21	0	0	0
1	G	385	2962	1858	510	573	21	0	0	0
1	H	385	2962	1858	510	573	21	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	169A	TYR	HIS	engineered mutation	UNP Q6DPL2
B	169A	TYR	HIS	engineered mutation	UNP Q6DPL2
C	169A	TYR	HIS	engineered mutation	UNP Q6DPL2
D	169A	TYR	HIS	engineered mutation	UNP Q6DPL2
E	169A	TYR	HIS	engineered mutation	UNP Q6DPL2
F	169A	TYR	HIS	engineered mutation	UNP Q6DPL2
G	169A	TYR	HIS	engineered mutation	UNP Q6DPL2
H	169A	TYR	HIS	engineered mutation	UNP Q6DPL2

- Molecule 2 is (3R,4R,5S)-4-(acetylamino)-5-amino-3-(pentan-3-yloxy)cyclohex-1-ene-1-carboxylic acid (three-letter code: G39) (formula: C₁₄H₂₄N₂O₄).

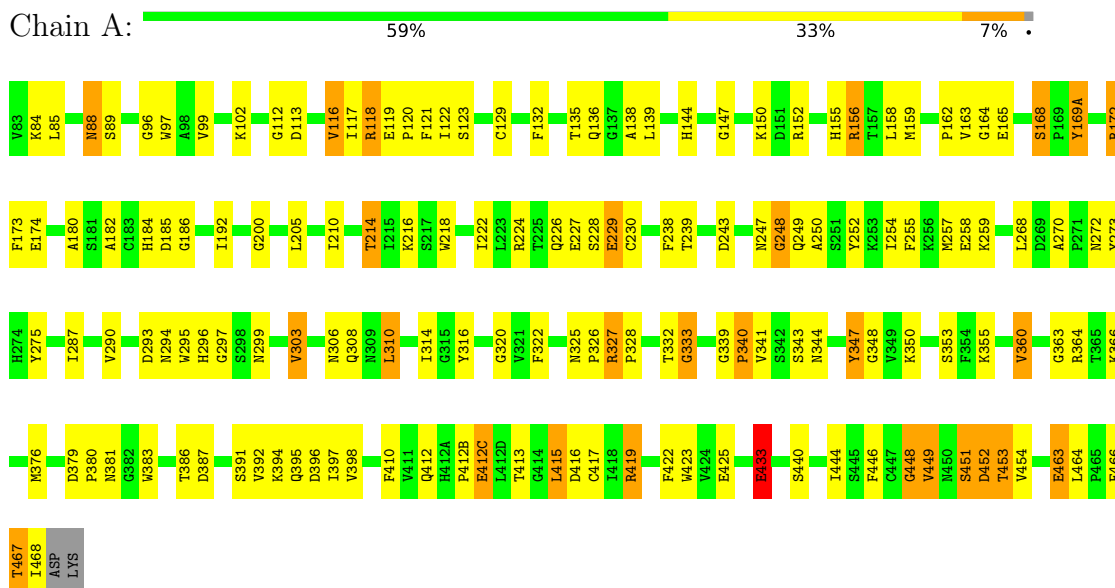


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	B	1	20	14	2	4	0	0

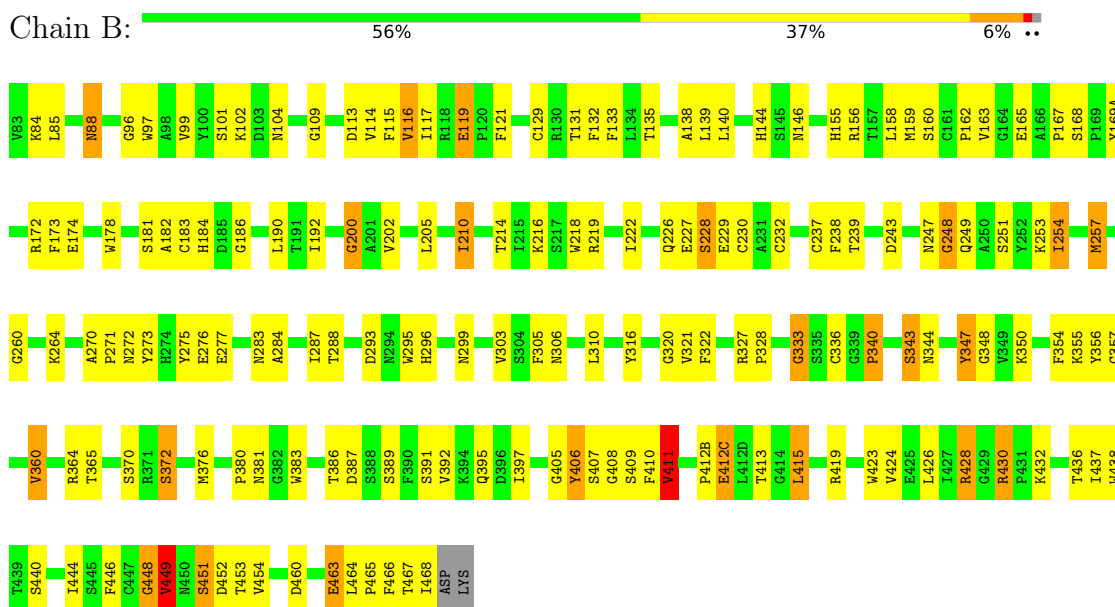
3 Residue-property plots [i](#)

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. 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. 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.

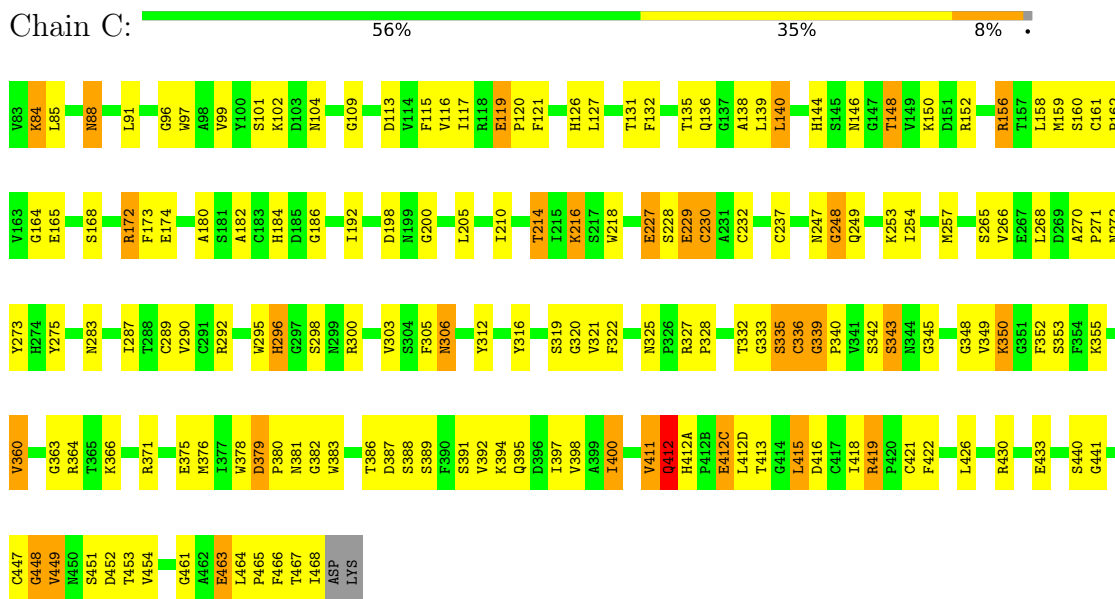
- Molecule 1: Neuraminidase



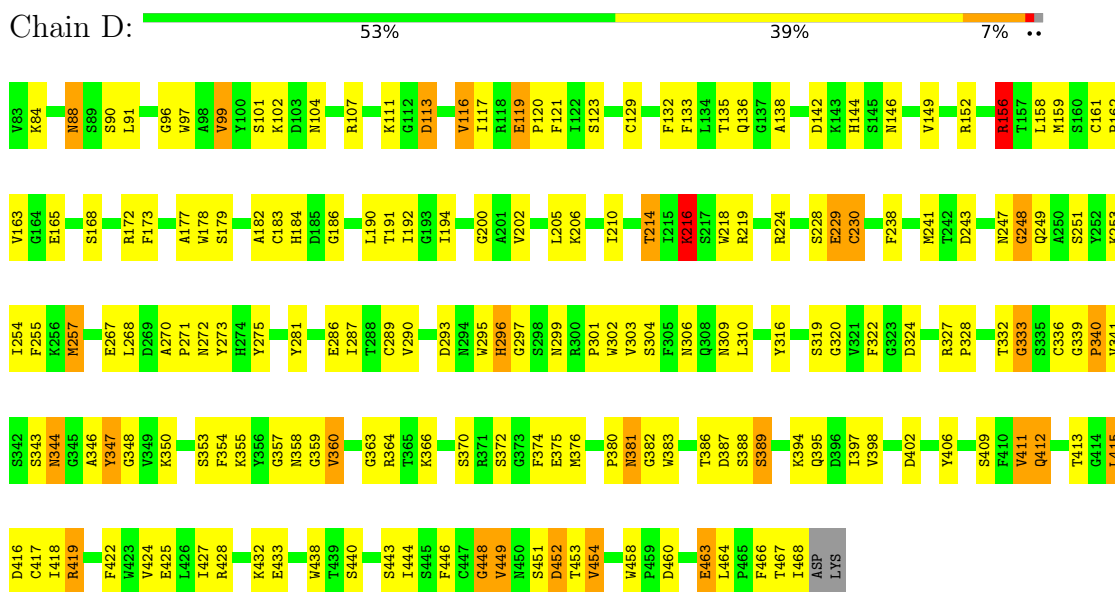
- Molecule 1: Neuraminidase



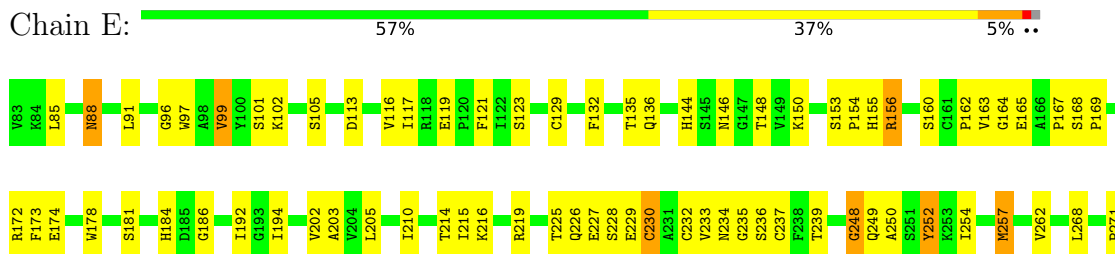
- Molecule 1: Neuraminidase

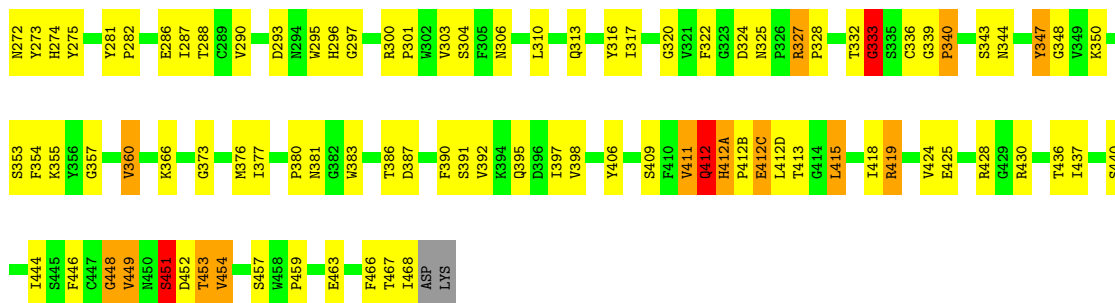


- Molecule 1: Neuraminidase



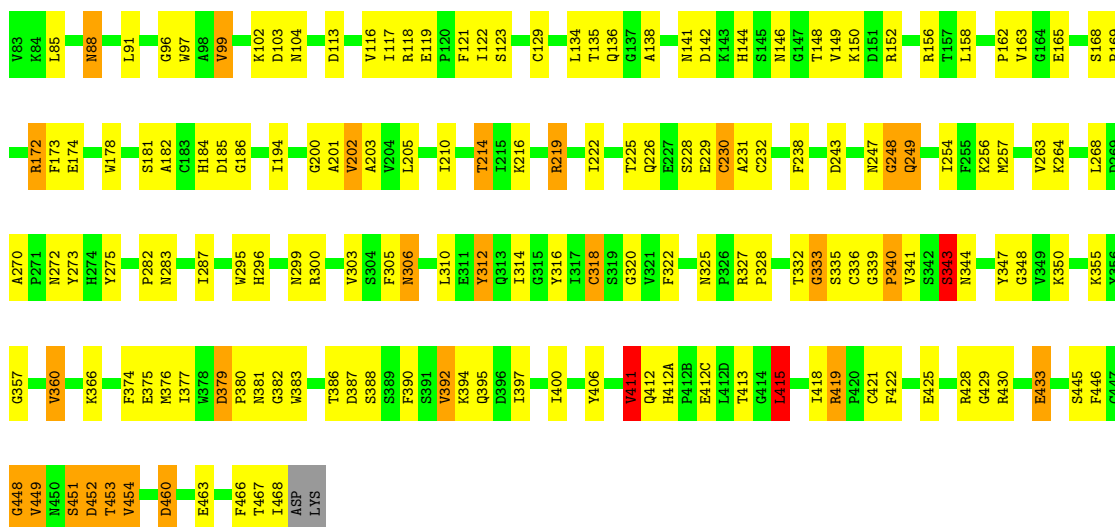
- Molecule 1: Neuraminidase





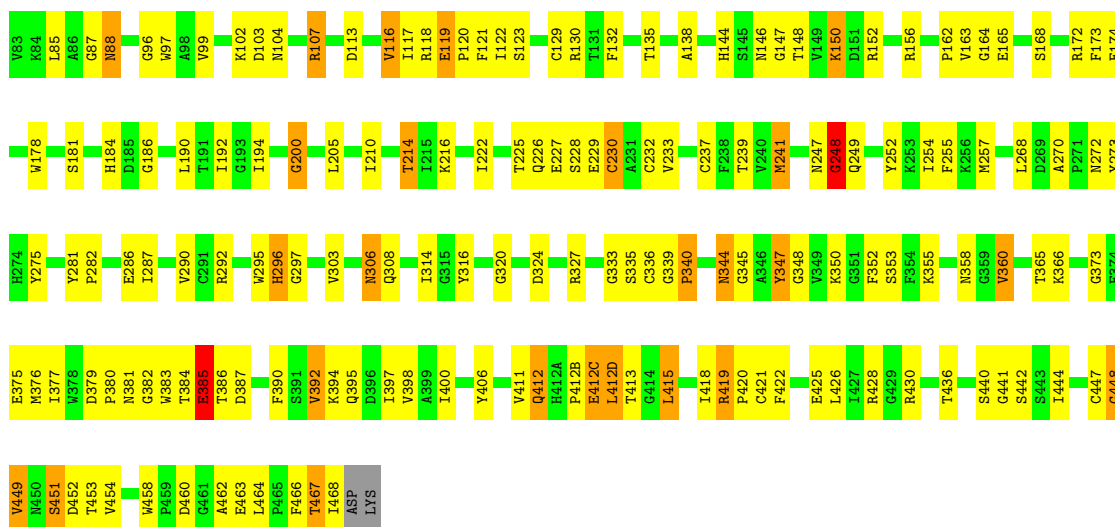
- Molecule 1: Neuraminidase

Chain F: 58% 34% 7% ..



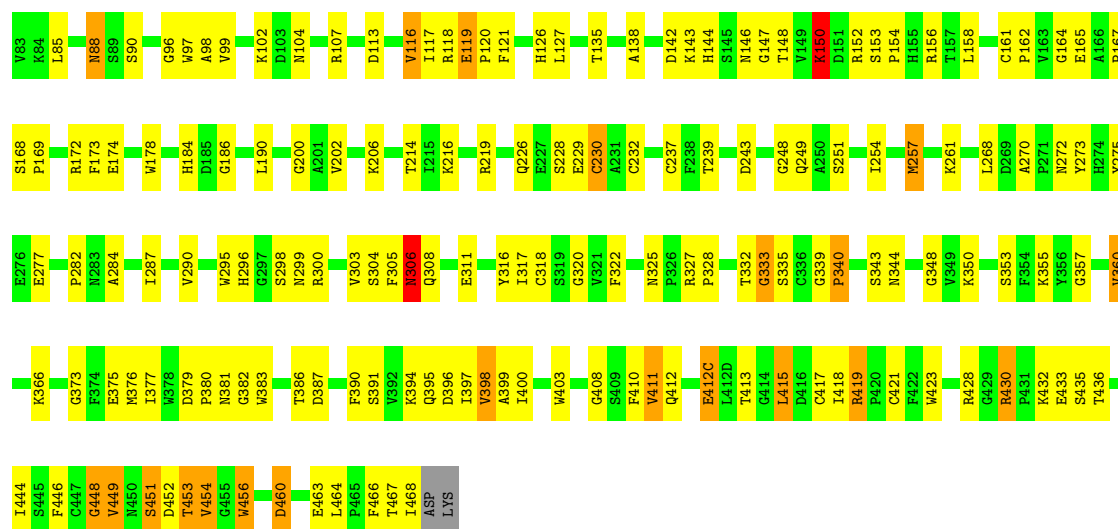
- Molecule 1: Neuraminidase

Chain G: 57% 36% 6% ..



- Molecule 1: Neuraminidase

Chain H:  57% 36% 5% ..



