



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:50 PM UTC

PDB ID : 2XQA / pdb_00002xqa
Title : Pentameric ligand gated ion channel GLIC in complex with tetrabutylantimony (TBSb)
Authors : Hilf, R.J.C.; Bertozzi, C.; Zimmermann, I.; Reiter, A.; Trauner, D.; Dutzler, R.
Deposited on : 2010-09-01
Resolution : 3.70 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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

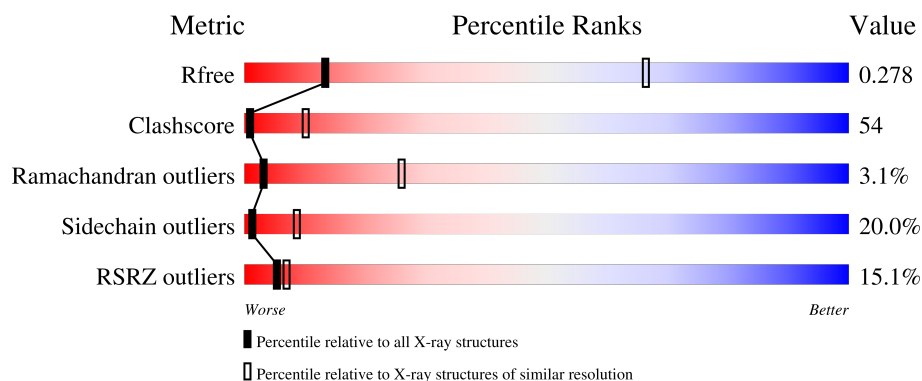
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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}	180053	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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	317	18% 30% 52% 15% ..
1	B	317	15% 28% 54% 15% ..
1	C	317	13% 30% 51% 15% ..
1	D	317	14% 29% 53% 15% ..
1	E	317	14% 30% 52% 15% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12606 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 GLR4197 PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2521	1662	403	452	4			
1	B	310	Total	C	N	O	S	0	0	0
			2521	1662	403	452	4			
1	C	310	Total	C	N	O	S	0	0	0
			2521	1662	403	452	4			
1	D	310	Total	C	N	O	S	0	0	0
			2521	1662	403	452	4			
1	E	310	Total	C	N	O	S	0	0	0
			2521	1662	403	452	4			

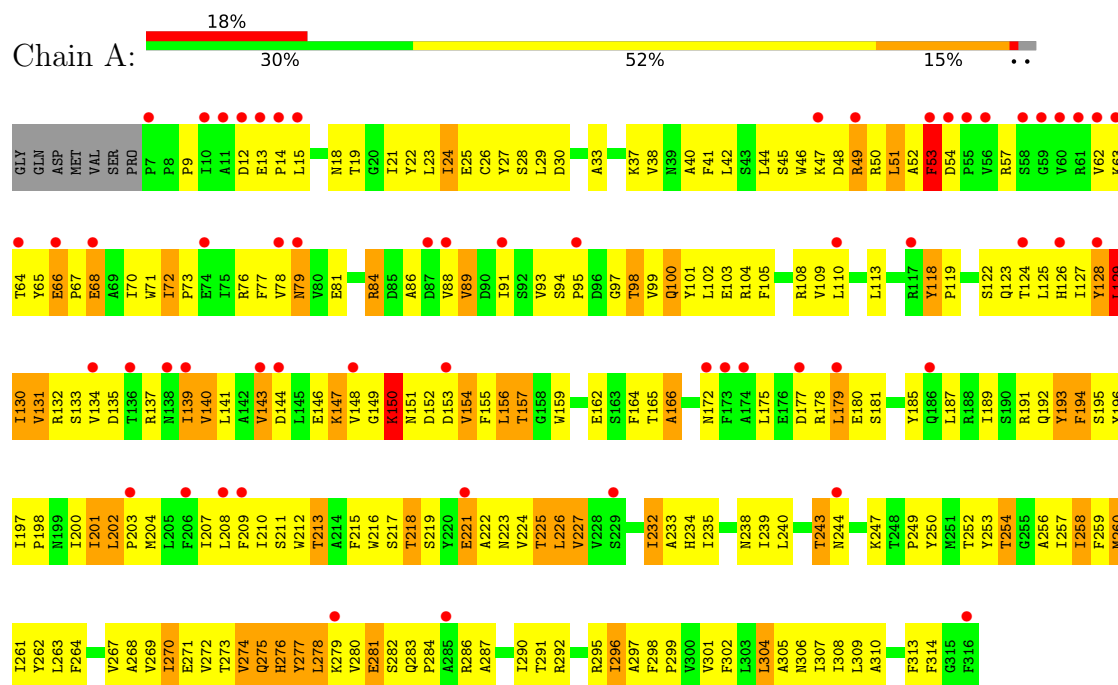
- Molecule 2 is ANTIMONY (III) ION (CCD ID: SB) (formula: Sb).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	1	Total	Sb	0	0
			1	1		

3 Residue-property plots

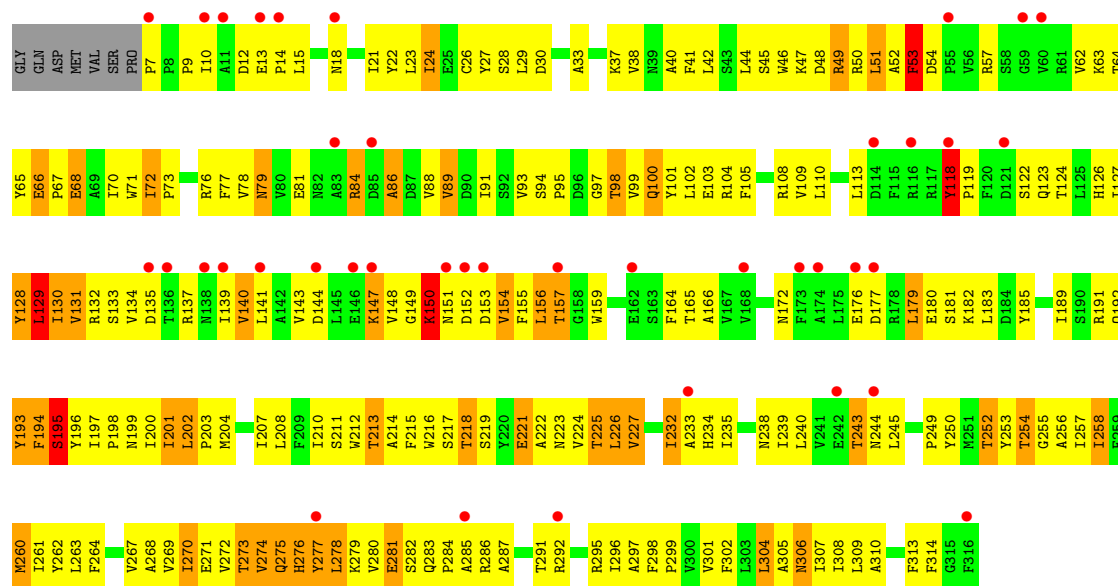
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: GLR4197 PROTEIN