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	198.08Å 200.58Å 210.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	142.86 – 2.95 19.70 – 2.86	Depositor EDS
% Data completeness (in resolution range)	79.1 (142.86-2.95) 77.7 (19.70-2.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.88Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.218 , 0.295 0.255 , 0.258	Depositor DCC
R_{free} test set	3705 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtrriage
Anisotropy	0.061	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , -18.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.023 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	23716	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.80% 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

Bond lengths and bond angles in the following residue types are not validated in this section: G39

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	1.26	7/3045 (0.2%)	1.18	13/4141 (0.3%)
1	B	1.35	13/3045 (0.4%)	1.15	11/4141 (0.3%)
1	C	1.38	19/3045 (0.6%)	1.27	19/4141 (0.5%)
1	D	1.36	16/3045 (0.5%)	1.20	18/4141 (0.4%)
1	E	1.19	6/3045 (0.2%)	1.11	11/4141 (0.3%)
1	F	1.22	9/3045 (0.3%)	1.09	8/4141 (0.2%)
1	G	1.30	12/3045 (0.4%)	1.12	6/4141 (0.1%)
1	H	1.25	8/3045 (0.3%)	1.09	7/4141 (0.2%)
All	All	1.29	90/24360 (0.4%)	1.15	93/33128 (0.3%)

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	A	0	2
1	B	0	1
1	C	0	4
1	D	0	2
1	E	0	3
1	F	0	3
1	G	0	3
1	H	0	3
All	All	0	21

All (90) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	411	VAL	CB-CG2	15.85	1.86	1.52
1	H	150	LYS	CE-NZ	13.79	1.83	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	411	VAL	CB-CG2	12.77	1.79	1.52
1	D	411	VAL	CB-CG2	12.26	1.78	1.52
1	C	336	CYS	C-N	11.22	1.53	1.33
1	C	411	VAL	CB-CG2	11.20	1.76	1.52
1	H	150	LYS	CD-CE	10.98	1.78	1.51
1	H	306	ASN	C-N	10.70	1.58	1.34
1	B	411	VAL	CB-CG1	-9.76	1.32	1.52
1	C	84	LYS	CG-CD	9.09	1.83	1.52
1	B	336	CYS	C-N	8.43	1.48	1.33
1	D	119	GLU	CD-OE1	7.98	1.34	1.25
1	E	333	GLY	C-N	7.91	1.52	1.34
1	F	343	SER	CB-OG	7.87	1.52	1.42
1	D	216	LYS	CD-CE	7.75	1.70	1.51
1	C	84	LYS	CD-CE	7.71	1.70	1.51
1	C	343	SER	CB-OG	7.69	1.52	1.42
1	C	463	GLU	CD-OE2	7.58	1.33	1.25
1	F	333	GLY	C-N	7.53	1.51	1.34
1	C	229	GLU	CB-CG	-7.52	1.37	1.52
1	C	339	GLY	N-CA	7.30	1.57	1.46
1	D	411	VAL	CB-CG1	-7.25	1.37	1.52
1	F	411	VAL	C-N	7.22	1.50	1.34
1	C	335	SER	CB-OG	-7.20	1.32	1.42
1	E	150	LYS	CD-CE	7.17	1.69	1.51
1	C	463	GLU	CD-OE1	7.11	1.33	1.25
1	G	150	LYS	CD-CE	7.02	1.68	1.51
1	C	352	PHE	CB-CG	-6.98	1.39	1.51
1	G	392	VAL	C-N	6.86	1.49	1.34
1	B	392	VAL	C-N	6.81	1.49	1.34
1	G	150	LYS	CE-NZ	6.73	1.65	1.49
1	B	463	GLU	CG-CD	6.72	1.62	1.51
1	H	119	GLU	CB-CG	-6.65	1.39	1.52
1	B	333	GLY	C-N	6.62	1.49	1.34
1	D	346	ALA	CA-CB	6.59	1.66	1.52
1	C	412	GLN	C-N	-6.57	1.19	1.34
1	H	333	GLY	C-N	6.52	1.49	1.34
1	A	229	GLU	CB-CG	-6.51	1.39	1.52
1	A	452	ASP	CB-CG	6.40	1.65	1.51
1	G	385	GLU	CD-OE2	6.40	1.32	1.25
1	B	84	LYS	CD-CE	6.39	1.67	1.51
1	B	356	TYR	CE2-CZ	6.37	1.46	1.38
1	F	312	TYR	CD1-CE1	6.29	1.48	1.39
1	C	227	GLU	CG-CD	6.22	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	412	GLN	CB-CG	6.16	1.69	1.52
1	D	336	CYS	C-N	6.15	1.44	1.33
1	A	84	LYS	CD-CE	6.03	1.66	1.51
1	B	119	GLU	CD-OE1	5.99	1.32	1.25
1	G	281	TYR	CE1-CZ	-5.96	1.30	1.38
1	G	385	GLU	CD-OE1	5.93	1.32	1.25
1	C	229	GLU	CD-OE1	5.93	1.32	1.25
1	C	216	LYS	CD-CE	5.84	1.65	1.51
1	D	84	LYS	CD-CE	5.84	1.65	1.51
1	A	169(A)	TYR	CD2-CE2	-5.79	1.30	1.39
1	B	84	LYS	CG-CD	5.79	1.72	1.52
1	D	463	GLU	CD-OE1	5.79	1.32	1.25
1	A	303	VAL	CB-CG2	-5.77	1.40	1.52
1	D	229	GLU	CB-CG	-5.76	1.41	1.52
1	D	389	SER	C-O	5.76	1.34	1.23
1	F	336	CYS	C-N	5.75	1.43	1.33
1	F	150	LYS	CD-CE	5.75	1.65	1.51
1	G	248	GLY	N-CA	5.75	1.54	1.46
1	D	412	GLN	CB-CG	5.71	1.68	1.52
1	E	412	GLN	C-N	-5.64	1.21	1.34
1	G	119	GLU	CD-OE1	5.63	1.31	1.25
1	H	398	VAL	CB-CG2	-5.61	1.41	1.52
1	E	297	GLY	C-O	5.60	1.32	1.23
1	B	405	GLY	N-CA	5.60	1.54	1.46
1	D	438	TRP	CB-CG	-5.51	1.40	1.50
1	C	216	LYS	CG-CD	5.51	1.71	1.52
1	A	463	GLU	CD-OE2	5.49	1.31	1.25
1	H	306	ASN	C-O	5.47	1.33	1.23
1	G	458	TRP	CG-CD1	5.47	1.44	1.36
1	D	216	LYS	CG-CD	5.41	1.70	1.52
1	D	406	TYR	CG-CD2	5.35	1.46	1.39
1	G	352	PHE	CE2-CZ	5.30	1.47	1.37
1	B	408	GLY	CA-C	-5.29	1.43	1.51
1	F	452	ASP	CB-CG	5.26	1.62	1.51
1	F	433	GLU	C-N	5.21	1.46	1.34
1	E	392	VAL	C-N	5.18	1.46	1.34
1	D	149	VAL	CA-CB	5.16	1.65	1.54
1	C	289	CYS	CB-SG	-5.15	1.73	1.81
1	C	119	GLU	CD-OE1	5.13	1.31	1.25
1	G	232	CYS	CB-SG	5.09	1.91	1.82
1	C	148	THR	CA-CB	5.08	1.66	1.53
1	D	463	GLU	CG-CD	5.07	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	232	CYS	CB-SG	5.06	1.90	1.82
1	A	453	THR	CB-CG2	5.06	1.69	1.52
1	H	251	SER	CB-OG	5.05	1.48	1.42
1	B	392	VAL	CB-CG1	5.03	1.63	1.52

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	412	GLN	O-C-N	-13.38	101.30	122.70
1	D	411	VAL	CA-CB-CG2	-12.09	92.77	110.90
1	H	306	ASN	O-C-N	-11.99	103.52	122.70
1	A	172	ARG	NE-CZ-NH1	-11.42	114.59	120.30
1	B	411	VAL	CA-CB-CG2	-11.21	94.08	110.90
1	H	150	LYS	CD-CE-NZ	-10.77	86.93	111.70
1	E	412	GLN	O-C-N	-10.44	105.99	122.70
1	C	379	ASP	CB-CG-OD1	9.51	126.86	118.30
1	D	172	ARG	NE-CZ-NH1	-9.41	115.59	120.30
1	F	172	ARG	NE-CZ-NH1	-9.39	115.61	120.30
1	E	411	VAL	CA-CB-CG2	-9.36	96.86	110.90
1	C	411	VAL	CA-CB-CG2	-9.31	96.93	110.90
1	F	172	ARG	NE-CZ-NH2	9.30	124.95	120.30
1	C	412	GLN	CA-C-N	8.70	136.34	117.20
1	E	411	VAL	CG1-CB-CG2	-8.58	97.17	110.90
1	C	336	CYS	C-N-CA	-8.32	104.83	122.30
1	F	306	ASN	O-C-N	-8.18	109.61	122.70
1	D	224	ARG	NE-CZ-NH2	8.02	124.31	120.30
1	A	379	ASP	CB-CG-OD1	7.84	125.36	118.30
1	B	336	CYS	C-N-CA	-7.34	106.88	122.30
1	D	107	ARG	NE-CZ-NH1	7.11	123.86	120.30
1	F	219	ARG	NE-CZ-NH1	-7.08	116.76	120.30
1	F	379	ASP	CB-CG-OD1	7.07	124.66	118.30
1	E	412	GLN	CA-C-N	6.99	132.57	117.20
1	C	140	LEU	CB-CG-CD2	-6.95	99.18	111.00
1	G	150	LYS	CD-CE-NZ	-6.92	95.79	111.70
1	C	172	ARG	NE-CZ-NH1	-6.85	116.88	120.30
1	D	336	CYS	C-N-CA	-6.81	108.00	122.30
1	G	412	GLN	CA-CB-CG	-6.74	98.57	113.40
1	B	306	ASN	O-C-N	-6.73	111.93	122.70
1	A	172	ARG	NE-CZ-NH2	6.58	123.59	120.30
1	F	415	LEU	CB-CG-CD1	6.53	122.11	111.00
1	C	292	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	G	292	ARG	NE-CZ-NH1	-6.39	117.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	306	ASN	O-C-N	-6.26	112.68	122.70
1	B	406	TYR	CB-CA-C	6.26	122.91	110.40
1	E	411	VAL	CA-CB-CG1	-6.24	101.54	110.90
1	H	430	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	E	219	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	A	224	ARG	NE-CZ-NH2	6.11	123.35	120.30
1	C	266	VAL	CG1-CB-CG2	-6.02	101.27	110.90
1	A	118	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	D	411	VAL	O-C-N	5.93	132.19	122.70
1	C	412	GLN	C-N-CA	5.91	136.49	121.70
1	B	449	VAL	CG1-CB-CG2	-5.88	101.49	110.90
1	G	107	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	C	363	GLY	N-CA-C	-5.76	98.69	113.10
1	D	363	GLY	N-CA-C	-5.75	98.72	113.10
1	F	392	VAL	O-C-N	5.74	131.88	122.70
1	D	432	LYS	CD-CE-NZ	-5.71	98.57	111.70
1	C	198	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	185	ASP	CB-CG-OD1	5.67	123.41	118.30
1	B	432	LYS	CD-CE-NZ	-5.64	98.73	111.70
1	C	350	LYS	N-CA-C	-5.62	95.82	111.00
1	B	293	ASP	CB-CG-OD1	-5.60	113.26	118.30
1	E	412(D)	LEU	CB-CG-CD2	-5.55	101.57	111.00
1	D	411	VAL	CG1-CB-CG2	-5.54	102.03	110.90
1	F	454	VAL	CB-CA-C	-5.53	100.89	111.40
1	D	152	ARG	NE-CZ-NH2	5.51	123.06	120.30
1	D	388	SER	N-CA-C	-5.50	96.16	111.00
1	B	430	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	A	268	LEU	CB-CG-CD2	-5.49	101.67	111.00
1	A	363	GLY	N-CA-C	-5.48	99.39	113.10
1	H	333	GLY	O-C-N	5.47	131.45	122.70
1	A	433	GLU	C-N-CA	-5.46	108.04	121.70
1	A	416	ASP	CB-CG-OD1	5.46	123.21	118.30
1	D	156	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	B	254	ILE	CB-CA-C	-5.40	100.80	111.60
1	G	241	MET	CG-SD-CE	-5.39	91.57	100.20
1	C	327	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	D	113	ASP	CB-CG-OD1	-5.35	113.49	118.30
1	E	306	ASN	C-N-CA	5.34	135.06	121.70
1	C	371	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	E	327	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	D	402	ASP	CB-CG-OD2	5.29	123.06	118.30
1	C	321	VAL	N-CA-C	-5.28	96.74	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	194	ILE	CG1-CB-CG2	-5.24	99.86	111.40
1	B	360	VAL	CB-CA-C	-5.23	101.47	111.40
1	C	306	ASN	O-C-N	-5.23	114.34	122.70
1	E	428	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	364	ARG	NE-CZ-NH2	5.21	122.91	120.30
1	C	364	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	H	142	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	B	428	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	327	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	H	396	ASP	CB-CG-OD1	5.10	122.89	118.30
1	D	433	GLU	C-N-CA	-5.08	108.99	121.70
1	G	412(D)	LEU	CA-CB-CG	5.08	126.98	115.30
1	C	388	SER	N-CA-C	-5.06	97.34	111.00
1	D	113	ASP	CB-CG-OD2	5.04	122.83	118.30
1	H	311	GLU	N-CA-C	-5.04	97.41	111.00
1	A	139	LEU	CB-CG-CD2	-5.03	102.44	111.00
1	D	324	ASP	CB-CG-OD2	-5.02	113.78	118.30

There are no chirality outliers.

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	333	GLY	Mainchain
1	A	433	GLU	Mainchain
1	B	411	VAL	Mainchain
1	C	306	ASN	Mainchain
1	C	336	CYS	Mainchain
1	C	412	GLN	Peptide,Mainchain
1	D	306	ASN	Mainchain
1	D	333	GLY	Mainchain
1	E	333	GLY	Mainchain
1	E	336	CYS	Mainchain
1	E	412	GLN	Peptide
1	F	306	ASN	Mainchain
1	F	333	GLY	Mainchain
1	F	411	VAL	Mainchain
1	G	306	ASN	Mainchain
1	G	336	CYS	Mainchain
1	G	392	VAL	Mainchain
1	H	306	ASN	Mainchain
1	H	411	VAL	Mainchain
1	H	433	GLU	Mainchain

5.2 Too-close contacts

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	2962	0	2783	161	0
1	B	2962	0	2782	171	0
1	C	2962	0	2782	177	5
1	D	2962	0	2783	183	8
1	E	2962	0	2780	194	0
1	F	2962	0	2783	173	0
1	G	2962	0	2783	171	3
1	H	2962	0	2783	166	0
2	B	20	0	23	4	0
All	All	23716	0	22282	1245	8

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 27.

All (1245) 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:E:411:VAL:CG2	1:E:411:VAL:CB	1.79	1.58
1:H:150:LYS:CE	1:H:150:LYS:CD	1.78	1.56
1:C:411:VAL:CG2	1:C:411:VAL:CB	1.76	1.56
1:D:411:VAL:CB	1:D:411:VAL:CG2	1.78	1.56
1:C:84:LYS:CD	1:C:84:LYS:CG	1.83	1.53
1:B:411:VAL:CB	1:B:411:VAL:CG2	1.86	1.48
1:H:150:LYS:CE	1:H:150:LYS:NZ	1.83	1.40
1:C:412:GLN:NE2	1:C:421:CYS:SG	2.03	1.32
1:B:452:ASP:HB3	1:D:216:LYS:HD3	1.21	1.19
1:G:453:THR:HG22	1:G:454:VAL:H	1.07	1.18
1:A:216:LYS:HD3	1:D:452:ASP:HB3	1.21	1.15
1:C:228:SER:HB3	1:C:350:LYS:HE2	1.13	1.13
1:E:413:THR:HG21	1:E:415:LEU:HD22	1.32	1.11
1:C:228:SER:HB3	1:C:350:LYS:CE	1.81	1.11
1:F:216:LYS:HD3	1:G:452:ASP:HB3	1.18	1.11
1:E:412:GLN:HG3	1:E:419:ARG:CB	1.81	1.10
1:B:97:TRP:O	1:B:453:THR:HG21	1.54	1.07
1:H:376:MET:HG2	1:H:397:ILE:HD11	1.37	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:453:THR:HG22	1:D:454:VAL:H	1.20	1.06
1:E:452:ASP:HB3	1:G:216:LYS:HD3	1.12	1.06
1:F:452:ASP:HB3	1:H:216:LYS:HD3	1.37	1.05
1:D:97:TRP:O	1:D:453:THR:HG21	1.59	1.02
1:E:452:ASP:HB3	1:G:216:LYS:CD	1.90	1.01
1:G:228:SER:HB3	1:G:350:LYS:HE2	1.41	1.01
1:A:453:THR:HG22	1:A:454:VAL:H	1.24	1.01
1:A:413:THR:HG21	1:A:415:LEU:HD22	1.41	1.00
1:B:333:GLY:H	1:B:386:THR:CG2	1.73	1.00
1:E:412:GLN:CG	1:E:419:ARG:CB	2.38	1.00
1:E:88:ASN:HD22	1:E:88:ASN:H	1.09	0.99
1:C:249:GLN:NE2	1:C:272:ASN:H	1.58	0.99
1:E:113:ASP:O	1:E:168:SER:HB2	1.63	0.99
1:E:412:GLN:CG	1:E:419:ARG:HB3	1.93	0.98
1:A:97:TRP:O	1:A:453:THR:HG21	1.64	0.98
1:G:453:THR:CG2	1:G:454:VAL:H	1.77	0.97
1:H:413:THR:HG21	1:H:415:LEU:HD22	1.46	0.96
1:B:276:GLU:OE2	2:B:800:G39:H92	1.65	0.96
1:B:144:HIS:HE1	1:C:463:GLU:H	1.00	0.96
1:E:412:GLN:HG3	1:E:419:ARG:HB3	1.45	0.96
1:D:411:VAL:CG2	1:D:411:VAL:CA	2.43	0.96
1:F:184:HIS:HD2	1:F:186:GLY:H	1.12	0.96
1:F:216:LYS:CD	1:G:452:ASP:HB3	1.95	0.96
1:C:413:THR:HG22	1:C:415:LEU:H	1.31	0.94
1:C:453:THR:HG22	1:C:454:VAL:H	1.33	0.94
1:B:85:LEU:HD12	1:B:412(C):GLU:HG3	1.46	0.93
1:C:412:GLN:CG	1:C:419:ARG:HB3	1.98	0.93
1:C:411:VAL:CG2	1:C:411:VAL:CA	2.46	0.93
1:D:249:GLN:HE21	1:D:272:ASN:H	1.13	0.93
1:D:411:VAL:CG2	1:D:411:VAL:CG1	2.46	0.93
1:B:463:GLU:H	1:D:144:HIS:HE1	1.17	0.92
1:A:88:ASN:H	1:A:88:ASN:HD22	1.17	0.92
1:A:463:GLU:H	1:C:144:HIS:HE1	0.98	0.92
1:E:249:GLN:NE2	1:E:272:ASN:H	1.67	0.92
1:B:411:VAL:CG2	1:B:411:VAL:CA	2.47	0.92
1:A:228:SER:HB3	1:A:350:LYS:HE2	1.51	0.92
1:A:144:HIS:HE1	1:D:463:GLU:H	1.12	0.92
1:C:249:GLN:HE21	1:C:272:ASN:H	0.97	0.92
1:F:375:GLU:OE1	1:F:394:LYS:HE3	1.71	0.91
1:B:452:ASP:HB3	1:D:216:LYS:CD	1.99	0.91
1:H:320:GLY:HA3	1:H:387:ASP:O	1.72	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:463:GLU:H	1:H:144:HIS:HE1	1.19	0.89
1:E:412:GLN:CG	1:E:419:ARG:HB2	2.01	0.89
1:E:411:VAL:CG2	1:E:411:VAL:CA	2.49	0.89
1:E:249:GLN:HE21	1:E:272:ASN:H	1.20	0.89
1:B:453:THR:HG22	1:B:454:VAL:H	1.37	0.88
1:D:359:GLY:CA	1:D:381:ASN:H	1.86	0.88
1:B:144:HIS:CE1	1:C:463:GLU:H	1.91	0.88
1:C:97:TRP:O	1:C:453:THR:HG21	1.73	0.88
1:D:333:GLY:H	1:D:386:THR:HG23	1.39	0.88
1:D:359:GLY:HA2	1:D:381:ASN:H	1.37	0.88
1:E:412:GLN:CB	1:E:419:ARG:HB2	2.04	0.88
1:G:282:PRO:HD2	1:G:411:VAL:HG21	1.55	0.88
1:A:216:LYS:CD	1:D:452:ASP:HB3	2.02	0.87
1:G:85:LEU:HD12	1:G:412(C):GLU:HG3	1.55	0.87
1:E:412:GLN:HB2	1:E:419:ARG:HB2	1.56	0.87
1:E:411:VAL:CG2	1:E:411:VAL:CG1	2.53	0.86
1:B:333:GLY:H	1:B:386:THR:HG23	1.40	0.86
1:B:448:GLY:O	1:B:449:VAL:HB	1.73	0.86
1:F:214:THR:HB	1:G:451:SER:OG	1.75	0.86
1:B:249:GLN:HE21	1:B:272:ASN:H	1.19	0.86
1:E:463:GLU:H	1:G:144:HIS:HE1	1.23	0.86
1:B:360:VAL:HG22	1:B:383:TRP:HB2	1.58	0.85
1:G:453:THR:HG22	1:G:454:VAL:N	1.89	0.85
1:D:359:GLY:HA2	1:D:381:ASN:N	1.90	0.85
1:B:214:THR:HG21	1:C:452:ASP:O	1.75	0.85
1:F:413:THR:HG21	1:F:415:LEU:HD22	1.59	0.84
1:F:214:THR:HG21	1:G:452:ASP:O	1.77	0.84
1:A:216:LYS:NZ	1:D:452:ASP:HB2	1.92	0.84
1:C:412:GLN:HG3	1:C:419:ARG:HB3	1.60	0.84
1:E:453:THR:HG22	1:E:454:VAL:H	1.42	0.84
1:F:184:HIS:CD2	1:F:186:GLY:H	1.94	0.84
1:A:448:GLY:O	1:A:449:VAL:HB	1.77	0.83
1:B:333:GLY:N	1:B:386:THR:CG2	2.42	0.83
1:E:452:ASP:O	1:G:214:THR:HG21	1.79	0.83
1:C:411:VAL:CG2	1:C:411:VAL:CG1	2.57	0.82
1:A:463:GLU:H	1:C:144:HIS:CE1	1.91	0.82
1:B:216:LYS:HD3	1:C:452:ASP:HB3	1.60	0.82
1:C:249:GLN:NE2	1:C:272:ASN:N	2.27	0.82
1:A:214:THR:HG21	1:D:452:ASP:O	1.79	0.82
1:F:452:ASP:O	1:H:214:THR:HG21	1.79	0.82
1:A:452:ASP:HB3	1:C:216:LYS:HD3	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:85:LEU:CD1	1:G:412(C):GLU:HG3	2.10	0.82
1:G:275:TYR:CE2	1:G:303:VAL:HG23	2.14	0.82
1:E:214:THR:HG21	1:H:452:ASP:O	1.80	0.82
1:F:97:TRP:O	1:F:453:THR:HG21	1.81	0.81
1:B:249:GLN:NE2	1:B:272:ASN:H	1.78	0.81
1:F:366:LYS:HD3	1:F:400:ILE:HG12	1.62	0.81
1:G:249:GLN:NE2	1:G:272:ASN:H	1.78	0.81
1:D:249:GLN:NE2	1:D:272:ASN:H	1.78	0.80
1:G:320:GLY:HA3	1:G:387:ASP:O	1.81	0.80
1:C:184:HIS:CD2	1:C:186:GLY:H	2.00	0.80
1:E:376:MET:HG2	1:E:397:ILE:HD11	1.63	0.80
1:B:452:ASP:O	1:D:214:THR:HG21	1.82	0.79
1:H:376:MET:HG2	1:H:397:ILE:CD1	2.12	0.79
1:B:85:LEU:CD1	1:B:412(C):GLU:HG3	2.12	0.79
1:D:113:ASP:O	1:D:168:SER:HB2	1.82	0.79
1:F:91:LEU:HG	1:F:283:ASN:ND2	1.96	0.79
1:D:376:MET:HG2	1:D:397:ILE:HD11	1.64	0.79
1:E:97:TRP:O	1:E:453:THR:HG21	1.82	0.79
1:E:144:HIS:HE1	1:H:463:GLU:H	1.30	0.78
1:F:316:TYR:CE1	1:F:340:PRO:HD3	2.18	0.78
1:H:448:GLY:O	1:H:449:VAL:HB	1.81	0.78
1:A:192:ILE:HG12	1:A:205:LEU:HD22	1.65	0.78
1:B:413:THR:HG21	1:B:415:LEU:HD22	1.65	0.78
1:A:452:ASP:HB2	1:C:216:LYS:NZ	1.98	0.78
1:H:316:TYR:CE1	1:H:340:PRO:HD3	2.19	0.78
1:F:144:HIS:HE1	1:G:463:GLU:H	1.32	0.78
1:G:229:GLU:HG2	1:G:230:CYS:O	1.84	0.78
1:F:249:GLN:NE2	1:F:272:ASN:H	1.83	0.77
1:C:162:PRO:HG2	1:C:165:GLU:CD	2.05	0.77
1:G:316:TYR:CE1	1:G:340:PRO:HD3	2.20	0.77
1:C:413:THR:HG21	1:C:415:LEU:HD22	1.67	0.77
1:D:358:ASN:O	1:D:381:ASN:HA	1.85	0.77
1:H:333:GLY:H	1:H:386:THR:HG23	1.49	0.77
1:H:411:VAL:CG1	1:H:418:ILE:HG23	2.15	0.77
1:B:264:LYS:HG2	1:B:310:LEU:HD22	1.66	0.76
1:A:144:HIS:CE1	1:D:463:GLU:H	2.01	0.76
1:C:275:TYR:CE2	1:C:303:VAL:HG23	2.21	0.76
1:D:448:GLY:O	1:D:449:VAL:HB	1.85	0.76
1:G:88:ASN:HD22	1:G:88:ASN:H	1.33	0.76
1:A:136:GLN:HE21	1:A:156:ARG:CD	1.99	0.76
1:C:412:GLN:HG2	1:C:419:ARG:HB3	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:453:THR:HG22	1:D:454:VAL:N	2.00	0.76
1:A:229:GLU:OE1	1:A:410:PHE:HA	1.86	0.75
1:G:333:GLY:H	1:G:386:THR:CG2	1.99	0.75
1:B:411:VAL:CG2	1:B:411:VAL:CG1	2.61	0.75
1:E:216:LYS:HD3	1:H:452:ASP:HB3	1.68	0.75
1:D:184:HIS:CD2	1:D:186:GLY:H	2.04	0.75
1:D:248:GLY:HA2	1:D:295:TRP:CE2	2.22	0.75
1:E:254:ILE:HD11	1:E:268:LEU:HD21	1.68	0.75
1:A:184:HIS:HD2	1:A:186:GLY:H	1.34	0.75
1:G:287:ILE:HD12	1:G:287:ILE:N	2.01	0.75
1:H:150:LYS:CD	1:H:150:LYS:NZ	2.49	0.75
1:D:316:TYR:CE1	1:D:340:PRO:HD3	2.22	0.75
1:G:117:ILE:HG22	1:G:135:THR:HG22	1.69	0.75
1:A:97:TRP:H	1:A:395:GLN:HE22	1.34	0.74
1:A:248:GLY:HA2	1:A:295:TRP:CE2	2.22	0.74
1:B:454:VAL:HG21	1:D:200:GLY:O	1.86	0.74
1:G:306:ASN:CG	1:G:308:GLN:H	1.89	0.74
1:F:453:THR:HG22	1:F:454:VAL:H	1.52	0.74
1:A:249:GLN:HE21	1:A:272:ASN:H	1.36	0.74
1:F:299:ASN:ND2	1:F:316:TYR:HB3	2.03	0.74
1:C:228:SER:CB	1:C:350:LYS:HE2	2.07	0.74
1:H:228:SER:HB3	1:H:350:LYS:HE2	1.69	0.74
1:B:192:ILE:HG12	1:B:205:LEU:HD22	1.68	0.73
1:H:333:GLY:H	1:H:386:THR:CG2	2.01	0.73
1:E:412:GLN:HG2	1:E:419:ARG:HB3	1.69	0.73
1:C:270:ALA:HB1	1:C:273:TYR:HB2	1.71	0.73
1:A:116:VAL:HG23	1:A:440:SER:HB2	1.71	0.73
1:F:228:SER:HB3	1:F:350:LYS:HE2	1.70	0.73
1:D:413:THR:HG21	1:D:415:LEU:HD22	1.70	0.73
1:F:248:GLY:HA2	1:F:295:TRP:CE2	2.24	0.73
1:H:306:ASN:CG	1:H:308:GLN:H	1.91	0.72
1:C:88:ASN:H	1:C:88:ASN:HD22	1.34	0.72
1:D:287:ILE:N	1:D:287:ILE:HD12	2.04	0.72
1:G:121:PHE:CG	1:G:228:SER:HA	2.24	0.72
1:H:248:GLY:HA2	1:H:295:TRP:CE2	2.24	0.72
1:B:463:GLU:H	1:D:144:HIS:CE1	2.06	0.72
1:D:333:GLY:N	1:D:386:THR:HG23	2.04	0.72
1:D:466:PHE:C	1:D:468:ILE:H	1.91	0.72
1:B:156:ARG:HG2	1:B:178:TRP:HA	1.72	0.72
1:C:150:LYS:HD3	1:C:152:ARG:O	1.88	0.72
1:C:412:GLN:HG3	1:C:419:ARG:CB	2.20	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:ASP:HB2	1:D:216:LYS:NZ	2.04	0.72
1:G:270:ALA:HB1	1:G:273:TYR:HB2	1.71	0.72
1:D:376:MET:HG2	1:D:397:ILE:CD1	2.19	0.72
1:G:397:ILE:HG22	1:G:398:VAL:HG23	1.72	0.72
1:G:412:GLN:HB2	1:G:419:ARG:HB2	1.72	0.72
1:H:97:TRP:O	1:H:453:THR:HG21	1.89	0.72
1:C:412:GLN:CG	1:C:419:ARG:CB	2.67	0.71
1:F:88:ASN:H	1:F:88:ASN:HD22	1.36	0.71
1:A:184:HIS:CD2	1:A:186:GLY:H	2.08	0.71
1:D:97:TRP:H	1:D:395:GLN:HE22	1.39	0.71
1:F:275:TYR:CE2	1:F:303:VAL:HG23	2.25	0.71
1:G:249:GLN:NE2	1:G:272:ASN:N	2.38	0.71
1:A:249:GLN:NE2	1:A:272:ASN:H	1.88	0.71
1:C:287:ILE:HD12	1:C:287:ILE:N	2.06	0.71
1:H:254:ILE:HD11	1:H:268:LEU:HD21	1.72	0.71
1:B:466:PHE:C	1:B:468:ILE:H	1.94	0.70
1:D:333:GLY:H	1:D:386:THR:CG2	2.04	0.70
1:G:413:THR:HG21	1:G:415:LEU:HD22	1.72	0.70
1:A:320:GLY:HA3	1:A:387:ASP:O	1.91	0.70
1:A:413:THR:HG22	1:A:415:LEU:H	1.57	0.70
1:D:453:THR:CG2	1:D:454:VAL:H	2.02	0.70
1:B:162:PRO:HG2	1:B:165:GLU:CD	2.11	0.70
1:B:287:ILE:N	1:B:287:ILE:HD12	2.06	0.70
1:C:84:LYS:CG	1:C:84:LYS:CE	2.70	0.70
1:G:448:GLY:O	1:G:449:VAL:HB	1.90	0.70
1:A:102:LYS:HG3	1:A:444:ILE:HG22	1.74	0.70
1:B:109:GLY:HA3	1:B:140:LEU:HD12	1.72	0.70
1:A:228:SER:HB3	1:A:350:LYS:CE	2.22	0.69
1:E:214:THR:HB	1:H:451:SER:OG	1.91	0.69
1:C:248:GLY:HA2	1:C:295:TRP:CE2	2.27	0.69
1:D:192:ILE:HG12	1:D:205:LEU:HD22	1.74	0.69
1:F:228:SER:HB3	1:F:350:LYS:CE	2.21	0.69
1:H:150:LYS:CE	1:H:150:LYS:CG	2.69	0.69
1:B:214:THR:HB	1:C:451:SER:CB	2.22	0.69
1:D:184:HIS:HD2	1:D:186:GLY:H	1.37	0.69
1:D:247:ASN:O	1:D:248:GLY:O	2.10	0.69
1:D:375:GLU:OE1	1:D:394:LYS:HE3	1.92	0.69
1:A:451:SER:OG	1:C:214:THR:HB	1.93	0.69
1:D:320:GLY:HA3	1:D:387:ASP:O	1.93	0.68
1:C:333:GLY:H	1:C:386:THR:HG23	1.58	0.68
1:F:88:ASN:HD22	1:F:88:ASN:N	1.88	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:121:PHE:CG	1:E:228:SER:HA	2.28	0.68
1:D:411:VAL:HG13	1:D:418:ILE:HG23	1.75	0.68
1:E:316:TYR:CE1	1:E:340:PRO:HD3	2.27	0.68
1:D:210:ILE:O	1:D:210:ILE:HG13	1.92	0.68
1:D:249:GLN:HE21	1:D:272:ASN:N	1.89	0.68
1:F:320:GLY:HA3	1:F:387:ASP:O	1.94	0.68
1:G:97:TRP:H	1:G:395:GLN:HE22	1.42	0.68
1:H:397:ILE:HG22	1:H:398:VAL:HG23	1.76	0.68
1:D:228:SER:HB3	1:D:350:LYS:HE2	1.74	0.68
1:D:249:GLN:NE2	1:D:272:ASN:N	2.42	0.68
1:E:320:GLY:HA3	1:E:387:ASP:O	1.94	0.68
1:H:184:HIS:CD2	1:H:186:GLY:H	2.11	0.68
1:E:249:GLN:NE2	1:E:272:ASN:N	2.41	0.67
1:C:413:THR:HG21	1:C:415:LEU:HB2	1.77	0.67
1:D:466:PHE:C	1:D:468:ILE:N	2.48	0.67
1:E:376:MET:HG2	1:E:397:ILE:CD1	2.23	0.67
1:G:248:GLY:HA2	1:G:295:TRP:CE2	2.29	0.67
1:H:282:PRO:HD2	1:H:411:VAL:HG21	1.76	0.67
1:E:412:GLN:HG3	1:E:419:ARG:HB2	1.62	0.67
1:F:376:MET:HG2	1:F:397:ILE:HD11	1.76	0.67
1:A:150:LYS:HD3	1:A:152:ARG:O	1.93	0.67
1:D:88:ASN:HD22	1:D:88:ASN:N	1.92	0.67
1:A:88:ASN:HD22	1:A:88:ASN:N	1.84	0.67
1:A:136:GLN:HE21	1:A:156:ARG:HD2	1.58	0.67
1:E:85:LEU:HD12	1:E:412(C):GLU:HG3	1.76	0.67
1:F:113:ASP:O	1:F:168:SER:HB2	1.95	0.67
1:C:413:THR:HG22	1:C:415:LEU:N	2.08	0.67
1:B:117:ILE:HG22	1:B:135:THR:HG22	1.77	0.67
1:H:411:VAL:HG13	1:H:418:ILE:HG23	1.76	0.66
1:D:270:ALA:O	1:D:273:TYR:HB2	1.95	0.66
1:E:463:GLU:H	1:G:144:HIS:CE1	2.09	0.66
1:F:116:VAL:HG12	1:F:138:ALA:O	1.96	0.66
1:E:88:ASN:HD22	1:E:88:ASN:N	1.81	0.66
1:G:306:ASN:CG	1:G:308:GLN:N	2.48	0.66
1:G:118:ARG:O	1:G:119:GLU:HG3	1.96	0.66
1:G:333:GLY:N	1:G:386:THR:CG2	2.58	0.66
1:C:413:THR:CG2	1:C:415:LEU:HB2	2.26	0.66
1:C:117:ILE:HG22	1:C:135:THR:HG22	1.77	0.66
1:D:88:ASN:HD22	1:D:88:ASN:H	1.41	0.66
1:F:377:ILE:HG23	1:F:390:PHE:CD1	2.29	0.66
1:D:254:ILE:CD1	1:D:268:LEU:HD21	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:88:ASN:HD22	1:G:88:ASN:N	1.89	0.66
1:G:97:TRP:O	1:G:453:THR:HG21	1.96	0.66
1:B:113:ASP:O	1:B:168:SER:HB2	1.96	0.66
1:C:113:ASP:O	1:C:168:SER:HB2	1.95	0.66
1:E:413:THR:HG21	1:E:415:LEU:CD2	2.19	0.66
1:F:463:GLU:H	1:H:144:HIS:CE1	2.09	0.66
1:H:226:GLN:NE2	1:H:239:THR:OG1	2.24	0.66
1:A:380:PRO:O	1:A:381:ASN:C	2.33	0.65
1:A:453:THR:CG2	1:A:454:VAL:H	2.03	0.65
1:H:156:ARG:HG2	1:H:178:TRP:HA	1.77	0.65
1:F:156:ARG:HG2	1:F:178:TRP:HA	1.79	0.65
1:H:184:HIS:HD2	1:H:186:GLY:H	1.42	0.65
1:C:333:GLY:N	1:C:386:THR:HG23	2.12	0.65
1:B:466:PHE:C	1:B:468:ILE:N	2.50	0.65
1:E:287:ILE:HD12	1:E:287:ILE:N	2.11	0.65
1:F:322:PHE:HB2	1:F:327:ARG:HD2	1.79	0.65
1:H:116:VAL:HG12	1:H:138:ALA:O	1.97	0.65
1:A:113:ASP:O	1:A:168:SER:HB2	1.96	0.65
1:B:214:THR:HB	1:C:451:SER:OG	1.97	0.65
1:B:216:LYS:CD	1:C:452:ASP:HB3	2.25	0.65
1:C:320:GLY:HA3	1:C:387:ASP:O	1.96	0.65
1:B:144:HIS:HE1	1:C:463:GLU:N	1.85	0.65
1:F:332:THR:HG23	1:F:386:THR:CG2	2.27	0.65
1:C:325:ASN:O	1:C:348:GLY:HA2	1.97	0.65
1:A:290:VAL:HG21	1:A:353:SER:HB2	1.79	0.64
1:A:303:VAL:HG22	1:A:314:ILE:HG22	1.79	0.64
1:D:162:PRO:HG2	1:D:165:GLU:CD	2.16	0.64
1:C:161:CYS:HB2	1:C:162:PRO:HD2	1.77	0.64
1:D:117:ILE:HG22	1:D:135:THR:HG22	1.78	0.64
1:A:135:THR:O	1:A:156:ARG:HA	1.98	0.64
1:B:249:GLN:NE2	1:B:272:ASN:N	2.43	0.64
1:E:184:HIS:HD2	1:E:186:GLY:H	1.46	0.64
1:F:452:ASP:HB3	1:H:216:LYS:CD	2.22	0.64
1:G:228:SER:HB3	1:G:350:LYS:CE	2.24	0.64
1:A:452:ASP:O	1:C:214:THR:HG21	1.97	0.64
1:B:248:GLY:HA2	1:B:295:TRP:CE2	2.32	0.64
1:C:184:HIS:HD2	1:C:186:GLY:H	1.44	0.64
1:F:247:ASN:O	1:F:248:GLY:O	2.15	0.64
1:G:412:GLN:HB2	1:G:419:ARG:CB	2.27	0.64
1:B:376:MET:HG2	1:B:397:ILE:CD1	2.27	0.64
1:C:88:ASN:HD22	1:C:88:ASN:N	1.92	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:ILE:HG12	1:C:205:LEU:HD22	1.79	0.64
1:F:287:ILE:N	1:F:287:ILE:HD12	2.12	0.64
1:B:406:TYR:OH	2:B:800:G39:C2	2.46	0.64
1:B:270:ALA:HB1	1:B:273:TYR:HB2	1.79	0.63