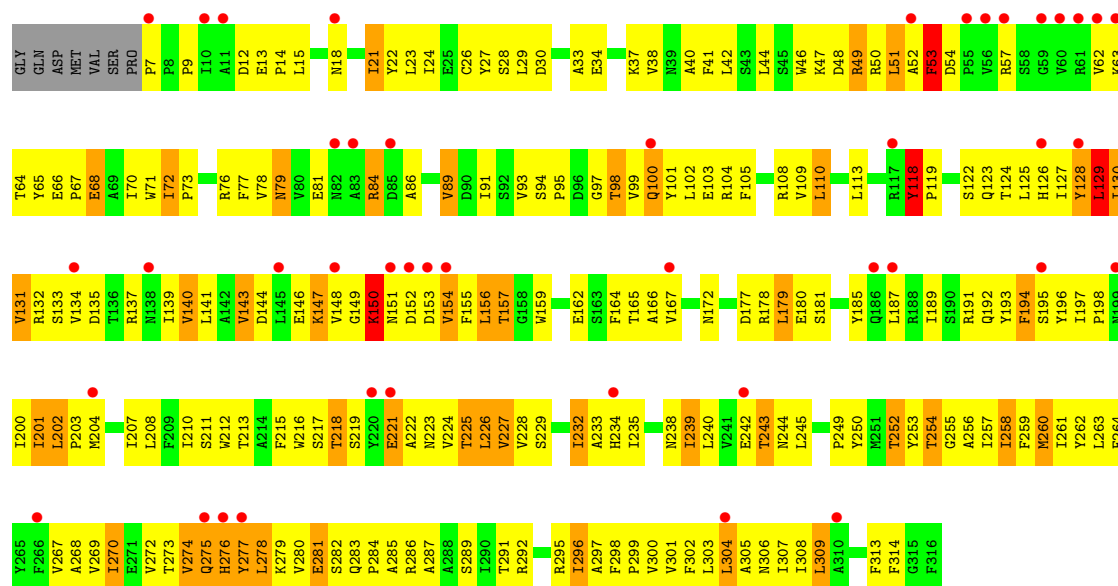




● Molecule 1: GLR4197 PROTEIN

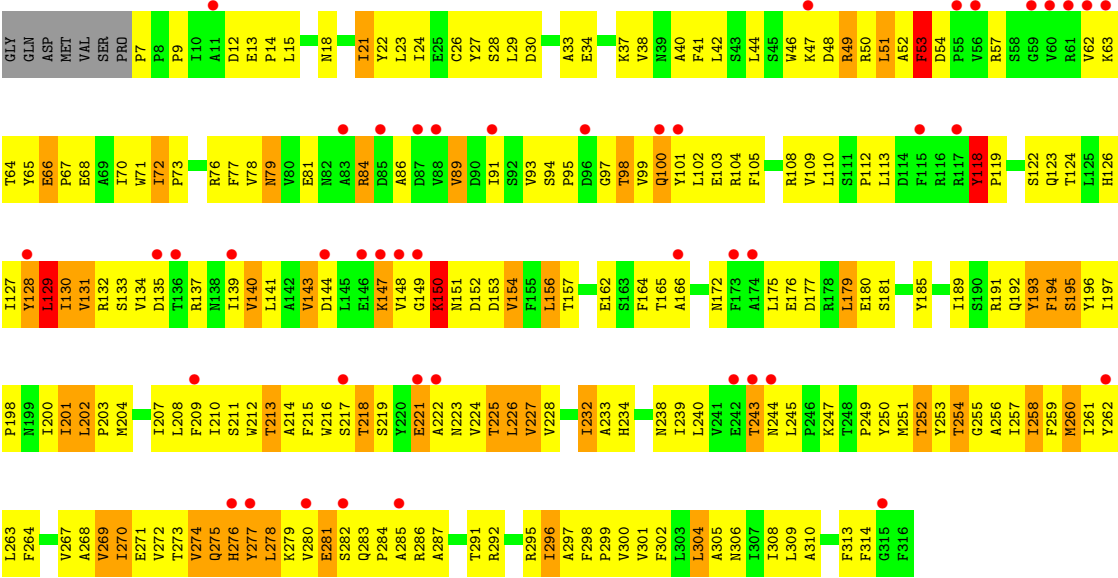


● Molecule 1: GLR4197 PROTEIN



● Molecule 1: GLR4197 PROTEIN





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	183.31Å 128.31Å 164.37Å 90.00° 104.04° 90.00°	Depositor
Resolution (Å)	40.20 – 3.70 40.20 – 3.70	Depositor EDS
% Data completeness (in resolution range)	95.7 (40.20-3.70) 95.6 (40.20-3.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 3.57Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.256 , 0.274 0.262 , 0.278	Depositor DCC
R_{free} test set	2172 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	94.3	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 108.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	12606	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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: SB

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	0.64	0/2589	1.08	20/3535 (0.6%)
1	B	0.69	0/2589	1.08	22/3535 (0.6%)
1	C	0.68	1/2589 (0.0%)	1.08	21/3535 (0.6%)
1	D	0.67	0/2589	1.08	17/3535 (0.5%)
1	E	0.69	0/2589	1.09	20/3535 (0.6%)
All	All	0.67	1/12945 (0.0%)	1.08	100/17675 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	273	THR	C-N	-6.17	1.25	1.33

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	128	TYR	N-CA-C	8.47	123.95	111.34
1	E	128	TYR	N-CA-C	8.42	123.88	111.34
1	C	128	TYR	N-CA-C	8.41	123.88	111.34
1	A	128	TYR	N-CA-C	8.41	123.87	111.34
1	B	128	TYR	N-CA-C	8.38	123.83	111.34
1	B	152	ASP	N-CA-C	-6.99	105.56	112.97
1	C	281	GLU	N-CA-C	-6.97	99.34	109.59
1	A	281	GLU	N-CA-C	-6.96	99.35	109.59
1	B	281	GLU	N-CA-C	-6.96	99.36	109.59
1	D	281	GLU	N-CA-C	-6.95	99.37	109.59
1	E	281	GLU	N-CA-C	-6.95	99.38	109.59
1	A	152	ASP	N-CA-C	-6.66	105.91	112.97
1	A	24	ILE	N-CA-C	-6.59	106.56	111.90
1	C	118	TYR	CA-C-N	-6.42	113.07	119.56
1	C	118	TYR	C-N-CA	-6.42	113.07	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	118	TYR	CA-C-N	-6.41	113.08	119.56
1	B	118	TYR	C-N-CA	-6.41	113.08	119.56
1	A	118	TYR	CA-C-N	-6.40	113.10	119.56
1	A	118	TYR	C-N-CA	-6.40	113.10	119.56
1	E	118	TYR	CA-C-N	-6.38	113.11	119.56
1	E	118	TYR	C-N-CA	-6.38	113.11	119.56
1	E	152	ASP	N-CA-C	-6.38	105.36	112.57
1	C	24	ILE	N-CA-C	-6.36	106.34	111.81
1	D	118	TYR	CA-C-N	-6.35	113.14	119.56
1	D	118	TYR	C-N-CA	-6.35	113.14	119.56
1	D	167	VAL	CB-CA-C	-6.18	105.25	111.80
1	E	193	TYR	N-CA-C	-6.01	102.18	110.35
1	B	129	LEU	N-CA-C	5.91	123.38	110.80
1	C	129	LEU	N-CA-C	5.90	123.37	110.80
1	E	129	LEU	N-CA-C	5.90	123.36	110.80
1	A	129	LEU	N-CA-C	5.89	123.34	110.80
1	B	134	VAL	CB-CA-C	5.88	120.94	111.29
1	D	129	LEU	N-CA-C	5.88	123.33	110.80
1	D	134	VAL	CB-CA-C	5.88	120.93	111.29
1	B	193	TYR	N-CA-C	-5.88	102.36	110.35
1	E	134	VAL	CB-CA-C	5.88	120.92	111.29
1	A	134	VAL	CB-CA-C	5.87	120.92	111.29
1	C	134	VAL	CB-CA-C	5.87	120.91	111.29
1	C	166	ALA	N-CA-C	5.86	118.02	108.76
1	C	53	PHE	N-CA-C	5.80	123.16	110.80
1	D	53	PHE	N-CA-C	5.80	123.15	110.80
1	A	53	PHE	N-CA-C	5.80	123.15	110.80
1	E	53	PHE	N-CA-C	5.79	123.13	110.80
1	B	53	PHE	N-CA-C	5.78	123.12	110.80
1	D	152	ASP	N-CA-C	-5.73	106.10	112.57
1	B	21	ILE	N-CA-C	5.65	116.08	108.17
1	B	167	VAL	CB-CA-C	-5.59	105.88	111.80
1	A	278	LEU	N-CA-CB	-5.59	103.61	110.98
1	D	278	LEU	N-CA-CB	-5.58	103.61	110.98
1	E	278	LEU	N-CA-CB	-5.58	103.61	110.98
1	B	278	LEU	N-CA-CB	-5.56	103.64	110.98
1	C	278	LEU	N-CA-CB	-5.56	103.64	110.98
1	A	166	ALA	N-CA-C	5.51	117.65	108.99
1	B	166	ALA	N-CA-C	5.47	117.41	108.76
1	C	152	ASP	N-CA-C	-5.46	106.40	112.57
1	B	7	PRO	CA-C-N	5.42	125.97	120.38
1	B	7	PRO	C-N-CA	5.42	125.97	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	147	LYS	CB-CA-C	-5.41	101.03	110.17
1	C	147	LYS	CB-CA-C	-5.41	101.03	110.17
1	A	147	LYS	CB-CA-C	-5.39	101.07	110.17
1	B	147	LYS	CB-CA-C	-5.38	101.07	110.17
1	E	147	LYS	CB-CA-C	-5.38	101.07	110.17
1	E	166	ALA	N-CA-C	5.37	117.42	108.99
1	C	86	ALA	N-CA-C	5.33	118.09	109.40
1	A	193	TYR	N-CA-C	-5.30	103.14	110.35
1	E	21	ILE	N-CA-C	5.29	115.57	108.17
1	E	135	ASP	N-CA-CB	-5.24	102.83	111.01
1	B	135	ASP	N-CA-CB	-5.24	102.84	111.01
1	C	7	PRO	CA-C-N	5.20	125.74	120.38
1	C	7	PRO	C-N-CA	5.20	125.74	120.38
1	C	66	GLU	CA-C-N	5.20	125.50	119.47
1	C	66	GLU	C-N-CA	5.20	125.50	119.47
1	A	135	ASP	N-CA-CB	-5.18	102.82	111.06
1	D	135	ASP	N-CA-CB	-5.16	102.86	111.06
1	B	66	GLU	CA-C-N	5.14	125.44	119.47
1	B	66	GLU	C-N-CA	5.14	125.44	119.47
1	C	135	ASP	N-CA-CB	-5.14	102.88	111.06
1	D	21	ILE	N-CA-C	5.14	115.37	108.17
1	D	150	LYS	N-CA-C	-5.12	99.89	110.80
1	C	150	LYS	N-CA-C	-5.12	99.90	110.80
1	A	150	LYS	N-CA-C	-5.11	99.91	110.80
1	B	150	LYS	N-CA-C	-5.11	99.92	110.80
1	D	7	PRO	CA-C-N	5.11	125.64	120.38
1	D	7	PRO	C-N-CA	5.11	125.64	120.38
1	E	66	GLU	CA-C-N	5.11	125.39	119.47
1	E	66	GLU	C-N-CA	5.11	125.39	119.47
1	E	150	LYS	N-CA-C	-5.11	99.92	110.80
1	A	66	GLU	N-CA-C	-5.10	103.76	110.39
1	B	220	TYR	N-CA-C	-5.08	105.82	111.36
1	A	139	ILE	N-CA-C	-5.08	101.17	108.53
1	C	193	TYR	N-CA-C	-5.06	103.46	110.35
1	E	7	PRO	CA-C-N	5.06	125.59	120.38
1	E	7	PRO	C-N-CA	5.06	125.59	120.38
1	C	276	HIS	N-CA-CB	-5.06	101.94	110.49
1	D	276	HIS	N-CA-CB	-5.05	101.95	110.49
1	A	276	HIS	N-CA-CB	-5.05	101.96	110.49
1	E	276	HIS	N-CA-CB	-5.04	101.96	110.49
1	A	66	GLU	CA-C-N	5.04	125.32	119.47
1	A	66	GLU	C-N-CA	5.04	125.32	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	276	HIS	N-CA-CB	-5.03	102.00	110.49