1:B:214:THR:HB	1:C:451:SER:HB2	1.79	0.63
1:E:148:THR:HG22	1:E:430:ARG:HH22	1.64	0.63
1:E:411:VAL:CG2	1:E:411:VAL:HA	2.28	0.63
1:H:300:ARG:HB2	1:H:317:ILE:HD12	1.80	0.63
1:A:451:SER:CB	1:C:214:THR:HB	2.28	0.63
1:C:380:PRO:O	1:C:381:ASN:C	2.35	0.63
1:F:136:GLN:HE21	1:F:156:ARG:CD	2.10	0.63
1:H:333:GLY:N	1:H:386:THR:HG23	2.14	0.63
1:A:121:PHE:CG	1:A:228:SER:HA	2.33	0.63
1:A:214:THR:HB	1:D:451:SER:OG	1.99	0.63
1:B:316:TYR:CE1	1:B:340:PRO:HD3	2.33	0.63
1:H:375:GLU:OE1	1:H:394:LYS:HE3	1.99	0.63
1:A:316:TYR:CE1	1:A:340:PRO:HD3	2.34	0.63
1:B:376:MET:HG2	1:B:397:ILE:HD11	1.80	0.63
1:C:412:GLN:HB2	1:C:419:ARG:HB2	1.81	0.63
1:B:333:GLY:N	1:B:386:THR:HG21	2.14	0.63
1:F:144:HIS:CE1	1:G:463:GLU:H	2.15	0.63
1:C:376:MET:HG2	1:C:397:ILE:CD1	2.29	0.63
1:F:380:PRO:O	1:F:381:ASN:C	2.35	0.63
1:G:156:ARG:HG2	1:G:178:TRP:HA	1.81	0.63
1:E:413:THR:CG2	1:E:415:LEU:HD22	2.21	0.62
1:F:181:SER:HB2	1:F:228:SER:O	1.99	0.62
1:H:202:VAL:CG2	1:H:214:THR:HG23	2.28	0.62
1:F:411:VAL:HG13	1:F:418:ILE:HG23	1.80	0.62
1:G:249:GLN:HE21	1:G:272:ASN:H	1.45	0.62
1:C:453:THR:CG2	1:C:454:VAL:H	2.11	0.62
1:D:116:VAL:HG12	1:D:138:ALA:O	1.98	0.62
1:F:256:LYS:HB2	1:F:310:LEU:HD11	1.81	0.62
1:F:327:ARG:HB2	1:F:328:PRO:HD2	1.81	0.62
1:G:148:THR:HG22	1:G:430:ARG:HH22	1.63	0.62
1:B:129:CYS:O	1:B:163:VAL:HG23	1.99	0.62
1:B:343:SER:O	1:B:344:ASN:CB	2.47	0.62
1:E:192:ILE:HG12	1:E:205:LEU:HD22	1.80	0.62
1:C:411:VAL:HG13	1:C:418:ILE:HG23	1.81	0.62
1:B:333:GLY:N	1:B:386:THR:HG23	2.12	0.62
1:B:411:VAL:CG2	1:B:411:VAL:HA	2.29	0.62
1:F:249:GLN:HE21	1:F:272:ASN:H	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:ASN:H	1:D:88:ASN:ND2	1.98	0.62
1:E:162:PRO:HG2	1:E:165:GLU:CD	2.20	0.62
1:H:102:LYS:HG3	1:H:444:ILE:HG22	1.82	0.62
1:H:412:GLN:HB2	1:H:419:ARG:HB2	1.81	0.62
1:F:202:VAL:HG11	1:G:454:VAL:HG23	1.82	0.62
1:F:316:TYR:CZ	1:F:340:PRO:HD3	2.34	0.62
1:G:275:TYR:CE2	1:G:303:VAL:CG2	2.82	0.62
1:A:452:ASP:HB2	1:C:216:LYS:HZ3	1.62	0.61
1:E:452:ASP:HB2	1:G:216:LYS:NZ	2.14	0.61
1:F:129:CYS:O	1:F:163:VAL:HG23	2.00	0.61
1:H:466:PHE:C	1:H:468:ILE:H	2.03	0.61
1:A:453:THR:HG22	1:A:454:VAL:N	2.06	0.61
1:E:216:LYS:CD	1:H:452:ASP:HB3	2.28	0.61
1:F:88:ASN:H	1:F:88:ASN:ND2	1.98	0.61
1:B:229:GLU:OE1	1:B:410:PHE:HA	2.00	0.61
1:C:84:LYS:CD	1:C:84:LYS:CB	2.75	0.61
1:D:190:LEU:HD21	1:D:257:MET:HE3	1.81	0.61
1:D:411:VAL:CG2	1:D:411:VAL:HA	2.29	0.61
1:E:168:SER:HB2	1:E:169:PRO:HD2	1.82	0.61
1:F:184:HIS:HD2	1:F:186:GLY:N	1.91	0.61
1:F:412:GLN:HB2	1:F:419:ARG:CB	2.31	0.61
1:G:103:ASP:O	1:G:104:ASN:HB2	2.00	0.61
1:D:254:ILE:HD11	1:D:268:LEU:HD21	1.81	0.61
1:G:184:HIS:CD2	1:G:186:GLY:H	2.18	0.61
1:G:333:GLY:H	1:G:386:THR:HG23	1.65	0.61
1:E:248:GLY:HA2	1:E:295:TRP:CE2	2.35	0.61
1:C:411:VAL:CG2	1:C:411:VAL:HA	2.30	0.61
1:E:333:GLY:H	1:E:386:THR:HG23	1.65	0.61
1:H:333:GLY:N	1:H:386:THR:CG2	2.63	0.61
1:B:380:PRO:O	1:B:381:ASN:C	2.40	0.60
1:E:117:ILE:HG22	1:E:135:THR:HG22	1.82	0.60
1:A:216:LYS:HZ3	1:D:452:ASP:HB2	1.64	0.60
1:E:184:HIS:CD2	1:E:186:GLY:H	2.19	0.60
1:F:282:PRO:HD2	1:F:411:VAL:HG21	1.83	0.60
1:A:216:LYS:NZ	1:D:452:ASP:CB	2.64	0.60
1:E:250:ALA:HB3	1:E:252:TYR:CE2	2.36	0.60
1:A:413:THR:HG21	1:A:415:LEU:CD2	2.25	0.60
1:C:387:ASP:HB3	1:C:389:SER:H	1.66	0.60
1:E:286:GLU:C	1:E:287:ILE:HD12	2.21	0.60
1:F:162:PRO:HG2	1:F:165:GLU:CD	2.22	0.60
1:F:451:SER:OG	1:H:214:THR:HB	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:161:CYS:HB2	1:H:162:PRO:HD2	1.83	0.60
1:H:379:ASP:OD2	1:H:382:GLY:HA3	2.02	0.60
1:A:250:ALA:HB3	1:A:252:TYR:CE2	2.36	0.60
1:G:290:VAL:HG21	1:G:353:SER:HB2	1.83	0.60
1:G:113:ASP:O	1:G:168:SER:HB2	2.01	0.60
1:H:228:SER:HB3	1:H:350:LYS:CE	2.32	0.60
1:H:254:ILE:CD1	1:H:268:LEU:HD21	2.32	0.60
1:B:452:ASP:CB	1:D:216:LYS:NZ	2.65	0.60
1:E:322:PHE:HB2	1:E:327:ARG:HD2	1.83	0.60
1:C:366:LYS:HD3	1:C:400:ILE:HG12	1.83	0.60
1:D:121:PHE:CG	1:D:228:SER:HA	2.36	0.60
1:E:88:ASN:H	1:E:88:ASN:ND2	1.91	0.60
1:E:144:HIS:CE1	1:H:463:GLU:H	2.17	0.60
1:F:299:ASN:HD22	1:F:316:TYR:HB3	1.66	0.60
1:A:216:LYS:HD3	1:D:452:ASP:CB	2.13	0.59
1:G:88:ASN:H	1:G:88:ASN:ND2	2.00	0.59
1:A:158:LEU:O	1:A:174:GLU:HB2	2.01	0.59
1:D:275:TYR:CE2	1:D:303:VAL:CG2	2.85	0.59
1:F:194:ILE:HG12	1:F:203:ALA:HB2	1.83	0.59
1:A:162:PRO:HG2	1:A:165:GLU:CD	2.22	0.59
1:F:332:THR:HG23	1:F:386:THR:HG21	1.84	0.59
1:A:144:HIS:HE1	1:D:463:GLU:N	1.93	0.59
1:B:364:ARG:HG3	1:B:365:THR:O	2.01	0.59
1:C:115:PHE:CE1	1:C:159:MET:HE3	2.38	0.59
1:F:412:GLN:HB2	1:F:419:ARG:HB2	1.84	0.59
1:A:216:LYS:HZ2	1:D:452:ASP:HB2	1.65	0.59
1:B:452:ASP:HB2	1:D:216:LYS:HZ2	1.67	0.59
1:E:96:GLY:O	1:E:448:GLY:O	2.20	0.59
1:F:96:GLY:O	1:F:448:GLY:O	2.19	0.59
1:H:355:LYS:HD2	1:H:383:TRP:CE2	2.38	0.59
1:C:464:LEU:HB3	1:C:465:PRO:HA	1.83	0.59
1:F:172:ARG:HD2	1:F:174:GLU:OE1	2.03	0.59
1:E:229:GLU:HG2	1:E:230:CYS:O	2.03	0.59
1:H:118:ARG:HB2	1:H:156:ARG:HH11	1.68	0.59
1:D:97:TRP:N	1:D:395:GLN:HE22	2.00	0.59
1:E:210:ILE:HG13	1:E:210:ILE:O	2.03	0.59
1:E:451:SER:HB2	1:G:214:THR:CG2	2.33	0.59
1:F:325:ASN:O	1:F:348:GLY:HA2	2.03	0.59
1:H:148:THR:HG23	1:H:430:ARG:HH12	1.68	0.59
1:A:454:VAL:HG21	1:C:200:GLY:O	2.02	0.58
1:F:229:GLU:HG2	1:F:230:CYS:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:VAL:HG12	1:B:138:ALA:O	2.04	0.58
1:E:148:THR:HG23	1:E:430:ARG:HH12	1.68	0.58
1:E:413:THR:CG2	1:E:415:LEU:HB2	2.32	0.58
1:F:216:LYS:CE	1:G:452:ASP:HB3	2.32	0.58
1:A:88:ASN:H	1:A:88:ASN:ND2	1.94	0.58
1:C:88:ASN:H	1:C:88:ASN:ND2	2.01	0.58
1:C:249:GLN:NE2	1:C:271:PRO:HA	2.18	0.58
1:A:451:SER:HB2	1:C:214:THR:CG2	2.33	0.58
1:A:466:PHE:O	1:A:468:ILE:N	2.36	0.58
1:B:322:PHE:HB2	1:B:327:ARG:HD2	1.84	0.58
1:C:85:LEU:HD12	1:C:412(C):GLU:HG3	1.85	0.58
1:E:320:GLY:CA	1:E:387:ASP:O	2.52	0.58
1:E:355:LYS:HD2	1:E:383:TRP:CE2	2.39	0.58
1:B:228:SER:HB3	1:B:350:LYS:NZ	2.17	0.58
1:B:247:ASN:O	1:B:248:GLY:O	2.21	0.58
1:D:182:ALA:O	1:D:229:GLU:HA	2.04	0.58
1:F:202:VAL:CG1	1:G:454:VAL:HG23	2.34	0.58
1:B:97:TRP:H	1:B:395:GLN:HE22	1.50	0.58
1:E:271:PRO:O	1:E:272:ASN:CB	2.51	0.58
1:F:168:SER:HB2	1:F:169:PRO:HD2	1.85	0.58
1:H:229:GLU:OE1	1:H:410:PHE:HA	2.04	0.58
1:A:466:PHE:C	1:A:468:ILE:H	2.06	0.58
1:F:451:SER:CB	1:H:214:THR:HB	2.34	0.58
1:H:88:ASN:N	1:H:88:ASN:HD22	2.02	0.58
1:H:113:ASP:O	1:H:168:SER:HB2	2.04	0.58
1:F:254:ILE:HD11	1:F:268:LEU:HD21	1.85	0.57
1:G:411:VAL:HG13	1:G:418:ILE:HG23	1.85	0.57
1:H:190:LEU:HD21	1:H:257:MET:HE3	1.85	0.57
1:A:249:GLN:NE2	1:A:272:ASN:N	2.52	0.57
1:A:466:PHE:C	1:A:468:ILE:N	2.56	0.57
1:B:249:GLN:HE21	1:B:272:ASN:N	1.93	0.57
1:G:254:ILE:HD11	1:G:268:LEU:HD21	1.85	0.57
1:A:120:PRO:HA	1:A:132:PHE:O	2.04	0.57
1:B:453:THR:CG2	1:B:454:VAL:H	2.10	0.57
1:E:411:VAL:CG1	1:E:412:GLN:N	2.66	0.57
1:F:316:TYR:CD1	1:F:340:PRO:HD3	2.39	0.57
1:B:275:TYR:CE2	1:B:303:VAL:CG2	2.88	0.57
1:D:322:PHE:HB2	1:D:327:ARG:HD2	1.86	0.57
1:E:343:SER:O	1:E:344:ASN:CB	2.53	0.57
1:F:216:LYS:NZ	1:G:452:ASP:CB	2.67	0.57
1:G:135:THR:O	1:G:156:ARG:HA	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:172:ARG:HD2	1:G:174:GLU:OE1	2.05	0.57
1:H:306:ASN:CG	1:H:308:GLN:N	2.58	0.57
1:E:227:GLU:HA	1:E:227:GLU:OE1	2.04	0.57
1:H:97:TRP:HD1	1:H:395:GLN:NE2	2.03	0.57
1:D:156:ARG:HB3	1:D:177:ALA:O	2.04	0.57
1:H:453:THR:HG22	1:H:454:VAL:H	1.70	0.57
1:F:152:ARG:CZ	1:F:222:ILE:HD13	2.35	0.57
1:F:173:PHE:CG	1:G:164:GLY:HA3	2.39	0.57
1:A:366:LYS:NZ	1:A:396:ASP:OD1	2.38	0.57
1:E:216:LYS:CE	1:H:452:ASP:HB3	2.35	0.57
1:B:119:GLU:HG3	1:B:119:GLU:O	2.05	0.56
1:B:451:SER:HB2	1:D:214:THR:CG2	2.35	0.56
1:F:332:THR:CG2	1:F:386:THR:HG21	2.34	0.56
1:A:452:ASP:CB	1:C:216:LYS:NZ	2.67	0.56
1:E:457:SER:OG	1:E:459:PRO:HD3	2.05	0.56
1:G:355:LYS:HD2	1:G:383:TRP:CE2	2.39	0.56
1:A:316:TYR:CZ	1:A:340:PRO:HD3	2.40	0.56
1:C:343:SER:C	1:C:345:GLY:H	2.07	0.56
1:F:210:ILE:HD13	1:G:413:THR:HA	1.87	0.56
1:H:88:ASN:O	1:H:284:ALA:HA	2.05	0.56
1:F:249:GLN:NE2	1:F:272:ASN:N	2.52	0.56
1:F:411:VAL:HG11	1:F:412(A):HIS:CD2	2.41	0.56
1:C:121:PHE:CG	1:C:228:SER:HA	2.41	0.56
1:D:299:ASN:ND2	1:D:316:TYR:HB3	2.19	0.56
1:F:318:CYS:HA	1:F:335:SER:O	2.05	0.56
1:H:277:GLU:OE1	1:H:350:LYS:HB2	2.04	0.56
1:A:162:PRO:HG2	1:A:165:GLU:OE1	2.05	0.56
1:B:115:PHE:CE1	1:B:159:MET:HE3	2.40	0.56
1:D:360:VAL:HG13	1:D:383:TRP:HE3	1.71	0.56
1:E:466:PHE:C	1:E:468:ILE:N	2.58	0.56
1:F:97:TRP:H	1:F:395:GLN:HE22	1.53	0.56
1:D:228:SER:HB3	1:D:350:LYS:CE	2.36	0.56
1:F:347:TYR:CG	1:F:348:GLY:N	2.74	0.56
1:G:247:ASN:O	1:G:248:GLY:O	2.23	0.56
1:B:370:SER:HB2	1:B:372:SER:OG	2.05	0.56
1:F:118:ARG:O	1:F:119:GLU:HG3	2.06	0.56
1:H:88:ASN:HD22	1:H:88:ASN:H	1.53	0.56
1:A:247:ASN:O	1:A:248:GLY:O	2.24	0.56
1:F:254:ILE:CD1	1:F:268:LEU:HD21	2.36	0.56
1:G:194:ILE:HD11	1:G:241:MET:HE2	1.88	0.56
1:C:96:GLY:O	1:C:448:GLY:O	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:325:ASN:O	1:E:348:GLY:HA2	2.06	0.56
1:G:466:PHE:C	1:G:468:ILE:H	2.10	0.56
1:A:376:MET:HG2	1:A:397:ILE:HD11	1.86	0.55
1:A:413:THR:CG2	1:A:415:LEU:HD22	2.27	0.55
1:B:406:TYR:OH	2:B:800:G39:C1	2.54	0.55
1:B:413:THR:HG22	1:B:415:LEU:H	1.70	0.55
1:D:116:VAL:HG23	1:D:440:SER:HB2	1.88	0.55
1:E:275:TYR:CE2	1:E:303:VAL:HG23	2.40	0.55
1:F:397:ILE:HD13	1:F:422:PHE:HZ	1.70	0.55
1:A:299:ASN:ND2	1:A:316:TYR:HB3	2.21	0.55
1:B:117:ILE:HG22	1:B:135:THR:CG2	2.37	0.55
1:F:452:ASP:O	1:H:214:THR:CG2	2.52	0.55
1:H:97:TRP:H	1:H:395:GLN:HE22	1.55	0.55
1:E:397:ILE:HG22	1:E:398:VAL:HG23	1.87	0.55
1:B:360:VAL:CG2	1:B:383:TRP:HB2	2.35	0.55
1:G:97:TRP:N	1:G:395:GLN:HE22	2.02	0.55
1:G:287:ILE:N	1:G:287:ILE:CD1	2.69	0.55
1:E:116:VAL:HG23	1:E:440:SER:HB2	1.88	0.55
1:E:252:TYR:HB2	1:E:268:LEU:HD12	1.87	0.55
1:E:412(B):PRO:HB3	1:E:415:LEU:O	2.07	0.55
1:A:136:GLN:HE21	1:A:156:ARG:HD3	1.71	0.55
1:B:321:VAL:HG13	1:B:364:ARG:NH2	2.22	0.55
1:D:290:VAL:HG11	1:D:353:SER:HB2	1.89	0.55
1:G:241:MET:HB2	1:G:255:PHE:HE1	1.72	0.55
1:H:162:PRO:HG2	1:H:165:GLU:CD	2.27	0.55
1:A:96:GLY:O	1:A:448:GLY:O	2.25	0.55
1:C:412:GLN:NE2	1:C:447:CYS:SG	2.78	0.55
1:D:412:GLN:HB2	1:D:419:ARG:HB2	1.89	0.55
1:F:136:GLN:HE21	1:F:156:ARG:HD3	1.70	0.55
1:A:275:TYR:CE2	1:A:303:VAL:HG23	2.42	0.54
1:A:452:ASP:HB3	1:C:216:LYS:CD	2.33	0.54
1:B:85:LEU:HD12	1:B:412(C):GLU:CG	2.30	0.54
1:B:133:PHE:O	1:B:158:LEU:HD12	2.07	0.54
1:E:210:ILE:CD1	1:H:413:THR:HG23	2.37	0.54
1:A:180:ALA:HB1	1:A:192:ILE:O	2.08	0.54
1:B:466:PHE:O	1:B:468:ILE:N	2.40	0.54
1:A:216:LYS:HE2	1:D:452:ASP:H	1.72	0.54
1:A:452:ASP:HB2	1:C:216:LYS:HZ2	1.71	0.54
1:B:413:THR:HA	1:D:210:ILE:HD13	1.88	0.54
1:C:290:VAL:HG11	1:C:353:SER:HB2	1.88	0.54
1:D:97:TRP:HD1	1:D:395:GLN:NE2	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:218:TRP:CZ2	1:D:253:LYS:HG3	2.42	0.54
1:H:366:LYS:HD2	1:H:398:VAL:O	2.08	0.54
1:H:322:PHE:HB2	1:H:327:ARG:HD2	1.89	0.54
1:H:428:ARG:NH2	1:H:460:ASP:OD1	2.40	0.54
1:A:333:GLY:N	1:A:386:THR:HG23	2.22	0.54
1:H:411:VAL:HG13	1:H:418:ILE:CG2	2.38	0.54
1:A:333:GLY:H	1:A:386:THR:HG23	1.73	0.54
1:D:411:VAL:CG2	1:D:411:VAL:HG13	2.37	0.54
1:F:102:LYS:HZ2	1:F:104:ASN:HD21	1.55	0.54
1:G:226:GLN:NE2	1:G:239:THR:OG1	2.38	0.54
1:H:436:THR:HG21	1:H:464:LEU:HD13	1.90	0.54
1:B:202:VAL:CG2	1:B:214:THR:HG23	2.37	0.54
1:E:452:ASP:HB3	1:G:216:LYS:CE	2.37	0.54
1:F:216:LYS:NZ	1:G:452:ASP:HB2	2.23	0.54
1:H:355:LYS:NZ	1:H:357:GLY:O	2.38	0.54
1:H:412:GLN:HB2	1:H:419:ARG:CB	2.37	0.54
1:B:190:LEU:HD21	1:B:257:MET:HE3	1.90	0.54
1:C:148:THR:HG23	1:C:430:ARG:HH12	1.72	0.54
1:D:184:HIS:HD2	1:D:186:GLY:N	2.05	0.54
1:E:85:LEU:CD1	1:E:412(C):GLU:HG3	2.37	0.54
1:F:467:THR:O	1:F:468:ILE:HB	2.07	0.54
1:D:466:PHE:O	1:D:468:ILE:N	2.42	0.53
1:H:229:GLU:HG2	1:H:230:CYS:O	2.08	0.53
1:C:120:PRO:HA	1:C:132:PHE:O	2.08	0.53
1:D:413:THR:HG22	1:D:415:LEU:H	1.73	0.53
1:H:275:TYR:CE2	1:H:303:VAL:HG23	2.43	0.53
1:B:343:SER:O	1:B:344:ASN:HB2	2.07	0.53
1:C:270:ALA:HB1	1:C:273:TYR:CB	2.37	0.53
1:C:397:ILE:HG22	1:C:398:VAL:HG23	1.89	0.53
1:B:454:VAL:HG23	1:D:202:VAL:CG1	2.38	0.53
1:D:101:SER:O	1:D:444:ILE:HA	2.09	0.53
1:H:290:VAL:HG21	1:H:353:SER:HB2	1.91	0.53
1:A:360:VAL:HG13	1:A:383:TRP:HE3	1.73	0.53
1:C:360:VAL:HG22	1:C:383:TRP:HB2	1.89	0.53
1:E:448:GLY:O	1:E:449:VAL:HB	2.08	0.53
1:E:454:VAL:HG21	1:G:200:GLY:O	2.08	0.53
1:B:463:GLU:N	1:D:144:HIS:HE1	1.97	0.53
1:C:332:THR:CG2	1:C:386:THR:HG21	2.39	0.53
1:C:416:ASP:OD1	1:C:416:ASP:N	2.36	0.53
1:F:355:LYS:NZ	1:F:357:GLY:O	2.36	0.53
1:G:413:THR:HG22	1:G:415:LEU:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:GLU:O	1:C:350:LYS:HE2	2.09	0.53
1:C:375:GLU:OE1	1:C:394:LYS:HE3	2.09	0.53
1:D:129:CYS:O	1:D:163:VAL:HG23	2.09	0.53
1:D:316:TYR:CZ	1:D:340:PRO:HD3	2.44	0.53
1:F:452:ASP:HB2	1:H:216:LYS:NZ	2.23	0.53
1:A:173:PHE:CZ	1:D:101:SER:HA	2.43	0.53
1:B:96:GLY:O	1:B:448:GLY:O	2.26	0.53
1:D:102:LYS:HZ2	1:D:104:ASN:HD21	1.56	0.53
1:D:467:THR:O	1:D:468:ILE:HB	2.08	0.53
1:F:299:ASN:OD1	1:F:341:VAL:HG23	2.08	0.53
1:A:97:TRP:N	1:A:395:GLN:HE22	2.06	0.52
1:G:442:SER:OG	1:G:460:ASP:OD2	2.27	0.52
1:G:466:PHE:O	1:G:468:ILE:N	2.42	0.52
1:B:101:SER:HA	1:D:173:PHE:CZ	2.44	0.52
1:C:467:THR:O	1:C:468:ILE:HB	2.08	0.52
1:E:105:SER:HB3	1:E:167:PRO:HD2	1.91	0.52
1:G:466:PHE:C	1:G:468:ILE:N	2.62	0.52
1:A:249:GLN:HE21	1:A:272:ASN:N	2.05	0.52
1:G:184:HIS:HD2	1:G:186:GLY:H	1.55	0.52
1:H:172:ARG:HD2	1:H:174:GLU:OE1	2.10	0.52
1:H:270:ALA:HB1	1:H:273:TYR:HB2	1.91	0.52
1:B:133:PHE:CD2	1:B:133:PHE:N	2.77	0.52
1:D:136:GLN:NE2	1:D:156:ARG:HD2	2.24	0.52
1:D:229:GLU:HG2	1:D:230:CYS:O	2.09	0.52
1:F:162:PRO:HG2	1:F:165:GLU:OE2	2.09	0.52
1:C:119:GLU:OE1	1:C:227:GLU:HB3	2.10	0.52
1:H:411:VAL:HG11	1:H:418:ILE:HG23	1.90	0.52
1:E:232:CYS:HA	1:E:236:SER:O	2.10	0.52
1:F:463:GLU:N	1:H:144:HIS:HE1	2.00	0.52
1:E:332:THR:HG23	1:E:386:THR:HG21	1.91	0.52