There are no chirality outliers.

There are no planarity outliers.

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	2521	0	2537	325	0
1	B	2521	0	2537	325	0
1	C	2521	0	2537	280	0
1	D	2521	0	2537	295	0
1	E	2521	0	2537	275	0
2	E	1	0	0	0	0
All	All	12606	0	12685	1362	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 54.

All (1362) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:PHE:CE1	1:B:112:PRO:HB3	1.83	1.12
1:B:76:ARG:NH2	1:B:130:ILE:HD12	1.68	1.08
1:D:76:ARG:NH2	1:D:130:ILE:HD12	1.70	1.06
1:A:76:ARG:NH2	1:A:130:ILE:HD12	1.73	1.03
1:A:104:ARG:HH22	1:B:78:VAL:HA	1.20	1.03
1:A:222:ALA:HB2	1:B:221:GLU:HA	1.38	1.02
1:C:76:ARG:NH2	1:C:130:ILE:HD12	1.76	1.01
1:E:76:ARG:NH2	1:E:130:ILE:HD12	1.76	1.01
1:C:22:TYR:HA	1:C:149:GLY:HA3	1.42	0.99
1:D:22:TYR:HA	1:D:149:GLY:HA3	1.46	0.98
1:B:257:ILE:O	1:B:261:ILE:HG12	1.63	0.97
1:B:22:TYR:HA	1:B:149:GLY:HA3	1.46	0.97
1:D:257:ILE:O	1:D:261:ILE:HG12	1.65	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ILE:O	1:A:261:ILE:HG12	1.63	0.96
1:D:155:PHE:CE1	1:E:112:PRO:HB3	1.99	0.96
1:E:257:ILE:O	1:E:261:ILE:HG12	1.65	0.96
1:A:104:ARG:NH2	1:B:78:VAL:HA	1.80	0.95
1:A:22:TYR:HA	1:A:149:GLY:HA3	1.47	0.95
1:C:257:ILE:O	1:C:261:ILE:HG12	1.66	0.94
1:D:104:ARG:HH22	1:E:78:VAL:HA	1.29	0.94
1:D:76:ARG:HH22	1:D:130:ILE:HD12	1.32	0.93
1:D:225:THR:CG2	1:E:224:VAL:HG23	1.98	0.93
1:E:22:TYR:HA	1:E:149:GLY:HA3	1.49	0.93
1:C:200:ILE:HD11	1:C:240:LEU:HD23	1.51	0.93
1:D:253:TYR:HA	1:D:313:PHE:CE2	2.03	0.93
1:A:253:TYR:HA	1:A:313:PHE:CE2	2.04	0.91
1:A:226:LEU:CD2	1:B:224:VAL:HB	2.00	0.91
1:A:253:TYR:HA	1:A:313:PHE:HE2	1.36	0.91
1:C:253:TYR:HA	1:C:313:PHE:CE2	2.06	0.90
1:E:253:TYR:HA	1:E:313:PHE:CE2	2.07	0.90
1:A:297:ALA:O	1:A:301:VAL:HG23	1.71	0.90
1:B:76:ARG:HH22	1:B:130:ILE:HD12	1.29	0.90
1:D:210:ILE:HG23	1:E:269:VAL:HG11	1.54	0.89
1:C:22:TYR:HA	1:C:149:GLY:CA	2.02	0.89
1:C:297:ALA:O	1:C:301:VAL:HG23	1.72	0.88
1:A:253:TYR:HD1	1:A:313:PHE:HD2	1.20	0.88
1:D:253:TYR:HA	1:D:313:PHE:HE2	1.36	0.88
1:B:253:TYR:HA	1:B:313:PHE:CE2	2.08	0.88
1:D:253:TYR:HD1	1:D:313:PHE:HD2	1.17	0.88
1:C:197:ILE:HB	1:C:198:PRO:HD3	1.55	0.87
1:E:200:ILE:HD11	1:E:240:LEU:HD23	1.56	0.87
1:C:139:ILE:HG12	1:C:172:ASN:HD21	1.37	0.87
1:D:304:LEU:O	1:D:308:ILE:HG12	1.74	0.87
1:E:139:ILE:HG12	1:E:172:ASN:HD21	1.36	0.87
1:C:253:TYR:HA	1:C:313:PHE:HE2	1.37	0.87
1:A:139:ILE:HG12	1:A:172:ASN:HD21	1.38	0.86
1:B:22:TYR:HA	1:B:149:GLY:CA	2.06	0.86
1:E:197:ILE:HB	1:E:198:PRO:HD3	1.58	0.86
1:D:22:TYR:HA	1:D:149:GLY:CA	2.06	0.85
1:E:253:TYR:HA	1:E:313:PHE:HE2	1.40	0.85
1:E:76:ARG:HH22	1:E:130:ILE:HD12	1.41	0.85
1:B:139:ILE:HG12	1:B:172:ASN:HD21	1.41	0.85
1:B:253:TYR:HA	1:B:313:PHE:HE2	1.40	0.85
1:D:139:ILE:HG12	1:D:172:ASN:HD21	1.41	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ASN:H	1:B:79:ASN:HD22	1.24	0.84
1:A:22:TYR:HA	1:A:149:GLY:CA	2.07	0.84
1:A:221:GLU:HB3	1:B:221:GLU:HG2	1.59	0.84
1:E:253:TYR:HD1	1:E:313:PHE:HD2	1.25	0.84
1:A:197:ILE:HB	1:A:198:PRO:HD3	1.60	0.83
1:B:253:TYR:HD1	1:B:313:PHE:HD2	1.27	0.83
1:C:76:ARG:HH22	1:C:130:ILE:HD12	1.42	0.83
1:C:234:HIS:CE1	1:C:261:ILE:HG21	2.14	0.83
1:C:199:ASN:HB3	1:D:242:GLU:CD	2.03	0.83
1:E:297:ALA:O	1:E:301:VAL:HG23	1.78	0.83
1:A:155:PHE:CZ	1:B:112:PRO:HB3	2.13	0.82
1:A:76:ARG:HH22	1:A:130:ILE:HD12	1.39	0.82
1:C:253:TYR:HD1	1:C:313:PHE:HD2	1.26	0.82
1:D:225:THR:HG21	1:E:224:VAL:HG23	1.59	0.82
1:A:27:TYR:CB	1:B:110:LEU:HD11	2.10	0.81
1:B:297:ALA:O	1:B:301:VAL:HG23	1.81	0.81
1:E:22:TYR:HA	1:E:149:GLY:CA	2.09	0.81
1:B:66:GLU:HG3	1:B:67:PRO:HD2	1.62	0.80
1:B:197:ILE:HB	1:B:198:PRO:HD3	1.64	0.80
1:E:66:GLU:HG3	1:E:67:PRO:HD2	1.64	0.80
1:D:41:PHE:HE2	1:E:175:LEU:HD23	1.45	0.80
1:E:304:LEU:O	1:E:308:ILE:HG12	1.83	0.79
1:B:304:LEU:O	1:B:308:ILE:HG12	1.82	0.79
1:D:297:ALA:O	1:D:301:VAL:HG23	1.83	0.79
1:E:89:VAL:HG11	1:E:102:LEU:HD23	1.64	0.79
1:A:283:GLN:N	1:A:284:PRO:HD3	1.98	0.79
1:D:197:ILE:HB	1:D:198:PRO:HD3	1.64	0.79
1:A:22:TYR:HB3	1:A:41:PHE:HB2	1.64	0.79
1:C:78:VAL:HG22	1:C:130:ILE:HG12	1.64	0.79
1:E:79:ASN:HD22	1:E:79:ASN:H	1.31	0.79
1:E:147:LYS:O	1:E:147:LYS:HG2	1.83	0.79
1:A:226:LEU:HD23	1:B:224:VAL:HB	1.64	0.78
1:C:147:LYS:HG2	1:C:147:LYS:O	1.83	0.78
1:C:149:GLY:O	1:C:164:PHE:HD1	1.67	0.78
1:B:22:TYR:CD1	1:B:149:GLY:HA2	2.19	0.78
1:D:22:TYR:CD1	1:D:149:GLY:HA2	2.19	0.77
1:D:66:GLU:HG3	1:D:67:PRO:HD2	1.67	0.77
1:A:147:LYS:O	1:A:147:LYS:HG2	1.83	0.77
1:D:283:GLN:N	1:D:284:PRO:HD3	2.00	0.77
1:E:149:GLY:O	1:E:164:PHE:HD1	1.68	0.77
1:B:254:THR:O	1:B:258:ILE:HB	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:ILE:HA	1:B:201:ILE:HB	1.67	0.77
1:E:78:VAL:HG22	1:E:130:ILE:HG12	1.66	0.77
1:B:200:ILE:HD11	1:B:240:LEU:HD23	1.66	0.77
1:B:283:GLN:N	1:B:284:PRO:HD3	2.00	0.77
1:A:89:VAL:HG11	1:A:102:LEU:HD23	1.67	0.76
1:A:217:SER:OG	1:B:220:TYR:HE2	1.67	0.76
1:C:283:GLN:N	1:C:284:PRO:HD3	1.99	0.76
1:A:234:HIS:CE1	1:A:261:ILE:HG21	2.20	0.76
1:A:254:THR:O	1:A:258:ILE:HB	1.86	0.76
1:D:225:THR:HG22	1:E:224:VAL:HG23	1.66	0.76
1:E:234:HIS:CE1	1:E:261:ILE:HG21	2.20	0.76
1:A:79:ASN:HD22	1:A:79:ASN:H	1.34	0.76
1:B:147:LYS:O	1:B:147:LYS:HG2	1.83	0.76
1:E:283:GLN:N	1:E:284:PRO:HD3	2.00	0.76
1:A:226:LEU:HD21	1:B:224:VAL:HB	1.66	0.76
1:B:78:VAL:HG22	1:B:130:ILE:HG12	1.66	0.75
1:B:234:HIS:CE1	1:B:261:ILE:HG21	2.22	0.75
1:D:89:VAL:HG11	1:D:102:LEU:HD23	1.68	0.75
1:C:22:TYR:CD1	1:C:149:GLY:HA2	2.21	0.75
1:D:147:LYS:O	1:D:147:LYS:HG2	1.83	0.75
1:A:66:GLU:HG3	1:A:67:PRO:HD2	1.69	0.75
1:D:200:ILE:HD11	1:D:240:LEU:HD23	1.67	0.75
1:D:78:VAL:HG22	1:D:130:ILE:HG12	1.69	0.75
1:D:197:ILE:HA	1:D:201:ILE:HB	1.69	0.75
1:D:234:HIS:CE1	1:D:261:ILE:HG21	2.22	0.75
1:D:254:THR:O	1:D:258:ILE:HB	1.87	0.74
1:A:200:ILE:HD11	1:A:240:LEU:HD23	1.69	0.74
1:D:104:ARG:NH2	1:E:78:VAL:HA	2.01	0.74
1:E:254:THR:O	1:E:258:ILE:HB	1.87	0.74
1:D:253:TYR:HD1	1:D:313:PHE:CD2	2.04	0.74
1:C:66:GLU:HG3	1:C:67:PRO:HD2	1.68	0.74
1:E:147:LYS:O	1:E:147:LYS:CG	2.35	0.74
1:A:217:SER:OG	1:B:220:TYR:CE2	2.39	0.74
1:B:149:GLY:O	1:B:164:PHE:HD1	1.70	0.74
1:C:226:LEU:HD21	1:D:224:VAL:HB	1.69	0.74
1:D:147:LYS:O	1:D:147:LYS:CG	2.35	0.74
1:B:147:LYS:O	1:B:147:LYS:CG	2.35	0.73
1:A:22:TYR:CD1	1:A:149:GLY:HA2	2.23	0.73
1:E:22:TYR:CD1	1:E:149:GLY:HA2	2.22	0.73
1:C:27:TYR:HB3	1:D:110:LEU:HD11	1.70	0.73
1:D:253:TYR:CD1	1:D:313:PHE:HD2	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:PHE:CE1	1:B:112:PRO:CB	2.69	0.73
1:A:198:PRO:CG	1:B:251:MET:HE1	2.19	0.73
1:B:100:GLN:HE21	1:B:100:GLN:HA	1.54	0.73
1:D:22:TYR:HB3	1:D:41:PHE:HB2	1.71	0.73
1:C:147:LYS:O	1:C:147:LYS:CG	2.35	0.73
1:D:100:GLN:HE21	1:D:100:GLN:HA	1.54	0.72
1:A:146:GLU:HG3	1:B:176:GLU:HG2	1.71	0.72
1:C:254:THR:O	1:C:258:ILE:HB	1.89	0.72
1:E:22:TYR:HB3	1:E:41:PHE:HB2	1.70	0.72
1:A:100:GLN:HE21	1:A:100:GLN:HA	1.54	0.72
1:C:22:TYR:HB3	1:C:41:PHE:HB2	1.71	0.72
1:A:149:GLY:O	1:A:164:PHE:HD1	1.73	0.72
1:A:253:TYR:CD1	1:A:313:PHE:HD2	2.06	0.72
1:C:304:LEU:O	1:C:308:ILE:HG12	1.89	0.72
1:B:238:ASN:HA	1:B:258:ILE:CD1	2.20	0.71
1:A:147:LYS:O	1:A:147:LYS:CG	2.35	0.71
1:B:54:ASP:HB2	1:B:57:ARG:HB2	1.72	0.71
1:A:104:ARG:HH22	1:B:78:VAL:CA	2.01	0.71
1:A:304:LEU:O	1:A:308:ILE:HG12	1.90	0.71
1:A:78:VAL:HG22	1:A:130:ILE:HG12	1.71	0.71
1:B:22:TYR:HB3	1:B:41:PHE:HB2	1.71	0.71
1:D:54:ASP:HB2	1:D:57:ARG:HG3	1.72	0.71
1:D:147:LYS:C	1:D:149:GLY:H	1.99	0.71
1:A:146:GLU:HG3	1:B:176:GLU:CG	2.20	0.71
1:B:89:VAL:HG11	1:B:102:LEU:HD23	1.73	0.71
1:D:79:ASN:H	1:D:79:ASN:HD22	1.36	0.71
1:D:146:GLU:HG3	1:E:176:GLU:HG2	1.73	0.71
1:D:149:GLY:O	1:D:164:PHE:HD1	1.73	0.71
1:B:15:LEU:HD11	1:B:46:TRP:HB2	1.73	0.70
1:D:54:ASP:HB2	1:D:57:ARG:HB2	1.73	0.70
1:C:147:LYS:C	1:C:149:GLY:H	1.99	0.70
1:C:157:THR:HG21	1:D:34:GLU:HG3	1.73	0.70
1:E:100:GLN:HA	1:E:100:GLN:HE21	1.55	0.70
1:A:202:LEU:HD12	1:B:259:PHE:CZ	2.26	0.70
1:A:253:TYR:HD1	1:A:313:PHE:CD2	2.06	0.70
1:E:54:ASP:HB2	1:E:57:ARG:HG3	1.74	0.70
1:A:27:TYR:CG	1:B:110:LEU:CD1	2.75	0.70
1:A:51:LEU:CD1	1:A:70:ILE:HD12	2.22	0.70
1:E:238:ASN:HA	1:E:258:ILE:CD1	2.22	0.70
1:C:79:ASN:HD22	1:C:79:ASN:H	1.39	0.70
1:E:147:LYS:C	1:E:149:GLY:H	1.99	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:LEU:HD11	1:E:46:TRP:HB2	1.74	0.69
1:B:54:ASP:HB2	1:B:57:ARG:HG3	1.74	0.69
1:C:54:ASP:HB2	1:C:57:ARG:HB2	1.74	0.69
1:B:51:LEU:CD1	1:B:70:ILE:HD12	2.22	0.69
1:B:147:LYS:C	1:B:149:GLY:H	1.99	0.69
1:E:84:ARG:HB2	1:E:84:ARG:NH1	2.07	0.69
1:B:253:TYR:HD1	1:B:313:PHE:CD2	2.10	0.69
1:C:193:TYR:O	1:C:194:PHE:HB2	1.92	0.69
1:E:197:ILE:HA	1:E:201:ILE:HB	1.75	0.69
1:B:29:LEU:HB2	1:B:156:LEU:HD11	1.74	0.69
1:E:267:VAL:HA	1:E:270:ILE:HB	1.74	0.69
1:D:238:ASN:HA	1:D:258:ILE:CD1	2.23	0.69
1:A:147:LYS:C	1:A:149:GLY:H	1.99	0.68
1:B:253:TYR:CD1	1:B:313:PHE:HD2	2.11	0.68
1:C:223:ASN:O	1:C:227:VAL:HG23	1.93	0.68
1:D:15:LEU:HD11	1:D:46:TRP:HB2	1.75	0.68
1:B:223:ASN:O	1:B:227:VAL:HG23	1.92	0.68