1:E:333:GLY:H	1:E:386:THR:CG2	2.23	0.52
1:C:397:ILE:HD13	1:C:422:PHE:HZ	1.74	0.52
1:E:99:VAL:HG13	1:E:446:PHE:CE2	2.44	0.52
1:G:406:TYR:HB2	1:G:425:GLU:OE1	2.10	0.52
1:D:333:GLY:N	1:D:386:THR:CG2	2.69	0.52
1:F:117:ILE:HG22	1:F:135:THR:HG22	1.91	0.52
1:F:231:ALA:HB1	1:F:282:PRO:HD3	1.92	0.52
1:F:428:ARG:NH2	1:F:460:ASP:OD1	2.42	0.52
1:B:347:TYR:CG	1:B:348:GLY:N	2.75	0.52
1:B:387:ASP:HB3	1:B:389:SER:H	1.76	0.52
1:C:376:MET:HG2	1:C:397:ILE:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:297:GLY:HA2	1:D:341:VAL:O	2.11	0.52
1:F:397:ILE:CD1	1:F:422:PHE:HZ	2.23	0.52
1:F:466:PHE:C	1:F:468:ILE:N	2.63	0.52
1:D:397:ILE:HD13	1:D:422:PHE:HZ	1.74	0.51
1:E:129:CYS:O	1:E:163:VAL:HG23	2.09	0.51
1:E:466:PHE:C	1:E:468:ILE:H	2.11	0.51
1:A:117:ILE:HG22	1:A:135:THR:HG22	1.91	0.51
1:E:136:GLN:HE21	1:E:156:ARG:CD	2.23	0.51
1:A:467:THR:O	1:A:468:ILE:HB	2.11	0.51
1:B:355:LYS:NZ	1:B:357:GLY:O	2.41	0.51
1:D:133:PHE:O	1:D:158:LEU:HD12	2.11	0.51
1:G:333:GLY:N	1:G:386:THR:HG23	2.24	0.51
1:H:97:TRP:N	1:H:395:GLN:HE22	2.07	0.51
1:H:135:THR:O	1:H:156:ARG:HA	2.10	0.51
1:B:113:ASP:HB3	1:B:139:LEU:HD13	1.92	0.51
1:D:413:THR:CG2	1:D:415:LEU:HD13	2.40	0.51
1:E:88:ASN:N	1:E:88:ASN:ND2	2.55	0.51
1:E:91:LEU:HD11	1:E:281:TYR:CE2	2.46	0.51
1:G:129:CYS:O	1:G:163:VAL:HG23	2.11	0.51
1:G:379:ASP:OD2	1:G:382:GLY:HA3	2.11	0.51
1:H:249:GLN:HE21	1:H:272:ASN:H	1.57	0.51
1:E:452:ASP:CB	1:G:216:LYS:NZ	2.74	0.51
1:A:129:CYS:O	1:A:163:VAL:HG23	2.11	0.51
1:A:287:ILE:N	1:A:287:ILE:HD12	2.26	0.51
1:A:413:THR:CG2	1:A:415:LEU:HB2	2.40	0.51
1:B:155:HIS:HD2	1:C:102:LYS:HE3	1.75	0.51
1:H:316:TYR:CZ	1:H:340:PRO:HD3	2.45	0.51
1:B:184:HIS:HD2	1:B:186:GLY:H	1.57	0.51
1:B:452:ASP:HB2	1:D:216:LYS:HZ3	1.74	0.51
1:D:428:ARG:HB3	1:D:464:LEU:HD11	1.93	0.51
1:G:162:PRO:HG2	1:G:165:GLU:CD	2.31	0.51
1:H:126:HIS:O	1:H:127:LEU:HD23	2.10	0.51
1:A:322:PHE:CE2	1:A:341:VAL:HG21	2.45	0.51
1:D:287:ILE:O	1:D:304:SER:HA	2.11	0.51
1:D:309:ASN:O	1:D:310:LEU:HB2	2.11	0.51
1:D:332:THR:HG22	1:D:386:THR:HG21	1.91	0.51
1:E:172:ARG:HD2	1:E:174:GLU:OE1	2.11	0.51
1:H:268:LEU:HD11	1:H:303:VAL:HG21	1.91	0.51
1:B:102:LYS:HG3	1:B:444:ILE:HG22	1.93	0.51
1:D:380:PRO:HB2	1:D:381:ASN:HD22	1.76	0.51
1:F:182:ALA:O	1:F:229:GLU:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:219:ARG:HB2	1:F:243:ASP:CG	2.31	0.51
1:A:136:GLN:NE2	1:A:156:ARG:HD2	2.23	0.51
1:A:226:GLN:NE2	1:A:239:THR:OG1	2.43	0.51
1:C:227:GLU:HB2	1:C:350:LYS:HD2	1.93	0.51
1:G:85:LEU:HD12	1:G:412(C):GLU:CG	2.33	0.51
1:G:87:GLY:HA3	1:G:233:VAL:HG22	1.93	0.51
1:A:397:ILE:CD1	1:A:422:PHE:HZ	2.24	0.50
1:C:218:TRP:CE2	1:C:253:LYS:HE3	2.46	0.50
1:C:366:LYS:HD2	1:C:398:VAL:O	2.12	0.50
1:D:119:GLU:O	1:D:119:GLU:HG3	2.11	0.50
1:D:366:LYS:HD2	1:D:398:VAL:O	2.10	0.50
1:F:282:PRO:HD2	1:F:411:VAL:CG2	2.41	0.50
1:B:114:VAL:HG13	1:B:167:PRO:O	2.12	0.50
1:D:290:VAL:HG21	1:D:353:SER:HB2	1.92	0.50
1:F:448:GLY:O	1:F:449:VAL:HB	2.10	0.50
1:A:376:MET:HG2	1:A:397:ILE:CD1	2.41	0.50
1:D:287:ILE:N	1:D:287:ILE:CD1	2.74	0.50
1:E:380:PRO:O	1:E:381:ASN:C	2.49	0.50
1:H:104:ASN:HD22	1:H:107:ARG:HD3	1.76	0.50
1:A:89:SER:HB2	1:A:417:CYS:HA	1.92	0.50
1:C:116:VAL:O	1:C:116:VAL:HG13	2.11	0.50
1:E:119:GLU:HG3	1:E:119:GLU:O	2.11	0.50
1:E:412:GLN:HG3	1:E:419:ARG:CG	2.39	0.50
1:G:118:ARG:HB2	1:G:156:ARG:HH11	1.77	0.50
1:B:249:GLN:NE2	1:B:271:PRO:HA	2.26	0.50
1:C:392:VAL:HG12	1:C:394:LYS:N	2.26	0.50
1:D:347:TYR:CG	1:D:348:GLY:N	2.77	0.50
1:C:229:GLU:HG2	1:C:230:CYS:O	2.12	0.50
1:C:275:TYR:CE2	1:C:303:VAL:CG2	2.93	0.50
1:C:466:PHE:C	1:C:468:ILE:H	2.14	0.50
1:F:451:SER:HB2	1:H:214:THR:HB	1.93	0.50
1:H:118:ARG:O	1:H:119:GLU:HG3	2.12	0.50
1:A:116:VAL:HG12	1:A:138:ALA:O	2.11	0.50
1:B:216:LYS:CE	1:C:452:ASP:HB3	2.42	0.50
1:F:122:ILE:HG22	1:F:123:SER:N	2.26	0.50
1:F:135:THR:O	1:F:156:ARG:HA	2.12	0.50
1:H:249:GLN:NE2	1:H:272:ASN:H	2.10	0.50
1:C:91:LEU:HG	1:C:283:ASN:ND2	2.27	0.50
1:D:183:CYS:HB3	1:D:230:CYS:O	2.12	0.50
1:E:202:VAL:CG1	1:H:454:VAL:HG23	2.42	0.50
1:H:466:PHE:C	1:H:468:ILE:N	2.65	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:354:PHE:CZ	1:D:409:SER:HB2	2.47	0.49
1:D:241:MET:HB2	1:D:255:PHE:HE1	1.76	0.49
1:E:194:ILE:HG12	1:E:203:ALA:HB2	1.93	0.49
1:E:453:THR:CG2	1:E:454:VAL:H	2.08	0.49
1:F:118:ARG:C	1:F:119:GLU:CG	2.80	0.49
1:G:118:ARG:C	1:G:119:GLU:CG	2.80	0.49
1:C:109:GLY:HA3	1:C:140:LEU:HD12	1.94	0.49
1:D:88:ASN:N	1:D:88:ASN:ND2	2.58	0.49
1:D:123:SER:OG	1:D:229:GLU:HG3	2.13	0.49
1:G:116:VAL:HG23	1:G:440:SER:HB2	1.94	0.49
1:G:296:HIS:HA	1:G:345:GLY:O	2.12	0.49
1:H:318:CYS:HA	1:H:335:SER:O	2.11	0.49
1:B:115:PHE:CE1	1:B:159:MET:CE	2.96	0.49
1:D:358:ASN:C	1:D:381:ASN:HA	2.33	0.49
1:E:102:LYS:HG3	1:E:444:ILE:HG22	1.94	0.49
1:H:448:GLY:O	1:H:449:VAL:CB	2.55	0.49
1:G:366:LYS:HD2	1:G:398:VAL:O	2.12	0.49
1:D:425:GLU:OE1	1:D:427:ILE:HD11	2.12	0.49
1:E:123:SER:OG	1:E:229:GLU:HG3	2.12	0.49
1:E:202:VAL:CG2	1:E:214:THR:HG23	2.43	0.49
1:A:216:LYS:CE	1:D:452:ASP:CB	2.91	0.49
1:C:249:GLN:HE21	1:C:272:ASN:N	1.81	0.49
1:E:135:THR:O	1:E:156:ARG:HA	2.12	0.49
1:E:463:GLU:N	1:G:144:HIS:HE1	2.00	0.49
1:F:136:GLN:O	1:G:107:ARG:NH1	2.43	0.49
1:F:248:GLY:O	1:F:249:GLN:C	2.51	0.49
1:F:343:SER:O	1:F:344:ASN:CB	2.59	0.49
1:G:376:MET:HG2	1:G:397:ILE:HD11	1.95	0.49
1:B:412(B):PRO:HB3	1:B:415:LEU:O	2.13	0.49
1:F:91:LEU:HG	1:F:283:ASN:HD22	1.75	0.49
1:G:303:VAL:HG22	1:G:314:ILE:HG22	1.95	0.49
1:B:275:TYR:CE2	1:B:303:VAL:HG23	2.47	0.49
1:F:454:VAL:HG21	1:H:200:GLY:O	2.12	0.49
1:C:343:SER:C	1:C:345:GLY:N	2.64	0.48
1:D:413:THR:HG21	1:D:415:LEU:HB2	1.95	0.48
1:F:85:LEU:HD21	1:F:412(A):HIS:CD2	2.48	0.48
1:F:360:VAL:HG13	1:F:383:TRP:HE3	1.78	0.48
1:C:162:PRO:HG2	1:C:165:GLU:OE1	2.14	0.48
1:C:355:LYS:HD2	1:C:383:TRP:CE2	2.47	0.48
1:E:327:ARG:HB2	1:E:328:PRO:HD2	1.95	0.48
1:E:411:VAL:HG12	1:E:412:GLN:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:452:ASP:H	1:G:216:LYS:HE2	1.79	0.48
1:B:216:LYS:NZ	1:C:452:ASP:CB	2.77	0.48
1:F:103:ASP:O	1:F:104:ASN:HB2	2.12	0.48
1:G:335:SER:OG	1:G:339:GLY:O	2.31	0.48
1:D:299:ASN:HD22	1:D:316:TYR:HB3	1.76	0.48
1:F:264:LYS:HG2	1:F:310:LEU:HD22	1.94	0.48
1:G:192:ILE:HG23	1:G:205:LEU:CD2	2.44	0.48
1:A:112:GLY:O	1:D:111:LYS:NZ	2.46	0.48
1:A:293:ASP:OD2	1:A:293:ASP:C	2.52	0.48
1:D:319:SER:HB2	1:D:382:GLY:O	2.14	0.48
1:E:105:SER:CB	1:E:167:PRO:HD2	2.43	0.48
1:E:168:SER:CB	1:E:169:PRO:HD2	2.40	0.48
1:F:102:LYS:HZ2	1:F:104:ASN:ND2	2.11	0.48
1:H:287:ILE:O	1:H:304:SER:HA	2.14	0.48
1:H:325:ASN:O	1:H:348:GLY:HA2	2.13	0.48
1:B:173:PHE:CZ	1:C:101:SER:HA	2.48	0.48
1:H:408:GLY:HA3	1:H:423:TRP:CZ2	2.49	0.48
1:A:463:GLU:N	1:C:144:HIS:HE1	1.84	0.48
1:B:184:HIS:CD2	1:B:186:GLY:H	2.32	0.48
1:F:216:LYS:NZ	1:G:452:ASP:HB3	2.29	0.48
1:B:226:GLN:O	1:B:227:GLU:HB2	2.13	0.48
1:E:333:GLY:N	1:E:386:THR:HG23	2.28	0.48
1:E:424:VAL:HG12	1:E:425:GLU:N	2.28	0.48
1:F:136:GLN:NE2	1:F:156:ARG:CD	2.76	0.48
1:G:144:HIS:C	1:G:146:ASN:H	2.17	0.48
1:A:332:THR:HG23	1:A:386:THR:HG21	1.95	0.48
1:B:135:THR:O	1:B:156:ARG:HA	2.13	0.48
1:E:287:ILE:N	1:E:287:ILE:CD1	2.77	0.48
1:G:146:ASN:O	1:G:148:THR:N	2.47	0.48
1:C:228:SER:CB	1:C:350:LYS:CE	2.73	0.47
1:D:413:THR:CG2	1:D:415:LEU:HB2	2.44	0.47
1:E:101:SER:HA	1:G:173:PHE:CZ	2.49	0.47
1:E:406:TYR:HB2	1:E:425:GLU:OE1	2.14	0.47
1:E:411:VAL:HG13	1:E:418:ILE:HG23	1.95	0.47
1:E:467:THR:O	1:E:468:ILE:HB	2.14	0.47
1:F:202:VAL:HG23	1:F:214:THR:HG23	1.95	0.47
1:G:297:GLY:N	1:G:345:GLY:O	2.47	0.47
1:A:164:GLY:HA3	1:C:173:PHE:CG	2.48	0.47
1:B:216:LYS:NZ	1:C:452:ASP:HB3	2.29	0.47
1:F:88:ASN:N	1:F:88:ASN:ND2	2.58	0.47
1:E:228:SER:HB3	1:E:350:LYS:CE	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:452:ASP:HB2	1:G:216:LYS:HZ2	1.79	0.47
1:F:148:THR:HG23	1:F:430:ARG:HH12	1.80	0.47
1:F:412:GLN:HB2	1:F:419:ARG:HB3	1.97	0.47
1:F:429:GLY:O	1:F:433:GLU:N	2.46	0.47
1:G:190:LEU:HD21	1:G:257:MET:HE3	1.96	0.47
1:A:99:VAL:HG12	1:A:446:PHE:CE2	2.50	0.47
1:B:413:THR:CG2	1:B:415:LEU:HB2	2.43	0.47
1:D:102:LYS:NZ	1:D:104:ASN:ND2	2.63	0.47
1:G:120:PRO:HA	1:G:132:PHE:O	2.13	0.47
1:H:85:LEU:HA	1:H:412(C):GLU:OE1	2.13	0.47
1:B:183:CYS:SG	1:B:190:LEU:HD23	2.54	0.47
1:D:453:THR:CG2	1:D:454:VAL:N	2.68	0.47
1:A:297:GLY:HA2	1:A:341:VAL:O	2.14	0.47
1:B:228:SER:HB3	1:B:350:LYS:CE	2.44	0.47
1:F:366:LYS:CD	1:F:400:ILE:HG12	2.40	0.47
1:G:121:PHE:CB	1:G:228:SER:HA	2.45	0.47
1:H:254:ILE:HD11	1:H:303:VAL:HG11	1.95	0.47
1:H:332:THR:HG23	1:H:386:THR:HG21	1.96	0.47
1:H:380:PRO:O	1:H:381:ASN:C	2.51	0.47
1:B:321:VAL:HG12	1:B:321:VAL:O	2.13	0.47
1:G:347:TYR:CG	1:G:348:GLY:N	2.83	0.47
1:H:339:GLY:O	1:H:340:PRO:C	2.52	0.47
1:A:412:GLN:HB2	1:A:419:ARG:HB2	1.97	0.47
1:B:182:ALA:O	1:B:229:GLU:HA	2.15	0.47
1:C:332:THR:HG23	1:C:386:THR:HG21	1.97	0.47
1:E:290:VAL:HG21	1:E:353:SER:HB2	1.97	0.47
1:E:366:LYS:HD2	1:E:398:VAL:O	2.15	0.47
1:F:397:ILE:HD13	1:F:422:PHE:CZ	2.49	0.47
1:A:451:SER:HB2	1:C:214:THR:HB	1.97	0.47
1:E:136:GLN:HE21	1:E:156:ARG:HD3	1.80	0.47
1:E:228:SER:HB3	1:E:350:LYS:HE2	1.96	0.47
1:E:451:SER:CB	1:G:214:THR:HB	2.45	0.47
1:A:216:LYS:CE	1:D:452:ASP:HB3	2.44	0.46
1:A:392:VAL:HG12	1:A:394:LYS:N	2.30	0.46
1:C:300:ARG:HH12	1:C:349:VAL:HG13	1.81	0.46
1:E:162:PRO:HG2	1:E:165:GLU:OE2	2.15	0.46
1:E:444:ILE:HG13	1:E:444:ILE:O	2.16	0.46
1:G:152:ARG:HH21	1:G:152:ARG:HG3	1.78	0.46
1:A:273:TYR:CD2	1:A:316:TYR:CE1	3.03	0.46
1:A:294:ASN:HA	1:A:347:TYR:O	2.16	0.46
1:A:327:ARG:O	1:A:344:ASN:ND2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:TRP:CE2	1:B:253:LYS:HE3	2.50	0.46
1:B:248:GLY:O	1:B:249:GLN:C	2.51	0.46
1:C:342:SER:O	1:C:343:SER:C	2.53	0.46
1:C:466:PHE:C	1:C:468:ILE:N	2.67	0.46
1:E:216:LYS:NZ	1:H:452:ASP:HB3	2.30	0.46
1:E:354:PHE:CZ	1:E:409:SER:HB2	2.49	0.46
1:F:216:LYS:HZ3	1:G:452:ASP:HB2	1.78	0.46
1:G:316:TYR:CD1	1:G:340:PRO:HD3	2.50	0.46
1:A:451:SER:HB2	1:C:214:THR:HG22	1.96	0.46
1:B:88:ASN:N	1:B:88:ASN:HD22	2.13	0.46
1:B:173:PHE:CG	1:C:164:GLY:HA3	2.51	0.46
1:B:287:ILE:HG22	1:B:288:THR:N	2.29	0.46
1:C:136:GLN:HE21	1:C:156:ARG:CD	2.28	0.46
1:D:136:GLN:HE21	1:D:156:ARG:HD2	1.79	0.46
1:E:287:ILE:HG22	1:E:288:THR:N	2.31	0.46
1:E:377:ILE:HG23	1:E:390:PHE:CD1	2.51	0.46
1:E:453:THR:HG22	1:E:454:VAL:N	2.20	0.46
1:G:102:LYS:HG3	1:G:444:ILE:HG22	1.96	0.46
1:H:411:VAL:HG12	1:H:412:GLN:N	2.30	0.46
1:H:413:THR:HB	1:H:415:LEU:HB2	1.97	0.46
1:A:325:ASN:O	1:A:348:GLY:HA2	2.15	0.46
1:D:397:ILE:HG22	1:D:398:VAL:HG23	1.97	0.46
1:F:102:LYS:NZ	1:F:104:ASN:ND2	2.64	0.46
1:F:411:VAL:HG13	1:F:418:ILE:CG2	2.44	0.46
1:F:419:ARG:NH1	1:F:419:ARG:HG3	2.31	0.46
1:H:88:ASN:H	1:H:88:ASN:ND2	2.12	0.46
1:C:453:THR:HG22	1:C:454:VAL:N	2.16	0.46
1:E:250:ALA:HB3	1:E:252:TYR:HE2	1.79	0.46
1:E:332:THR:HG23	1:E:386:THR:CG2	2.45	0.46
1:E:415:LEU:HD12	1:E:415:LEU:HA	1.71	0.46
1:G:249:GLN:HE21	1:G:272:ASN:N	2.09	0.46
1:G:397:ILE:HD11	1:G:422:PHE:HZ	1.79	0.46
1:H:150:LYS:NZ	1:H:150:LYS:HD2	2.31	0.46
1:A:88:ASN:N	1:A:88:ASN:ND2	2.57	0.46
1:A:172:ARG:HD2	1:A:174:GLU:OE1	2.15	0.46
1:B:254:ILE:HD13	1:B:305:PHE:CD2	2.51	0.46
1:B:407:SER:HA	1:B:423:TRP:O	2.16	0.46
1:E:271:PRO:O	1:E:272:ASN:HB3	2.15	0.46
1:B:277:GLU:OE1	1:B:350:LYS:HB2	2.16	0.46
1:C:305:PHE:HB3	1:C:312:TYR:HB3	1.97	0.46
1:C:332:THR:HG23	1:C:386:THR:CG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:LYS:HZ2	1:D:104:ASN:ND2	2.14	0.46
1:H:355:LYS:HB2	1:H:383:TRP:CE3	2.51	0.46
1:A:273:TYR:CD2	1:A:316:TYR:HE1	2.33	0.46
1:C:136:GLN:NE2	1:C:156:ARG:HD2	2.30	0.46
1:C:343:SER:O	1:C:345:GLY:N	2.49	0.46
1:D:286:GLU:C	1:D:287:ILE:HD12	2.36	0.46
1:E:413:THR:HG23	1:G:210:ILE:HD12	1.98	0.46
1:F:390:PHE:CD2	1:F:390:PHE:N	2.83	0.46
1:G:412(B):PRO:HB3	1:G:415:LEU:O	2.16	0.46
1:B:121:PHE:CG	1:B:228:SER:HA	2.51	0.46
1:G:152:ARG:HG3	1:G:152:ARG:NH2	2.31	0.46
1:D:96:GLY:O	1:D:448:GLY:O	2.34	0.45
1:E:324:ASP:O	1:E:327:ARG:HD3	2.15	0.45
1:C:254:ILE:HD11	1:C:268:LEU:HD21	1.97	0.45
1:E:452:ASP:CB	1:G:216:LYS:CE	2.94	0.45
1:F:225:THR:OG1	1:F:226:GLN:N	2.48	0.45
1:G:181:SER:OG	1:G:192:ILE:HD12	2.16	0.45
1:H:411:VAL:CG1	1:H:418:ILE:CG2	2.91	0.45
1:E:97:TRP:H	1:E:395:GLN:HE22	1.64	0.45
1:E:227:GLU:OE1	1:E:227:GLU:CA	2.64	0.45
1:G:467:THR:HG22	1:G:467:THR:O	2.15	0.45
1:A:325:ASN:HA	1:A:326:PRO:C	2.36	0.45
1:E:274:HIS:HB3	1:E:293:ASP:OD2	2.15	0.45
1:E:320:GLY:N	1:E:387:ASP:O	2.49	0.45
1:F:136:GLN:NE2	1:F:156:ARG:HD3	2.31	0.45
1:F:275:TYR:CE2	1:F:303:VAL:CG2	2.95	0.45
1:G:237:CYS:O	1:G:257:MET:HG2	2.16	0.45
1:H:153:SER:HB2	1:H:154:PRO:HD2	1.97	0.45
1:A:270:ALA:O	1:A:273:TYR:HB2	2.17	0.45
1:A:433:GLU:OE2	1:A:464:LEU:HD12	2.15	0.45
1:B:146:ASN:O	1:B:437:ILE:O	2.35	0.45
1:B:219:ARG:HB2	1:B:243:ASP:CG	2.37	0.45
1:B:287:ILE:N	1:B:287:ILE:CD1	2.78	0.45
1:B:354:PHE:CZ	1:B:409:SER:HB2	2.51	0.45
1:E:254:ILE:CD1	1:E:268:LEU:HD21	2.41	0.45
1:H:320:GLY:CA	1:H:387:ASP:O	2.56	0.45
1:H:453:THR:CG2	1:H:454:VAL:H	2.30	0.45
1:A:328:PRO:HD3	1:A:343:SER:O	2.17	0.45
1:D:136:GLN:HE21	1:D:156:ARG:CD	2.30	0.45
1:E:300:ARG:HB2	1:E:317:ILE:HD12	1.99	0.45
1:F:116:VAL:O	1:F:116:VAL:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:366:LYS:HG3	1:F:374:PHE:N	2.32	0.45
1:A:136:GLN:NE2	1:A:156:ARG:CD	2.75	0.45
1:A:210:ILE:HD13	1:D:413:THR:HA	1.99	0.45
1:A:226:GLN:O	1:A:227:GLU:HB2	2.17	0.45
1:A:397:ILE:HG22	1:A:398:VAL:HG23	1.98	0.45
1:B:232:CYS:HA	1:B:237:CYS:HA	1.97	0.45
1:B:424:VAL:HB	1:B:444:ILE:HG13	1.98	0.45
1:E:233:VAL:O	1:E:235:GLY:N	2.50	0.45
1:E:332:THR:CG2	1:E:386:THR:HG21	2.47	0.45
1:E:412(B):PRO:HD3	1:E:418:ILE:HA	1.98	0.45
1:F:287:ILE:N	1:F:287:ILE:CD1	2.78	0.45
1:G:467:THR:O	1:G:468:ILE:HB	2.16	0.45
1:A:397:ILE:HG23	1:A:446:PHE:CZ	2.52	0.45
1:B:226:GLN:NE2	1:B:239:THR:OG1	2.39	0.45
1:D:156:ARG:HG2	1:D:178:TRP:HA	1.98	0.45
1:G:275:TYR:HE2	1:G:303:VAL:HG23	1.76	0.45
1:H:96:GLY:O	1:H:448:GLY:O	2.34	0.45
1:H:150:LYS:CE	1:H:150:LYS:CB	2.94	0.45
1:B:426:LEU:HD13	1:B:460:ASP:N	2.32	0.45
1:E:85:LEU:HD21	1:E:412(A):HIS:CD2	2.52	0.45
1:H:202:VAL:HG21	1:H:214:THR:HG23	1.98	0.45
1:H:360:VAL:HG13	1:H:383:TRP:HE3	1.81	0.45
1:H:375:GLU:OE1	1:H:394:LYS:CE	2.65	0.45
1:A:343:SER:O	1:A:344:ASN:HB3	2.17	0.45
1:C:113:ASP:HB3	1:C:139:LEU:HD13	1.99	0.45
1:G:360:VAL:HG13	1:G:383:TRP:HE3	1.82	0.45
1:H:98:ALA:O	1:H:446:PHE:HA	2.17	0.45
1:A:347:TYR:CG	1:A:348:GLY:N	2.83	0.44
1:A:413:THR:HG21	1:A:415:LEU:HB2	1.98	0.44
1:C:159:MET:HA	1:C:174:GLU:HG2	1.99	0.44
1:D:99:VAL:HG13	1:D:446:PHE:CE2	2.52	0.44
1:D:322:PHE:CE1	1:D:328:PRO:HG2	2.51	0.44
1:E:343:SER:O	1:E:344:ASN:HB2	2.16	0.44
1:F:113:ASP:O	1:F:169:PRO:HD2	2.17	0.44
1:F:210:ILE:CD1	1:G:413:THR:HA	2.46	0.44
1:G:152:ARG:NH1	1:G:222:ILE:HD13	2.32	0.44
1:H:377:ILE:HG23	1:H:390:PHE:CD1	2.52	0.44
1:A:113:ASP:OD2	1:A:169(A):TYR:OH	2.33	0.44
1:B:430:ARG:HD2	1:B:436:THR:O	2.16	0.44
1:E:411:VAL:HG13	1:E:418:ILE:CG2	2.47	0.44
1:F:121:PHE:CG	1:F:228:SER:HA	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:144:HIS:HE1	1:G:463:GLU:N	2.08	0.44
1:F:419:ARG:HG3	1:F:419:ARG:HH11	1.82	0.44
1:G:375:GLU:OE1	1:G:394:LYS:HE3	2.17	0.44
1:H:117:ILE:HD13	1:H:167:PRO:HG3	1.98	0.44
1:H:355:LYS:HB2	1:H:383:TRP:CZ3	2.53	0.44
1:A:320:GLY:CA	1:A:387:ASP:O	2.63	0.44
1:E:373:GLY:HA2	1:E:398:VAL:O	2.17	0.44
1:F:466:PHE:C	1:F:468:ILE:H	2.21	0.44
1:G:226:GLN:O	1:G:227:GLU:HB2	2.17	0.44
1:H:172:ARG:HG2	1:H:173:PHE:N	2.31	0.44
1:H:232:CYS:HA	1:H:237:CYS:HA	1.99	0.44
1:E:328:PRO:HD3	1:E:343:SER:O	2.18	0.44
1:F:119:GLU:CD	1:F:134:LEU:HD12	2.38	0.44
1:F:300:ARG:HG2	1:F:300:ARG:HH21	1.82	0.44
1:G:377:ILE:HG23	1:G:390:PHE:CD1	2.52	0.44
1:A:85:LEU:HD12	1:A:412(C):GLU:HG3	1.99	0.44
1:A:118:ARG:O	1:A:119:GLU:HG3	2.17	0.44
1:B:132:PHE:HB3	1:B:158:LEU:HD11	2.00	0.44
1:C:192:ILE:HG23	1:C:205:LEU:CD2	2.48	0.44
1:E:452:ASP:O	1:G:214:THR:CG2	2.56	0.44
1:G:413:THR:CG2	1:G:415:LEU:HD13	2.47	0.44
1:B:451:SER:CB	1:D:214:THR:HB	2.48	0.44
1:C:355:LYS:HB2	1:C:383:TRP:CZ3	2.52	0.44
1:F:406:TYR:HB2	1:F:425:GLU:OE1	2.18	0.44
1:H:85:LEU:HD12	1:H:412(C):GLU:HG3	2.00	0.44
1:C:254:ILE:CD1	1:C:268:LEU:HD21	2.48	0.44
1:C:412:GLN:CB	1:C:419:ARG:HB2	2.46	0.44
1:D:249:GLN:NE2	1:D:271:PRO:HA	2.33	0.44
1:E:451:SER:HB2	1:G:214:THR:HG22	1.99	0.44
1:G:152:ARG:CZ	1:G:222:ILE:HD13	2.46	0.44
1:G:286:GLU:C	1:G:287:ILE:HD12	2.38	0.44
1:G:365:THR:HA	1:G:373:GLY:O	2.18	0.44
1:H:148:THR:HG22	1:H:430:ARG:HH22	1.82	0.44
1:A:238:PHE:HA	1:A:255:PHE:O	2.18	0.44
1:D:251:SER:OG	1:D:267:GLU:OE2	2.34	0.44
1:F:270:ALA:HB1	1:F:273:TYR:HB2	1.99	0.44
1:G:397:ILE:CD1	1:G:422:PHE:HZ	2.31	0.44
1:H:146:ASN:O	1:H:148:THR:N	2.50	0.44
1:D:270:ALA:HB1	1:D:273:TYR:HB2	1.99	0.43
1:D:328:PRO:HD3	1:D:343:SER:O	2.18	0.43
1:E:164:GLY:HA3	1:G:173:PHE:CG	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:360:VAL:HG22	1:E:383:TRP:HB2	2.00	0.43
1:F:248:GLY:HA2	1:F:295:TRP:CZ2	2.53	0.43
1:B:116:VAL:HG23	1:B:440:SER:HB2	2.01	0.43
1:B:210:ILE:HD13	1:C:413:THR:HA	2.00	0.43
1:B:397:ILE:HG23	1:B:446:PHE:CZ	2.53	0.43
1:F:332:THR:HG23	1:F:386:THR:HG22	2.01	0.43
1:F:421:CYS:HB3	1:F:446:PHE:O	2.18	0.43
1:G:366:LYS:HB3	1:G:400:ILE:HG12	2.00	0.43
1:H:85:LEU:CD1	1:H:412(C):GLU:HG3	2.48	0.43
1:H:117:ILE:HD12	1:H:120:PRO:HB3	2.00	0.43
1:D:161:CYS:HB2	1:D:162:PRO:HD2	2.00	0.43
1:D:184:HIS:CD2	1:D:186:GLY:N	2.80	0.43
1:G:324:ASP:O	1:G:327:ARG:HD3	2.19	0.43
1:H:152:ARG:HG3	1:H:152:ARG:HH21	1.82	0.43
1:A:412(B):PRO:HB3	1:A:415:LEU:O	2.19	0.43
1:B:299:ASN:OD1	1:B:299:ASN:N	2.38	0.43
1:C:136:GLN:HE21	1:C:156:ARG:HD2	1.84	0.43
1:C:158:LEU:O	1:C:174:GLU:HB2	2.18	0.43
1:D:293:ASP:OD2	1:D:293:ASP:C	2.56	0.43
1:E:210:ILE:HD13	1:H:413:THR:HG23	2.00	0.43
1:E:282:PRO:HD2	1:E:411:VAL:HG21	1.99	0.43
1:E:413:THR:HG21	1:E:415:LEU:HB2	2.01	0.43
1:F:397:ILE:HG23	1:F:446:PHE:CZ	2.54	0.43
1:G:150:LYS:HD3	1:G:152:ARG:O	2.17	0.43
1:G:411:VAL:HG13	1:G:418:ILE:CG2	2.48	0.43
1:G:412(D):LEU:O	1:G:412(D):LEU:HD12	2.19	0.43
1:B:190:LEU:HD13	1:B:260:GLY:HA2	2.00	0.43
1:C:335:SER:OG	1:C:339:GLY:O	2.36	0.43
1:F:453:THR:CG2	1:F:454:VAL:H	2.22	0.43
1:H:190:LEU:HA	1:H:206:LYS:O	2.18	0.43
1:B:172:ARG:HD2	1:B:174:GLU:OE1	2.18	0.43
1:B:438:TRP:CZ2	1:B:464:LEU:HD22	2.54	0.43
1:C:97:TRP:H	1:C:395:GLN:HE22	1.65	0.43
1:B:88:ASN:HD22	1:B:88:ASN:H	1.65	0.43
1:D:364:ARG:O	1:D:374:PHE:HA	2.19	0.43
1:E:451:SER:OG	1:G:214:THR:HB	2.19	0.43
1:G:358:ASN:HB3	1:G:381:ASN:HA	2.00	0.43
1:A:116:VAL:HG23	1:A:440:SER:CB	2.45	0.43
1:A:295:TRP:CD1	1:A:295:TRP:C	2.90	0.43
1:A:449:VAL:HG13	1:A:451:SER:OG	2.19	0.43
1:C:140:LEU:HD23	1:C:140:LEU:HA	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:316:TYR:CZ	1:E:340:PRO:HD3	2.54	0.43
1:H:421:CYS:HB3	1:H:446:PHE:O	2.19	0.43
1:D:413:THR:HG22	1:D:415:LEU:HD13	2.00	0.43
1:E:156:ARG:HG2	1:E:178:TRP:HA	2.00	0.43
1:F:263:VAL:O	1:F:264:LYS:HB2	2.19	0.43
1:G:380:PRO:O	1:G:381:ASN:C	2.57	0.43
1:H:428:ARG:NH1	1:H:464:LEU:HG	2.34	0.43
1:A:343:SER:O	1:A:344:ASN:CB	2.66	0.43
1:B:451:SER:HB2	1:D:214:THR:HG22	2.01	0.43
1:C:116:VAL:HG12	1:C:138:ALA:O	2.19	0.43
1:E:210:ILE:HD12	1:H:413:THR:HG23	2.00	0.43
1:G:355:LYS:HB2	1:G:383:TRP:CZ3	2.53	0.43
1:G:428:ARG:NH1	1:G:464:LEU:HG	2.34	0.43
1:G:430:ARG:HD2	1:G:436:THR:O	2.18	0.43
1:H:90:SER:O	1:H:417:CYS:HB2	2.19	0.43
1:B:228:SER:HB3	1:B:350:LYS:HE2	2.00	0.42
1:B:238:PHE:N	1:B:238:PHE:CD1	2.87	0.42
1:E:154:PRO:HB3	1:H:456:TRP:CZ3	2.54	0.42
1:E:225:THR:OG1	1:E:226:GLN:N	2.52	0.42
1:H:158:LEU:HG	1:H:174:GLU:HB2	2.00	0.42
1:H:343:SER:O	1:H:344:ASN:CB	2.66	0.42
1:A:397:ILE:HD13	1:A:422:PHE:HZ	1.83	0.42
1:B:102:LYS:HZ2	1:B:104:ASN:ND2	2.17	0.42
1:B:283:ASN:O	1:B:284:ALA:C	2.54	0.42
1:B:320:GLY:HA3	1:B:387:ASP:O	2.19	0.42
1:C:287:ILE:N	1:C:287:ILE:CD1	2.77	0.42
1:C:319:SER:HB2	1:C:382:GLY:O	2.19	0.42
1:D:289:CYS:O	1:D:302:TRP:HA	2.19	0.42
1:E:85:LEU:CD2	1:E:412(A):HIS:CD2	3.02	0.42
1:G:116:VAL:HG12	1:G:138:ALA:O	2.19	0.42
1:A:306:ASN:OD1	1:A:308:GLN:N	2.53	0.42
1:D:120:PRO:HA	1:D:132:PHE:O	2.19	0.42
1:D:191:THR:OG1	1:D:206:LYS:HB2	2.20	0.42
1:D:355:LYS:NZ	1:D:357:GLY:O	2.51	0.42
1:E:202:VAL:HG23	1:E:214:THR:HG23	2.02	0.42
1:E:273:TYR:CD2	1:E:316:TYR:HE1	2.37	0.42
1:E:301:PRO:HB3	1:E:316:TYR:CZ	2.55	0.42
1:G:421:CYS:HA	1:G:447:CYS:HA	2.01	0.42
1:H:102:LYS:HG3	1:H:444:ILE:CG2	2.47	0.42
1:H:316:TYR:CD1	1:H:340:PRO:HD3	2.54	0.42
1:B:452:ASP:O	1:D:214:THR:CG2	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:102:LYS:NZ	1:D:104:ASN:HD21	2.16	0.42
1:E:226:GLN:HE22	1:E:230:CYS:HA	1.85	0.42
1:E:412(C):GLU:H	1:E:412(C):GLU:HG2	1.64	0.42
1:F:85:LEU:HB2	1:F:185:ASP:O	2.19	0.42
1:H:430:ARG:HD2	1:H:436:THR:O	2.19	0.42
1:B:131:THR:O	1:B:160:SER:HA	2.18	0.42
1:D:142:ASP:OD2	1:D:144:HIS:HD2	2.03	0.42
1:E:333:GLY:N	1:E:386:THR:CG2	2.83	0.42
1:E:411:VAL:CG2	1:E:411:VAL:HG13	2.44	0.42
1:A:182:ALA:O	1:A:229:GLU:HA	2.20	0.42
1:B:322:PHE:CE1	1:B:328:PRO:HG2	2.54	0.42
1:B:467:THR:HG22	1:B:467:THR:O	2.20	0.42
1:C:426:LEU:O	1:C:441:GLY:HA2	2.20	0.42
1:F:122:ILE:HD12	1:F:445:SER:HB3	2.02	0.42
1:H:403:TRP:CH2	1:H:432:LYS:HB3	2.54	0.42
1:B:200:GLY:O	1:C:454:VAL:HG21	2.19	0.42
1:B:438:TRP:HZ2	1:B:464:LEU:HD22	1.84	0.42
1:E:347:TYR:CG	1:E:348:GLY:N	2.88	0.42
1:F:303:VAL:HG22	1:F:314:ILE:HG22	2.00	0.42
1:G:148:THR:HG23	1:G:430:ARG:HH12	1.85	0.42
1:D:91:LEU:HD11	1:D:281:TYR:CE2	2.54	0.42
1:D:301:PRO:HB3	1:D:316:TYR:CZ	2.55	0.42
1:D:366:LYS:HG3	1:D:374:PHE:N	2.35	0.42
1:E:202:VAL:HG11	1:H:454:VAL:HG23	2.02	0.42
1:F:99:VAL:HG13	1:F:446:PHE:CE2	2.55	0.42
1:F:202:VAL:CG1	1:G:454:VAL:CG2	2.97	0.42
1:H:299:ASN:ND2	1:H:316:TYR:HB3	2.35	0.42
1:A:120:PRO:HD2	1:A:425:GLU:HB2	2.00	0.42
1:A:355:LYS:HD2	1:A:383:TRP:CE2	2.55	0.42
1:C:119:GLU:OE1	1:C:227:GLU:OE1	2.38	0.42
1:C:135:THR:O	1:C:156:ARG:HA	2.19	0.42
1:C:378:TRP:HB3	1:C:392:VAL:HB	2.02	0.42
1:D:397:ILE:HD13	1:D:422:PHE:CZ	2.55	0.42
1:F:392:VAL:HG12	1:F:394:LYS:N	2.34	0.42
1:F:452:ASP:HB2	1:H:216:LYS:HZ3	1.85	0.42
1:H:257:MET:HA	1:H:261:LYS:O	2.19	0.42
1:A:258:GLU:O	1:A:259:LYS:HB2	2.20	0.42
1:C:102:LYS:NZ	1:C:104:ASN:ND2	2.68	0.42
1:C:270:ALA:O	1:C:273:TYR:HB2	2.20	0.42
1:E:181:SER:HB2	1:E:228:SER:O	2.20	0.42
1:E:216:LYS:NZ	1:H:452:ASP:CB	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:232:CYS:HA	1:E:237:CYS:HA	2.02	0.42
1:H:327:ARG:HB2	1:H:328:PRO:HD2	2.01	0.42
1:A:180:ALA:CB	1:A:192:ILE:O	2.68	0.41
2:B:800:G39:H811	2:B:800:G39:H912	1.86	0.41
1:C:158:LEU:HD22	1:C:180:ALA:HB1	2.02	0.41
1:C:182:ALA:O	1:C:229:GLU:HA	2.20	0.41
1:D:370:SER:HB2	1:D:372:SER:OG	2.21	0.41
1:F:142:ASP:OD2	1:F:144:HIS:HB2	2.20	0.41
1:F:452:ASP:CB	1:H:216:LYS:NZ	2.83	0.41
1:C:316:TYR:CE1	1:C:340:PRO:HD3	2.55	0.41
1:C:411:VAL:CG1	1:C:412:GLN:N	2.83	0.41
1:E:155:HIS:HB3	1:H:104:ASN:HD21	1.85	0.41
1:E:287:ILE:O	1:E:304:SER:HA	2.20	0.41
1:G:192:ILE:HG23	1:G:205:LEU:HD22	2.01	0.41
1:A:155:HIS:HD2	1:D:102:LYS:HZ2	1.66	0.41
1:A:248:GLY:HA2	1:A:295:TRP:NE1	2.35	0.41
1:B:135:THR:OG1	1:B:159:MET:HE2	2.19	0.41
1:B:428:ARG:HB3	1:B:464:LEU:HD11	2.01	0.41
1:C:254:ILE:O	1:C:265:SER:HA	2.20	0.41
1:C:320:GLY:CA	1:C:387:ASP:O	2.67	0.41
1:C:322:PHE:CD1	1:C:328:PRO:HG2	2.55	0.41
1:C:379:ASP:OD2	1:C:382:GLY:HA3	2.19	0.41
1:E:132:PHE:CD2	1:E:160:SER:HB3	2.56	0.41
1:B:226:GLN:O	1:B:227:GLU:CB	2.66	0.41
1:B:321:VAL:CG1	1:B:364:ARG:NH2	2.83	0.41
1:B:453:THR:HG22	1:B:454:VAL:N	2.20	0.41
1:C:172:ARG:HD2	1:C:174:GLU:OE1	2.21	0.41
1:D:99:VAL:HG11	1:D:458:TRP:CE2	2.56	0.41
1:D:135:THR:OG1	1:D:159:MET:HE2	2.20	0.41
1:D:238:PHE:CD1	1:D:238:PHE:N	2.89	0.41
1:E:116:VAL:O	1:E:116:VAL:HG13	2.21	0.41
1:F:339:GLY:HA2	1:F:340:PRO:HD2	1.67	0.41
1:G:184:HIS:HD2	1:G:186:GLY:N	2.18	0.41
1:H:373:GLY:HA2	1:H:399:ALA:O	2.20	0.41
1:A:250:ALA:HB3	1:A:252:TYR:HE2	1.85	0.41
1:B:169(A):TYR:CD2	1:B:169(A):TYR:N	2.84	0.41
1:C:379:ASP:C	1:C:380:PRO:O	2.58	0.41
1:C:433:GLU:CD	1:C:464:LEU:HD12	2.41	0.41
1:D:142:ASP:OD2	1:D:144:HIS:CD2	2.73	0.41
1:D:343:SER:O	1:D:344:ASN:HB2	2.21	0.41
1:E:174:GLU:HA	1:E:174:GLU:OE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:239:THR:CG2	1:E:257:MET:HE1	2.51	0.41
1:F:202:VAL:HG12	1:G:454:VAL:CG2	2.51	0.41
1:H:121:PHE:CG	1:H:228:SER:HA	2.55	0.41
1:B:102:LYS:NZ	1:B:104:ASN:ND2	2.69	0.41
1:B:155:HIS:CE1	1:C:461:GLY:HA3	2.56	0.41
1:B:181:SER:OG	1:B:192:ILE:HD12	2.21	0.41
1:C:448:GLY:O	1:C:449:VAL:HB	2.19	0.41
1:A:218:TRP:N	1:A:243:ASP:OD1	2.52	0.41
1:A:310:LEU:HA	1:A:310:LEU:HD12	1.87	0.41
1:B:448:GLY:O	1:B:449:VAL:CB	2.50	0.41
1:C:116:VAL:HG23	1:C:440:SER:HB2	2.02	0.41
1:E:355:LYS:NZ	1:E:357:GLY:O	2.54	0.41
1:F:122:ILE:CG2	1:F:123:SER:N	2.83	0.41
1:A:102:LYS:HG3	1:A:444:ILE:CG2	2.47	0.41
1:A:159:MET:HA	1:A:174:GLU:HG2	2.02	0.41
1:B:155:HIS:NE2	1:C:461:GLY:HA3	2.36	0.41
1:B:454:VAL:HG23	1:D:202:VAL:HG11	2.02	0.41
1:C:144:HIS:C	1:C:146:ASN:H	2.24	0.41
1:C:332:THR:HG22	1:C:386:THR:HG21	2.03	0.41
1:D:90:SER:O	1:D:417:CYS:HB2	2.21	0.41
1:A:210:ILE:HD12	1:D:413:THR:HG23	2.02	0.41
1:A:332:THR:CG2	1:A:386:THR:HG21	2.50	0.41
1:B:264:LYS:HG2	1:B:310:LEU:CD2	2.45	0.41
1:B:451:SER:HB2	1:D:214:THR:HB	2.03	0.41
1:C:247:ASN:O	1:C:248:GLY:O	2.39	0.41
1:D:102:LYS:HG3	1:D:444:ILE:HG22	2.03	0.41
1:D:327:ARG:HB2	1:D:328:PRO:HD2	2.03	0.41
1:E:146:ASN:O	1:E:437:ILE:O	2.38	0.41
1:E:430:ARG:HD2	1:E:436:THR:O	2.21	0.41
1:F:152:ARG:HB3	1:F:178:TRP:CG	2.55	0.41
1:F:238:PHE:CD1	1:F:238:PHE:N	2.89	0.41
1:F:256:LYS:HG2	1:F:263:VAL:CG2	2.51	0.41
1:G:225:THR:OG1	1:G:226:GLN:N	2.53	0.41
1:G:420:PRO:O	1:G:448:GLY:N	2.48	0.41
1:H:366:LYS:HB3	1:H:400:ILE:HG12	2.02	0.41
1:A:122:ILE:CG2	1:A:123:SER:N	2.84	0.41
1:A:339:GLY:O	1:A:340:PRO:C	2.60	0.41
1:B:464:LEU:HB3	1:B:465:PRO:HA	2.02	0.41
1:D:219:ARG:HB2	1:D:243:ASP:CG	2.41	0.41
1:F:226:GLN:HE22	1:F:230:CYS:HB3	1.86	0.41
1:F:300:ARG:HG2	1:F:300:ARG:NH2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:118:ARG:C	1:H:119:GLU:CG	2.89	0.41
1:H:254:ILE:HD13	1:H:305:PHE:CD2	2.56	0.41
1:A:121:PHE:HB3	1:A:423:TRP:CZ2	2.56	0.40
1:B:219:ARG:HE	1:B:251:SER:HB2	1.86	0.40
1:D:360:VAL:CG1	1:D:383:TRP:HE3	2.34	0.40
1:F:158:LEU:O	1:F:174:GLU:HB2	2.21	0.40
1:H:113:ASP:O	1:H:169:PRO:HD2	2.21	0.40
1:H:219:ARG:HB2	1:H:243:ASP:CG	2.41	0.40
1:A:270:ALA:HB1	1:A:273:TYR:HB2	2.02	0.40
1:B:218:TRP:CD1	1:B:219:ARG:HG2	2.56	0.40
1:C:126:HIS:CD2	1:C:127:LEU:HG	2.55	0.40
1:E:313:GLN:HE21	1:E:313:GLN:HB3	1.65	0.40
1:F:379:ASP:OD2	1:F:382:GLY:HA3	2.20	0.40
1:G:96:GLY:O	1:G:448:GLY:O	2.39	0.40
1:G:400:ILE:H	1:G:400:ILE:HG13	1.49	0.40
1:G:426:LEU:O	1:G:441:GLY:HA2	2.21	0.40
1:H:466:PHE:O	1:H:468:ILE:N	2.54	0.40
1:A:254:ILE:HD13	1:A:254:ILE:HG21	1.89	0.40
1:A:413:THR:HA	1:C:210:ILE:HD13	2.02	0.40
1:C:232:CYS:HA	1:C:237:CYS:HA	2.02	0.40
1:D:387:ASP:HB3	1:D:389:SER:H	1.86	0.40
1:E:339:GLY:O	1:E:340:PRO:C	2.60	0.40
1:F:144:HIS:CE1	1:G:462:ALA:HA	2.56	0.40
1:F:463:GLU:HB2	1:H:143:LYS:HE3	2.04	0.40
1:G:122:ILE:HG22	1:G:123:SER:N	2.36	0.40
1:G:130:ARG:HG2	1:G:130:ARG:HH21	1.87	0.40
1:D:424:VAL:O	1:D:443:SER:HA	2.21	0.40
1:E:173:PHE:CG	1:H:164:GLY:HA3	2.56	0.40
1:F:305:PHE:HB3	1:F:312:TYR:HB3	2.02	0.40
1:G:118:ARG:HD2	1:G:118:ARG:HA	1.77	0.40
1:H:287:ILE:HD12	1:H:287:ILE:N	2.36	0.40
1:B:438:TRP:CD1	1:B:438:TRP:N	2.90	0.40
1:C:131:THR:O	1:C:160:SER:HA	2.21	0.40
1:C:453:THR:CG2	1:C:454:VAL:N	2.81	0.40
1:E:215:ILE:HD11	1:E:262:VAL:CG2	2.51	0.40
1:E:239:THR:HG22	1:E:257:MET:CE	2.51	0.40
1:E:446:PHE:CD1	1:E:446:PHE:N	2.89	0.40
1:F:202:VAL:HG12	1:G:454:VAL:HG21	2.04	0.40