1:E:54:ASP:HB2	1:E:57:ARG:HB2	1.74	0.68
1:A:238:ASN:HA	1:A:258:ILE:CD1	2.23	0.68
1:C:238:ASN:HA	1:C:258:ILE:CD1	2.23	0.68
1:A:54:ASP:HB2	1:A:57:ARG:HG3	1.75	0.68
1:A:197:ILE:HA	1:A:201:ILE:HB	1.76	0.68
1:C:274:VAL:C	1:C:276:HIS:H	2.02	0.68
1:B:274:VAL:C	1:B:276:HIS:H	2.02	0.68
1:D:53:PHE:CE1	1:D:95:PRO:HA	2.29	0.68
1:C:132:ARG:HA	1:C:180:GLU:HG2	1.76	0.68
1:E:84:ARG:HB2	1:E:84:ARG:HH11	1.58	0.68
1:B:216:TRP:HA	1:B:295:ARG:HH21	1.59	0.68
1:C:118:TYR:CE1	1:C:245:LEU:HD11	2.29	0.68
1:C:216:TRP:HA	1:C:295:ARG:HH21	1.57	0.68
1:D:94:SER:OG	1:D:95:PRO:HD2	1.94	0.68
1:D:216:TRP:HA	1:D:295:ARG:HH21	1.57	0.68
1:D:218:THR:HG22	1:D:279:LYS:HE2	1.76	0.68
1:C:54:ASP:HB2	1:C:57:ARG:HG3	1.75	0.67
1:A:157:THR:CG2	1:B:34:GLU:OE1	2.42	0.67
1:A:194:PHE:HE2	1:B:250:TYR:O	1.77	0.67
1:C:197:ILE:HA	1:C:201:ILE:HB	1.75	0.67
1:E:218:THR:HG22	1:E:279:LYS:HE2	1.74	0.67
1:A:27:TYR:CG	1:B:110:LEU:HD11	2.29	0.67
1:E:53:PHE:CE1	1:E:95:PRO:HA	2.29	0.67
1:A:192:GLN:CD	1:B:249:PRO:HB3	2.19	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:THR:HG22	1:B:279:LYS:HE2	1.77	0.67
1:C:94:SER:OG	1:C:95:PRO:HD2	1.95	0.67
1:D:65:TYR:CD1	1:D:70:ILE:HD11	2.30	0.67
1:A:41:PHE:HE2	1:B:175:LEU:HD23	1.58	0.67
1:D:155:PHE:HE1	1:E:112:PRO:HB3	1.52	0.67
1:D:225:THR:CG2	1:E:224:VAL:CG2	2.71	0.67
1:A:94:SER:OG	1:A:95:PRO:HD2	1.95	0.67
1:D:51:LEU:CD1	1:D:70:ILE:HD12	2.25	0.67
1:A:132:ARG:HA	1:A:180:GLU:HG2	1.77	0.67
1:A:202:LEU:HD12	1:B:259:PHE:CE1	2.30	0.67
1:C:29:LEU:HB2	1:C:156:LEU:HD11	1.77	0.67
1:A:54:ASP:HB2	1:A:57:ARG:HB2	1.76	0.67
1:A:218:THR:HG22	1:A:279:LYS:HE2	1.77	0.67
1:A:274:VAL:C	1:A:276:HIS:H	2.02	0.67
1:C:89:VAL:HG11	1:C:102:LEU:HD23	1.75	0.67
1:C:216:TRP:HA	1:C:295:ARG:NH2	2.09	0.67
1:E:29:LEU:HB2	1:E:156:LEU:HD11	1.76	0.67
1:E:193:TYR:O	1:E:194:PHE:HB2	1.94	0.67
1:C:267:VAL:HA	1:C:270:ILE:HB	1.77	0.66
1:E:253:TYR:HD1	1:E:313:PHE:CD2	2.10	0.66
1:A:194:PHE:HE2	1:B:250:TYR:C	2.03	0.66
1:A:216:TRP:HA	1:A:295:ARG:HH21	1.60	0.66
1:A:223:ASN:O	1:A:227:VAL:HG23	1.94	0.66
1:B:267:VAL:HA	1:B:270:ILE:HB	1.77	0.66
1:C:218:THR:HG22	1:C:279:LYS:HE2	1.76	0.66
1:D:24:ILE:HD13	1:D:104:ARG:HE	1.60	0.66
1:D:132:ARG:HA	1:D:180:GLU:HG2	1.77	0.66
1:A:15:LEU:HD11	1:A:46:TRP:HB2	1.76	0.66
1:C:53:PHE:CE1	1:C:95:PRO:HA	2.31	0.66
1:C:118:TYR:CE1	1:C:245:LEU:CD1	2.78	0.66
1:A:225:THR:HG21	1:B:225:THR:OG1	1.96	0.66
1:B:13:GLU:HB3	1:B:14:PRO:HD2	1.78	0.66
1:D:274:VAL:C	1:D:276:HIS:H	2.02	0.66
1:E:223:ASN:O	1:E:227:VAL:HG23	1.95	0.66
1:C:100:GLN:HE21	1:C:100:GLN:HA	1.61	0.66
1:B:118:TYR:CE1	1:B:245:LEU:CD1	2.79	0.66
1:E:274:VAL:C	1:E:276:HIS:H	2.02	0.66
1:A:77:PHE:CD1	1:A:84:ARG:HD2	2.30	0.66
1:A:137:ARG:HD2	1:A:179:LEU:HG	1.78	0.66
1:B:21:ILE:O	1:B:149:GLY:HA3	1.96	0.66
1:E:118:TYR:CE1	1:E:245:LEU:CD1	2.79	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:253:TYR:CD1	1:E:313:PHE:HD2	2.10	0.66
1:C:199:ASN:HB3	1:D:242:GLU:OE1	1.96	0.66
1:C:202:LEU:HD12	1:D:259:PHE:HE1	1.60	0.66
1:D:118:TYR:CE1	1:D:245:LEU:CD1	2.79	0.66
1:B:53:PHE:CE1	1:B:95:PRO:HA	2.31	0.66
1:B:84:ARG:NH1	1:B:84:ARG:HB2	2.11	0.66
1:E:47:LYS:HD3	1:E:49:ARG:NH2	2.10	0.66
1:E:84:ARG:HH11	1:E:84:ARG:CB	2.08	0.66
1:D:198:PRO:CG	1:E:251:MET:HE1	2.26	0.66
1:C:253:TYR:HD1	1:C:313:PHE:CD2	2.10	0.65
1:C:48:ASP:O	1:C:51:LEU:HD23	1.96	0.65
1:A:77:PHE:H	1:A:84:ARG:HD3	1.60	0.65
1:C:253:TYR:CD1	1:C:313:PHE:HD2	2.10	0.65
1:E:216:TRP:HA	1:E:295:ARG:HH21	1.61	0.65
1:A:84:ARG:NH1	1:A:84:ARG:HB2	2.11	0.65
1:C:15:LEU:HD11	1:C:46:TRP:HB2	1.77	0.65
1:D:21:ILE:O	1:D:149:GLY:HA3	1.97	0.65
1:A:21:ILE:O	1:A:149:GLY:HA3	1.97	0.65
1:B:53:PHE:HE2	1:B:63:LYS:HB3	1.61	0.65
1:B:216:TRP:HA	1:B:295:ARG:NH2	2.11	0.65
1:E:137:ARG:HD2	1:E:179:LEU:HG	1.79	0.65
1:C:84:ARG:HB2	1:C:84:ARG:NH1	2.11	0.65
1:A:93:VAL:HG22	1:A:99:VAL:HG22	1.78	0.65
1:C:53:PHE:HE2	1:C:63:LYS:HB3	1.62	0.65
1:D:41:PHE:HE2	1:E:175:LEU:CD2	2.09	0.65
1:E:132:ARG:HA	1:E:180:GLU:HG2	1.79	0.65
1:C:222:ALA:HB2	1:D:221:GLU:OE1	1.97	0.65
1:E:118:TYR:CE1	1:E:245:LEU:HD11	2.31	0.65
1:A:216:TRP:HA	1:A:295:ARG:NH2	2.12	0.64
1:C:51:LEU:CD1	1:C:70:ILE:HD12	2.27	0.64
1:C:137:ARG:HD2	1:C:179:LEU:HG	1.79	0.64
1:D:84:ARG:NH1	1:D:84:ARG:HB2	2.12	0.64
1:E:249:PRO:HD2	1:E:250:TYR:CD1	2.31	0.64
1:C:21:ILE:O	1:C:149:GLY:HA3	1.98	0.64
1:A:29:LEU:HB2	1:A:156:LEU:HD11	1.80	0.64
1:C:128:TYR:O	1:C:129:LEU:HB2	1.98	0.64
1:E:89:VAL:CG1	1:E:102:LEU:HD23	2.28	0.64
1:A:219:SER:OG	1:A:222:ALA:HB3	1.98	0.64