All (8) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:HIS:CD2	1:D:272:ASN:OD1[8_456]	1.92	0.28
1:D:381:ASN:OD1	1:G:384:THR:O[3_565]	1.93	0.27
1:D:416:ASP:OD2	1:G:344:ASN:N[3_565]	2.05	0.15
1:C:332:THR:OG1	1:D:332:THR:OG1[8_456]	2.12	0.08
1:C:272:ASN:OD1	1:D:296:HIS:CD2[8_456]	2.15	0.05
1:C:342:SER:OG	1:D:339:GLY:C[8_456]	2.18	0.02
1:C:342:SER:OG	1:D:339:GLY:O[8_456]	2.19	0.01
1:D:381:ASN:ND2	1:G:385:GLU:CB[3_565]	2.19	0.01

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	383/387 (99%)	339 (88%)	34 (9%)	10 (3%)	5	24
1	B	383/387 (99%)	345 (90%)	30 (8%)	8 (2%)	7	29
1	C	383/387 (99%)	339 (88%)	40 (10%)	4 (1%)	15	48
1	D	383/387 (99%)	341 (89%)	36 (9%)	6 (2%)	9	36
1	E	383/387 (99%)	344 (90%)	31 (8%)	8 (2%)	7	29
1	F	383/387 (99%)	339 (88%)	32 (8%)	12 (3%)	4	19
1	G	383/387 (99%)	345 (90%)	29 (8%)	9 (2%)	6	27
1	H	383/387 (99%)	339 (88%)	36 (9%)	8 (2%)	7	29
All	All	3064/3096 (99%)	2731 (89%)	268 (9%)	65 (2%)	7	29