1:C:194:PHE:C	1:C:196:TYR:N	2.54	0.64
1:A:203:PRO:HB3	1:B:262:TYR:CZ	2.33	0.64
1:D:192:GLN:OE1	1:E:249:PRO:HB3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:ASN:O	1:D:227:VAL:HG23	1.96	0.64
1:E:51:LEU:CD1	1:E:70:ILE:HD12	2.28	0.64
1:E:128:TYR:O	1:E:129:LEU:HB2	1.98	0.64
1:A:193:TYR:O	1:A:194:PHE:HB2	1.96	0.64
1:A:221:GLU:HB3	1:B:221:GLU:CG	2.27	0.64
1:B:221:GLU:OE2	1:C:221:GLU:CD	2.40	0.64
1:A:53:PHE:CE1	1:A:95:PRO:HA	2.32	0.64
1:A:232:ILE:HG22	1:A:233:ALA:N	2.12	0.64
1:A:283:GLN:N	1:A:284:PRO:CD	2.60	0.64
1:C:24:ILE:HD13	1:C:104:ARG:HE	1.63	0.64
1:D:47:LYS:HD3	1:D:49:ARG:NH2	2.13	0.64
1:E:224:VAL:C	1:E:226:LEU:H	2.05	0.64
1:A:53:PHE:HE2	1:A:63:LYS:HB3	1.63	0.64
1:B:132:ARG:HA	1:B:180:GLU:HG2	1.79	0.64
1:E:48:ASP:O	1:E:51:LEU:HD23	1.98	0.64
1:E:139:ILE:HG12	1:E:172:ASN:ND2	2.12	0.64
1:C:65:TYR:CG	1:C:70:ILE:HD11	2.33	0.63
1:C:222:ALA:HB2	1:D:221:GLU:HA	1.80	0.63
1:A:128:TYR:O	1:A:129:LEU:HB2	1.98	0.63
1:B:47:LYS:HD3	1:B:49:ARG:NH2	2.13	0.63
1:E:216:TRP:HA	1:E:295:ARG:NH2	2.13	0.63
1:A:104:ARG:NH1	1:B:77:PHE:O	2.29	0.63
1:B:276:HIS:O	1:B:280:VAL:HG22	1.98	0.63
1:D:13:GLU:HB3	1:D:14:PRO:HD2	1.80	0.63
1:B:84:ARG:HB2	1:B:84:ARG:HH11	1.64	0.63
1:D:118:TYR:CE1	1:D:245:LEU:HD11	2.32	0.63
1:A:224:VAL:C	1:A:226:LEU:N	2.56	0.63
1:A:267:VAL:HA	1:A:270:ILE:HB	1.80	0.63
1:C:149:GLY:O	1:C:164:PHE:CD1	2.51	0.63
1:D:51:LEU:HD11	1:D:70:ILE:HD12	1.79	0.63
1:D:77:PHE:H	1:D:84:ARG:HD3	1.62	0.63
1:B:193:TYR:O	1:B:194:PHE:HB2	1.97	0.63
1:C:47:LYS:HD3	1:C:49:ARG:NH2	2.14	0.63
1:C:65:TYR:CD1	1:C:70:ILE:HD11	2.34	0.63
1:C:77:PHE:H	1:C:84:ARG:HD3	1.62	0.63
1:D:232:ILE:HG22	1:D:233:ALA:N	2.13	0.63
1:D:53:PHE:HE2	1:D:63:LYS:HB3	1.64	0.63
1:E:53:PHE:HE2	1:E:63:LYS:HB3	1.61	0.63
1:A:48:ASP:O	1:A:51:LEU:HD23	1.99	0.62
1:A:224:VAL:C	1:A:226:LEU:H	2.05	0.62
1:E:144:ASP:HA	1:E:147:LYS:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:TYR:O	1:B:129:LEU:HB2	1.98	0.62
1:D:216:TRP:HA	1:D:295:ARG:NH2	2.13	0.62
1:B:118:TYR:CE1	1:B:245:LEU:HD11	2.33	0.62
1:B:283:GLN:N	1:B:284:PRO:CD	2.63	0.62
1:D:267:VAL:HA	1:D:270:ILE:HB	1.80	0.62
1:E:21:ILE:O	1:E:149:GLY:HA3	1.98	0.62
1:C:193:TYR:O	1:C:194:PHE:CB	2.46	0.62
1:D:84:ARG:CB	1:D:84:ARG:HH11	2.12	0.62
1:B:224:VAL:C	1:B:226:LEU:H	2.07	0.62
1:C:283:GLN:N	1:C:284:PRO:CD	2.62	0.62
1:A:13:GLU:HB3	1:A:14:PRO:HD2	1.81	0.62
1:B:249:PRO:HD2	1:B:250:TYR:CD1	2.35	0.62
1:D:249:PRO:HD2	1:D:250:TYR:CD1	2.35	0.62
1:C:202:LEU:HD12	1:D:259:PHE:CE1	2.35	0.61
1:D:65:TYR:CG	1:D:70:ILE:HD11	2.35	0.61
1:E:283:GLN:N	1:E:284:PRO:CD	2.62	0.61
1:B:48:ASP:O	1:B:51:LEU:HD23	2.00	0.61
1:B:84:ARG:HH11	1:B:84:ARG:CB	2.13	0.61
1:D:128:TYR:O	1:D:129:LEU:HB2	1.98	0.61
1:D:283:GLN:N	1:D:284:PRO:CD	2.62	0.61
1:C:84:ARG:HB2	1:C:84:ARG:HH11	1.65	0.61
1:C:219:SER:OG	1:C:222:ALA:HB3	1.99	0.61
1:D:29:LEU:HB2	1:D:156:LEU:HD11	1.81	0.61
1:D:192:GLN:CD	1:E:249:PRO:HB3	2.26	0.61
1:A:89:VAL:CG1	1:A:102:LEU:HD23	2.30	0.61
1:C:13:GLU:HB3	1:C:14:PRO:HD2	1.82	0.61
1:C:93:VAL:HG22	1:C:99:VAL:HG22	1.83	0.61
1:D:77:PHE:CD1	1:D:84:ARG:HD2	2.36	0.61
1:E:194:PHE:C	1:E:196:TYR:N	2.56	0.61
1:A:131:VAL:HG11	1:A:140:VAL:HG13	1.83	0.61
1:B:77:PHE:H	1:B:84:ARG:HD3	1.66	0.61
1:D:193:TYR:O	1:D:194:PHE:HB2	1.98	0.61
1:E:29:LEU:C	1:E:29:LEU:HD23	2.25	0.61
1:E:224:VAL:C	1:E:226:LEU:N	2.56	0.61
1:C:194:PHE:C	1:C:196:TYR:H	2.06	0.61
1:D:131:VAL:HG11	1:D:140:VAL:HG13	1.82	0.61
1:B:51:LEU:HD11	1:B:70:ILE:HD12	1.82	0.61
1:B:238:ASN:HA	1:B:258:ILE:HD11	1.81	0.61
1:D:137:ARG:HD2	1:D:179:LEU:HG	1.82	0.61
1:E:200:ILE:O	1:E:204:MET:HB2	2.01	0.61
1:B:131:VAL:HG11	1:B:140:VAL:HG13	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:GLU:O	1:B:283:GLN:N	2.34	0.61
1:C:77:PHE:CD1	1:C:84:ARG:HD2	2.35	0.61
1:C:224:VAL:C	1:C:226:LEU:H	2.08	0.61
1:D:215:PHE:HZ	1:D:298:PHE:CD1	2.18	0.61
1:E:94:SER:OG	1:E:95:PRO:HD2	2.01	0.61
1:A:194:PHE:C	1:A:196:TYR:N	2.58	0.61
1:A:24:ILE:HD13	1:A:104:ARG:HE	1.64	0.60
1:A:149:GLY:O	1:A:164:PHE:CD1	2.54	0.60
1:B:144:ASP:HA	1:B:147:LYS:HB3	1.83	0.60
1:B:224:VAL:C	1:B:226:LEU:N	2.57	0.60
1:C:215:PHE:HZ	1:C:298:PHE:CD1	2.17	0.60
1:B:260:MET:HE2	1:B:309:LEU:HD22	1.83	0.60
1:C:86:ALA:HB2	1:C:105:PHE:HB3	1.83	0.60
1:C:276:HIS:C	1:C:278:LEU:H	2.09	0.60
1:D:89:VAL:CG1	1:D:102:LEU:HD23	2.31	0.60
1:A:157:THR:HG21	1:B:34:GLU:HG3	1.84	0.60
1:B:232:ILE:HG22	1:B:233:ALA:N	2.16	0.60
1:C:84:ARG:HH11	1:C:84:ARG:CB	2.14	0.60
1:A:84:ARG:HB2	1:A:84:ARG:HH11	1.67	0.60
1:B:193:TYR:O	1:B:194:PHE:CB	2.48	0.60
1:E:193:TYR:O	1:E:194:PHE:CB	2.49	0.60
1:A:249:PRO:HD2	1:A:250:TYR:CD1	2.37	0.60
1:B:94:SER:OG	1:B:95:PRO:HD2	2.02	0.60
1:B:137:ARG:HD2	1:B:179:LEU:HG	1.83	0.60
1:D:276:HIS:C	1:D:278:LEU:H	2.09	0.60
1:E:276:HIS:C	1:E:278:LEU:H	2.09	0.60
1:A:225:THR:HG22	1:B:224:VAL:HG23	1.83	0.60
1:B:77:PHE:CD1	1:B:84:ARG:HD2	2.36	0.60
1:A:51:LEU:HD11	1:A:70:ILE:HD12	1.84	0.60
1:A:198:PRO:HG3	1:B:251:MET:HE1	1.83	0.60
1:B:194:PHE:C	1:B:196:TYR:N	2.57	0.60
1:B:276:HIS:C	1:B:278:LEU:H	2.09	0.60
1:D:76:ARG:HH22	1:D:130:ILE:CD1	2.10	0.60
1:C:29:LEU:C	1:C:29:LEU:HD23	2.27	0.59
1:C:144:ASP:HA	1:C:147:LYS:HB3	1.84	0.59
1:C:194:PHE:HA	1:C:197:ILE:HD12	1.84	0.59
1:D:281:GLU:O	1:D:283:GLN:N	2.35	0.59
1:E:13:GLU:HB3	1:E:14:PRO:HD2	1.83	0.59
1:E:65:TYR:CD1	1:E:70:ILE:HD11	2.37	0.59
1:E:86:ALA:HB2	1:E:105:PHE:HB3	1.84	0.59
1:A:194:PHE:CE2	1:B:250:TYR:C	2.80	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:ARG:NH2	1:B:130:ILE:CD1	2.55	0.59
1:C:27:TYR:CB	1:D:110:LEU:HD11	2.31	0.59
1:A:238:ASN:HA	1:A:258:ILE:HD11	1.84	0.59
1:A:276:HIS:C	1:A:278:LEU:H	2.09	0.59
1:C:200:ILE:CD1	1:C:240:LEU:HD23	2.30	0.59
1:A:193:TYR:O	1:A:194:PHE:CB	2.49	0.59
1:D:194:PHE:C	1:D:196:TYR:N	2.57	0.59
1:E:65:TYR:CG	1:E:70:ILE:HD11	2.36	0.59
1:B:200:ILE:O	1:B:204:MET:HB2	2.02	0.59
1:E:24:ILE:HD13	1:E:104:ARG:HE	1.67	0.59
1:A:84:ARG:HH11	1:A:84:ARG:CB	2.14	0.59
1:B:215:PHE:HZ	1:B:298:PHE:CD1	2.20	0.59
1:A:215:PHE:HZ	1:A:298:PHE:CD1	2.20	0.59
1:A:226:LEU:HD23	1:B:224:VAL:CB	2.32	0.59
1:C:194:PHE:HE2	1:D:250:TYR:O	1.86	0.59
1:C:281:GLU:O	1:C:283:GLN:N	2.36	0.59
1:B:93:VAL:HG22	1:B:99:VAL:HG22	1.85	0.59
1:C:224:VAL:C	1:C:226:LEU:N	2.60	0.59
1:C:249:PRO:HD2	1:C:250:TYR:CD1	2.37	0.59
1:E:194:PHE:C	1:E:196:TYR:H	2.10	0.59
1:C:139:ILE:HG12	1:C:172:ASN:ND2	2.14	0.59
1:D:54:ASP:HB2	1:D:57:ARG:CG	2.32	0.59
1:B:139:ILE:HG12	1:B:172:ASN:ND2	2.16	0.58
1:C:234:HIS:CE1	1:C:261:ILE:CG2	2.85	0.58
1:E:276:HIS:O	1:E:280:VAL:HG22	2.03	0.58
1:A:86:ALA:HB2	1:A:105:PHE:HB3	1.85	0.58
1:B:54:ASP:HB2	1:B:57:ARG:CG	2.33	0.58
1:B:65:TYR:CD1	1:B:70:ILE:HD11	2.38	0.58
1:D:224:VAL:C	1:D:226:LEU:H	2.11	0.58
1:D:225:THR:HG22	1:E:224:VAL:CG2	2.30	0.58
1:E:194:PHE:HA	1:E:197:ILE:HD12	1.85	0.58
1:C:131:VAL:HG11	1:C:140:VAL:HG13	1.84	0.58
1:E:131:VAL:HG11	1:E:140:VAL:HG13	1.86	0.58
1:E:232:ILE:HG22	1:E:233:ALA:N	2.18	0.58
1:C:275:GLN:O	1:C:275:GLN:HG2	2.04	0.58
1:C:276:HIS:O	1:C:280:VAL:HG22	2.03	0.58
1:E:215:PHE:HZ	1:E:298:PHE:CD1	2.21	0.58
1:E:281:GLU:O	1:E:283:GLN:N	2.37	0.58
1:D:139:ILE:HG12	1:D:172:ASN:ND2	2.17	0.58
1:A:65:TYR:CG	1:A:70:ILE:HD11	2.38	0.58
1:D:76:ARG:NH2	1:D:130:ILE:CD1	2.56	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:TYR:CG	1:B:70:ILE:HD11	2.38	0.58
1:D:140:VAL:HG22	1:D:181:SER:HB3	1.86	0.58
1:E:149:GLY:O	1:E:164:PHE:CD1	2.53	0.58
1:E:298:PHE:HB2	1:E:299:PRO:HD3	1.85	0.58
1:B:86:ALA:HB2	1:B:105:PHE:HB3	1.86	0.58
1:C:200:ILE:O	1:C:204:MET:HB2	2.04	0.58
1:D:48:ASP:O	1:D:51:LEU:HD23	2.04	0.58
1:E:219:SER:OG	1:E:222:ALA:HB3	2.04	0.58
1:E:77:PHE:H	1:E:84:ARG:HD3	1.68	0.58
1:D:86:ALA:HB2	1:D:105:PHE:HB3	1.85	0.57
1:D:193:TYR:O	1:D:194:PHE:CB	2.51	0.57
1:E:47:LYS:CD	1:E:49:ARG:HH21	2.17	0.57
1:E:215:PHE:HZ	1:E:298:PHE:CE1	2.21	0.57
1:E:275:GLN:O	1:E:275:GLN:HG2	2.04	0.57
1:A:281:GLU:O	1:A:283:GLN:N	2.37	0.57
1:C:118:TYR:CD1	1:C:245:LEU:HD11	2.39	0.57
1:C:215:PHE:HZ	1:C:298:PHE:CE1	2.22	0.57
1:E:54:ASP:HB2	1:E:57:ARG:CG	2.34	0.57
1:A:65:TYR:CD1	1:A:70:ILE:HD11	2.39	0.57
1:A:140:VAL:HG22	1:A:181:SER:HB3	1.86	0.57
1:B:275:GLN:HG2	1:B:275:GLN:O	2.04	0.57
1:E:264:PHE:CE2	1:E:302:PHE:HB2	2.39	0.57
1:A:41:PHE:HZ	1:B:76:ARG:NH2	2.03	0.57
1:C:44:LEU:HD12	1:C:101:TYR:CD2	2.40	0.57
1:A:47:LYS:HD3	1:A:49:ARG:NH2	2.19	0.57
1:B:29:LEU:HD23	1:B:29:LEU:C	2.30	0.57
1:B:194:PHE:C	1:B:196:TYR:H	2.12	0.57
1:E:93:VAL:HG22	1:E:99:VAL:HG22	1.86	0.57
1:A:275:GLN:O	1:A:275:GLN:HG2	2.04	0.57
1:B:47:LYS:CD	1:B:49:ARG:HH21	2.18	0.57
1:C:54:ASP:HB2	1:C:57:ARG:CG	2.34	0.57
1:E:62:VAL:HG13	1:E:93:VAL:O	2.05	0.57
1:B:149:GLY:O	1:B:164:PHE:CD1	2.56	0.57
1:D:29:LEU:HD23	1:D:29:LEU:C	2.29	0.57
1:B:76:ARG:HH22	1:B:130:ILE:CD1	2.09	0.57
1:C:86:ALA:HB2	1:C:105:PHE:CB	2.35	0.57
1:A:194:PHE:C	1:A:196:TYR:H	2.12	0.56
1:D:276:HIS:O	1:D:280:VAL:HG22	2.05	0.56
1:A:29:LEU:C	1:A:29:LEU:HD23	2.29	0.56
1:A:139:ILE:HG12	1:A:172:ASN:ND2	2.14	0.56