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	412(A)	HIS
1	C	448	GLY
1	D	248	GLY
1	D	448	GLY
1	E	412(A)	HIS

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Mol	Chain	Res	Type
1	F	201	ALA
1	F	340	PRO
1	F	448	GLY
1	F	451	SER
1	G	248	GLY
1	A	147	GLY
1	A	248	GLY
1	A	448	GLY
1	A	449	VAL
1	A	451	SER
1	A	467	THR
1	B	248	GLY
1	B	448	GLY
1	B	449	VAL
1	C	248	GLY
1	D	340	PRO
1	E	234	ASN
1	E	248	GLY
1	E	340	PRO
1	E	448	GLY
1	F	248	GLY
1	F	343	SER
1	G	147	GLY
1	G	340	PRO
1	G	448	GLY
1	G	451	SER
1	H	306	ASN
1	H	340	PRO
1	H	448	GLY
1	H	451	SER
1	A	340	PRO
1	C	449	VAL
1	D	146	ASN
1	D	449	VAL
1	E	449	VAL
1	F	449	VAL
1	G	449	VAL
1	G	467	THR
1	H	435	SER
1	H	449	VAL
1	H	467	THR
1	B	200	GLY

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Mol	Chain	Res	Type
1	B	343	SER
1	B	347	TYR
1	D	347	TYR
1	E	347	TYR
1	F	249	GLN
1	F	388	SER
1	A	347	TYR
1	F	146	ASN
1	G	347	TYR
1	B	340	PRO
1	E	451	SER
1	H	147	GLY
1	G	200	GLY
1	A	200	GLY
1	F	149	VAL
1	B	222	ILE
1	F	200	GLY
1	A	222	ILE

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	329/331 (99%)	315 (96%)	14 (4%)	29	62
1	B	329/331 (99%)	315 (96%)	14 (4%)	29	62
1	C	329/331 (99%)	314 (95%)	15 (5%)	27	60
1	D	329/331 (99%)	311 (94%)	18 (6%)	21	53
1	E	329/331 (99%)	312 (95%)	17 (5%)	23	56
1	F	329/331 (99%)	312 (95%)	17 (5%)	23	56
1	G	329/331 (99%)	316 (96%)	13 (4%)	31	64
1	H	329/331 (99%)	312 (95%)	17 (5%)	23	56
All	All	2632/2648 (99%)	2507 (95%)	125 (5%)	26	59

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	116	VAL
1	A	156	ARG
1	A	168	SER
1	A	214	THR
1	A	230	CYS
1	A	257	MET
1	A	296	HIS
1	A	310	LEU
1	A	360	VAL
1	A	391	SER
1	A	412(C)	GLU
1	A	415	LEU
1	A	419	ARG
1	B	88	ASN
1	B	99	VAL
1	B	116	VAL
1	B	210	ILE
1	B	228	SER
1	B	230	CYS
1	B	257	MET
1	B	296	HIS
1	B	372	SER
1	B	391	SER
1	B	412(C)	GLU
1	B	415	LEU
1	B	419	ARG
1	B	451	SER
1	C	88	ASN
1	C	99	VAL
1	C	156	ARG
1	C	214	THR
1	C	230	CYS
1	C	257	MET
1	C	296	HIS
1	C	298	SER
1	C	360	VAL
1	C	391	SER
1	C	400	ILE
1	C	412(C)	GLU
1	C	412(D)	LEU
1	C	415	LEU
1	C	419	ARG

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Mol	Chain	Res	Type
1	D	88	ASN
1	D	99	VAL
1	D	116	VAL
1	D	156	ARG
1	D	179	SER
1	D	214	THR
1	D	216	LYS
1	D	230	CYS
1	D	257	MET
1	D	296	HIS
1	D	344	ASN
1	D	360	VAL
1	D	381	ASN
1	D	415	LEU
1	D	419	ARG
1	D	452	ASP
1	D	454	VAL
1	D	460	ASP
1	E	88	ASN
1	E	99	VAL
1	E	153	SER
1	E	156	ARG
1	E	230	CYS
1	E	252	TYR
1	E	257	MET
1	E	296	HIS
1	E	310	LEU
1	E	360	VAL
1	E	391	SER
1	E	412(C)	GLU
1	E	415	LEU
1	E	419	ARG
1	E	451	SER
1	E	453	THR
1	E	454	VAL
1	F	88	ASN
1	F	99	VAL
1	F	141	ASN
1	F	202	VAL
1	F	205	LEU
1	F	214	THR
1	F	230	CYS

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Mol	Chain	Res	Type
1	F	257	MET
1	F	296	HIS
1	F	318	CYS
1	F	343	SER
1	F	360	VAL
1	F	412(C)	GLU
1	F	415	LEU
1	F	419	ARG
1	F	453	THR
1	F	460	ASP
1	G	88	ASN
1	G	99	VAL
1	G	116	VAL
1	G	214	THR
1	G	230	CYS
1	G	252	TYR
1	G	296	HIS
1	G	344	ASN
1	G	360	VAL
1	G	385	GLU
1	G	412(C)	GLU
1	G	415	LEU
1	G	419	ARG
1	H	88	ASN
1	H	99	VAL
1	H	116	VAL
1	H	150	LYS
1	H	230	CYS
1	H	257	MET
1	H	296	HIS
1	H	298	SER
1	H	360	VAL
1	H	391	SER
1	H	412(C)	GLU
1	H	415	LEU
1	H	419	ARG
1	H	453	THR
1	H	454	VAL
1	H	456	TRP
1	H	460	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	A	104	ASN
1	A	136	GLN
1	A	144	HIS
1	A	155	HIS
1	A	184	HIS
1	A	208	ASN
1	A	226	GLN
1	A	249	GLN
1	A	313	GLN
1	A	395	GLN
1	B	88	ASN
1	B	104	ASN
1	B	144	HIS
1	B	146	ASN
1	B	155	HIS
1	B	184	HIS
1	B	226	GLN
1	B	249	GLN
1	B	313	GLN
1	B	395	GLN
1	C	88	ASN
1	C	104	ASN
1	C	136	GLN
1	C	144	HIS
1	C	146	ASN
1	C	155	HIS
1	C	184	HIS
1	C	226	GLN
1	C	249	GLN
1	C	313	GLN
1	C	395	GLN
1	D	88	ASN
1	D	104	ASN
1	D	136	GLN
1	D	144	HIS
1	D	184	HIS
1	D	226	GLN
1	D	249	GLN
1	D	381	ASN
1	D	395	GLN
1	E	88	ASN
1	E	104	ASN

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Mol	Chain	Res	Type
1	E	136	GLN
1	E	144	HIS
1	E	146	ASN
1	E	184	HIS
1	E	208	ASN
1	E	226	GLN
1	E	249	GLN
1	E	313	GLN
1	E	395	GLN
1	E	412(A)	HIS
1	F	88	ASN
1	F	104	ASN
1	F	136	GLN
1	F	144	HIS
1	F	155	HIS
1	F	184	HIS
1	F	226	GLN
1	F	249	GLN
1	F	313	GLN
1	F	344	ASN
1	F	395	GLN
1	F	412(A)	HIS
1	G	88	ASN
1	G	104	ASN
1	G	136	GLN
1	G	144	HIS
1	G	146	ASN
1	G	184	HIS
1	G	226	GLN
1	G	249	GLN
1	G	313	GLN
1	G	395	GLN
1	H	88	ASN
1	H	104	ASN
1	H	144	HIS
1	H	146	ASN
1	H	155	HIS
1	H	184	HIS
1	H	208	ASN
1	H	226	GLN
1	H	249	GLN
1	H	313	GLN

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Mol	Chain	Res	Type
1	H	395	GLN

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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	G39	B	800	-	17,20,20	1.44	3 (17%)	15,27,27	1.12	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	G39	B	800	-	-	4/12/32/32	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	800	G39	C3-C2	2.87	1.55	1.50
2	B	800	G39	C6-C5	2.80	1.56	1.53
2	B	800	G39	C6-C7	2.77	1.54	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	G39	C4-C3-C2	2.80	113.06	109.75
2	B	800	G39	C3-C4-N4	2.10	115.14	110.88

There are no chirality outliers.

All (4) torsion outliers are listed below:

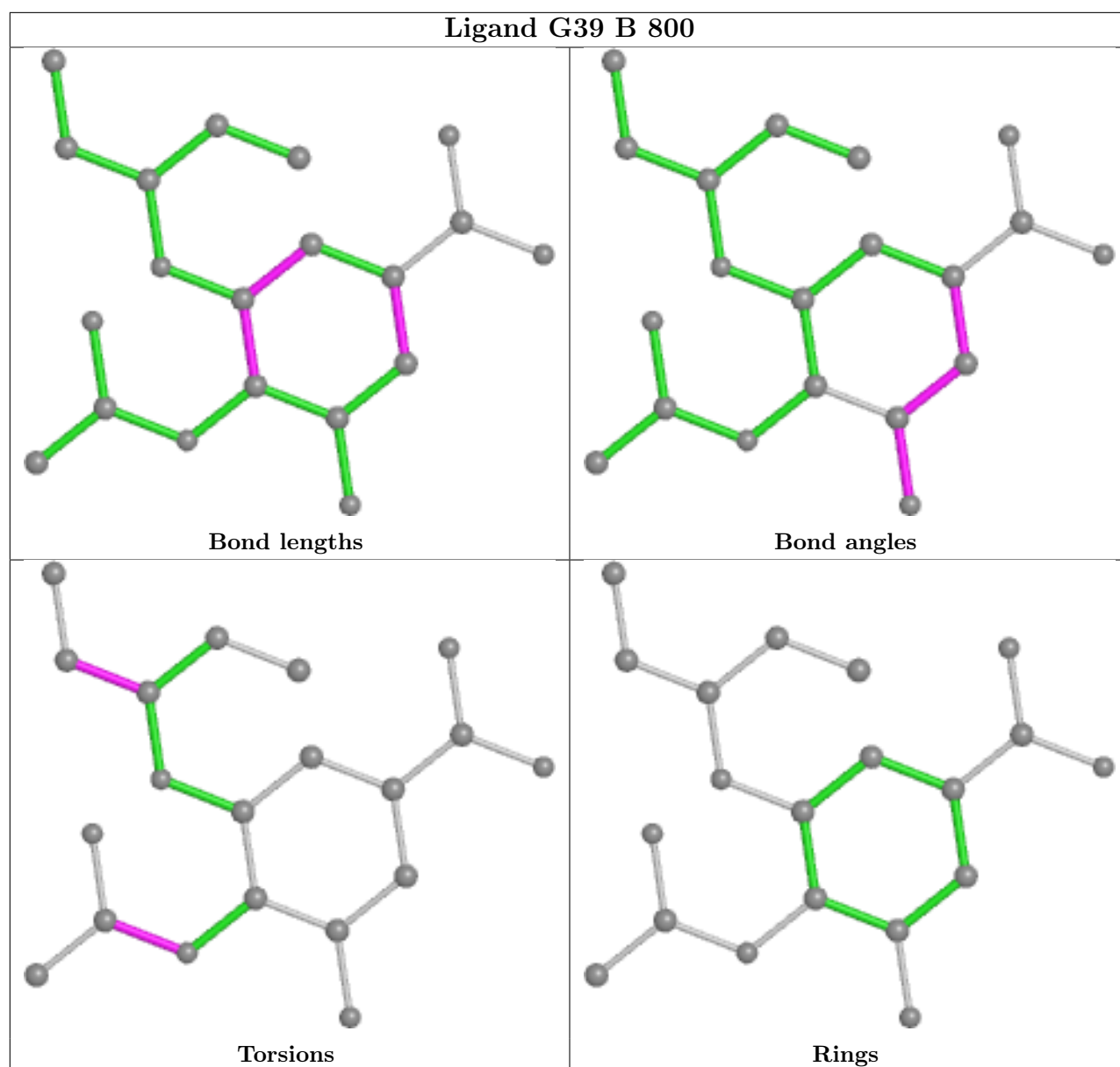
Mol	Chain	Res	Type	Atoms
2	B	800	G39	C11-C10-N5-C5
2	B	800	G39	O10-C10-N5-C5
2	B	800	G39	O7-C8-C81-C82
2	B	800	G39	C9-C8-C81-C82

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	800	G39	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	412:GLN	C	412(A):HIS	N	1.18

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

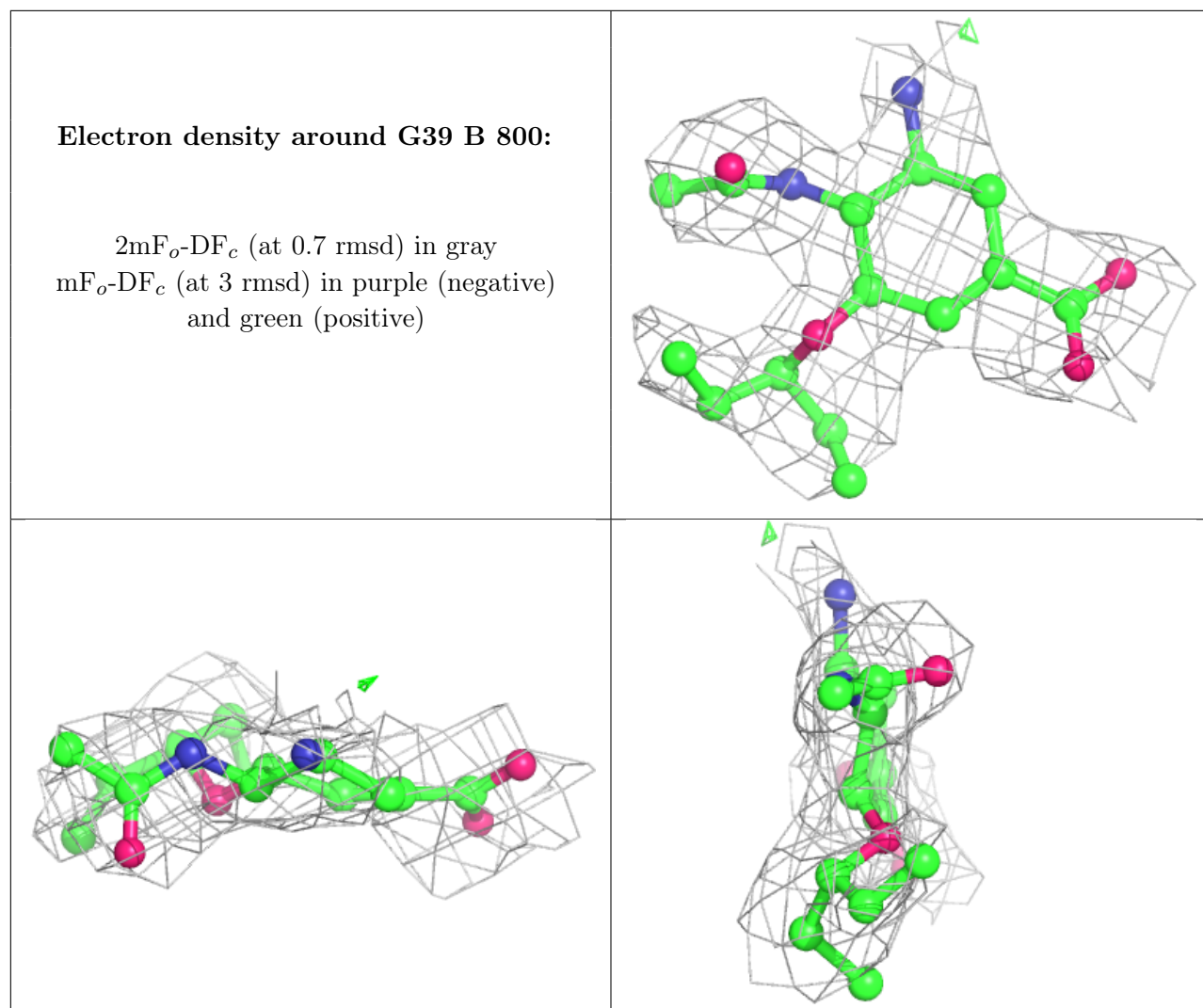
6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

Unable to reproduce the depositor's R factor - this section is therefore empty.