1:B:194:PHE:HA	1:B:197:ILE:HD12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:ARG:NH2	1:C:130:ILE:CD1	2.62	0.56
1:C:89:VAL:CG1	1:C:102:LEU:HD23	2.35	0.56
1:C:147:LYS:HE2	1:C:165:THR:HA	1.87	0.56
1:D:53:PHE:CD1	1:D:95:PRO:HA	2.41	0.56
1:D:215:PHE:HZ	1:D:298:PHE:CE1	2.23	0.56
1:E:77:PHE:CD1	1:E:84:ARG:HD2	2.40	0.56
1:D:194:PHE:HA	1:D:197:ILE:HD12	1.86	0.56
1:A:215:PHE:HZ	1:A:298:PHE:CE1	2.23	0.56
1:A:222:ALA:O	1:A:226:LEU:HB2	2.06	0.56
1:D:224:VAL:C	1:D:226:LEU:N	2.61	0.56
1:D:238:ASN:HA	1:D:258:ILE:HD11	1.86	0.56
1:D:37:LYS:HG2	1:D:108:ARG:HB3	1.88	0.56
1:D:48:ASP:O	1:D:50:ARG:N	2.39	0.56
1:D:149:GLY:O	1:D:164:PHE:CD1	2.57	0.56
1:E:238:ASN:HA	1:E:258:ILE:HD11	1.86	0.56
1:A:147:LYS:O	1:A:147:LYS:HD3	2.06	0.56
1:B:147:LYS:O	1:B:147:LYS:HD3	2.06	0.56
1:B:215:PHE:HZ	1:B:298:PHE:CE1	2.24	0.56
1:D:275:GLN:O	1:D:275:GLN:HG2	2.04	0.56
1:A:76:ARG:NH2	1:A:130:ILE:CD1	2.60	0.56
1:A:147:LYS:HE2	1:A:165:THR:HA	1.86	0.56
1:E:70:ILE:HD13	1:E:70:ILE:N	2.21	0.56
1:A:25:GLU:HG3	1:B:79:ASN:HA	1.86	0.56
1:B:298:PHE:HB2	1:B:299:PRO:HD3	1.88	0.56
1:A:54:ASP:HB2	1:A:57:ARG:CG	2.35	0.56
1:A:253:TYR:O	1:A:256:ALA:HB3	2.06	0.56
1:B:54:ASP:HB2	1:B:57:ARG:CB	2.36	0.56
1:E:51:LEU:HD11	1:E:70:ILE:HD12	1.88	0.56
1:E:305:ALA:O	1:E:309:LEU:HB2	2.06	0.56
1:B:23:LEU:HA	1:B:40:ALA:HB2	1.87	0.55
1:B:24:ILE:HD13	1:B:104:ARG:HE	1.71	0.55
1:B:140:VAL:HG22	1:B:181:SER:HB3	1.88	0.55
1:E:147:LYS:O	1:E:147:LYS:HD3	2.06	0.55
1:A:23:LEU:HA	1:A:40:ALA:HB2	1.87	0.55
1:B:253:TYR:O	1:B:256:ALA:HB3	2.06	0.55
1:C:147:LYS:O	1:C:147:LYS:HD3	2.06	0.55
1:C:238:ASN:HA	1:C:258:ILE:HD11	1.88	0.55
1:D:23:LEU:HA	1:D:40:ALA:HB2	1.88	0.55
1:D:147:LYS:O	1:D:147:LYS:HD3	2.06	0.55
1:C:47:LYS:CD	1:C:49:ARG:HH21	2.20	0.55
1:A:42:LEU:HD23	1:A:103:GLU:OE1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:VAL:CG1	1:B:102:LEU:HD23	2.35	0.55
1:C:215:PHE:CZ	1:C:298:PHE:CD1	2.94	0.55
1:D:118:TYR:CE2	1:D:196:TYR:HE2	2.25	0.55
1:D:123:GLN:HA	1:D:123:GLN:NE2	2.21	0.55
1:D:298:PHE:HB2	1:D:299:PRO:HD3	1.88	0.55
1:E:200:ILE:CD1	1:E:240:LEU:HD23	2.32	0.55
1:A:86:ALA:HB2	1:A:105:PHE:CB	2.37	0.55
1:A:240:LEU:HD13	1:B:239:ILE:CG1	2.37	0.55
1:D:84:ARG:HB2	1:D:84:ARG:HH11	1.70	0.55
1:B:118:TYR:CE2	1:B:196:TYR:HE2	2.25	0.55
1:C:298:PHE:HB2	1:C:299:PRO:HD3	1.88	0.55
1:A:44:LEU:HD12	1:A:101:TYR:CD2	2.42	0.55
1:A:194:PHE:HA	1:A:197:ILE:HD12	1.88	0.55
1:B:118:TYR:CE1	1:B:245:LEU:HD13	2.41	0.55
1:D:215:PHE:CZ	1:D:298:PHE:CD1	2.95	0.55
1:D:278:LEU:HD23	1:D:287:ALA:HA	1.88	0.55
1:A:276:HIS:O	1:A:280:VAL:HG22	2.06	0.55
1:D:41:PHE:CE2	1:E:175:LEU:CD2	2.90	0.55
1:E:53:PHE:CD1	1:E:95:PRO:HA	2.42	0.55
1:A:157:THR:HG21	1:B:34:GLU:OE1	2.05	0.54
1:A:278:LEU:HD23	1:A:287:ALA:HA	1.89	0.54
1:B:62:VAL:HG13	1:B:93:VAL:O	2.07	0.54
1:A:200:ILE:O	1:A:204:MET:HB2	2.07	0.54
1:B:53:PHE:CD1	1:B:95:PRO:HA	2.42	0.54
1:C:118:TYR:CE2	1:C:196:TYR:HE2	2.25	0.54
1:C:23:LEU:CD2	1:C:38:VAL:HG21	2.37	0.54
1:C:42:LEU:HD23	1:C:103:GLU:OE1	2.06	0.54
1:D:118:TYR:CE1	1:D:245:LEU:HD13	2.41	0.54
1:E:98:THR:HG22	1:E:98:THR:O	2.07	0.54
1:D:93:VAL:HG22	1:D:99:VAL:HG22	1.88	0.54
1:C:215:PHE:O	1:C:291:THR:HG22	2.08	0.54
1:D:153:ASP:O	1:D:154:VAL:C	2.51	0.54
1:A:298:PHE:HB2	1:A:299:PRO:HD3	1.88	0.54
1:B:305:ALA:O	1:B:309:LEU:HB2	2.08	0.54
1:C:264:PHE:CE2	1:C:302:PHE:HB2	2.43	0.54
1:D:18:ASN:O	1:D:44:LEU:HA	2.08	0.54
1:D:222:ALA:O	1:D:226:LEU:HB2	2.08	0.54
1:E:86:ALA:HB2	1:E:105:PHE:CB	2.37	0.54
1:A:37:LYS:HG2	1:A:108:ARG:HB3	1.89	0.54
1:B:23:LEU:CD2	1:B:38:VAL:HG21	2.38	0.54
1:C:41:PHE:HZ	1:D:76:ARG:NH2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:ASP:HA	1:D:147:LYS:HB3	1.89	0.54
1:E:278:LEU:HD23	1:E:287:ALA:HA	1.89	0.54
1:B:123:GLN:HA	1:B:123:GLN:NE2	2.22	0.54
1:B:267:VAL:HG23	1:B:298:PHE:CZ	2.42	0.54
1:B:278:LEU:HD23	1:B:287:ALA:HA	1.89	0.54
1:C:153:ASP:O	1:C:154:VAL:C	2.51	0.54
1:D:194:PHE:C	1:D:196:TYR:H	2.14	0.54
1:E:54:ASP:HB2	1:E:57:ARG:CB	2.37	0.54
1:A:18:ASN:O	1:A:44:LEU:HA	2.07	0.53
1:A:274:VAL:C	1:A:276:HIS:N	2.66	0.53
1:E:274:VAL:C	1:E:276:HIS:N	2.66	0.53
1:C:155:PHE:HD1	1:D:110:LEU:CD2	2.22	0.53
1:C:232:ILE:HG22	1:C:233:ALA:N	2.22	0.53
1:D:86:ALA:HB2	1:D:105:PHE:CB	2.38	0.53
1:E:118:TYR:CD1	1:E:245:LEU:HD11	2.43	0.53
1:A:234:HIS:CE1	1:A:261:ILE:CG2	2.92	0.53
1:B:118:TYR:CD1	1:B:245:LEU:HD11	2.43	0.53
1:D:47:LYS:CD	1:D:49:ARG:HH21	2.21	0.53
1:E:260:MET:HE2	1:E:309:LEU:HD22	1.91	0.53
1:C:51:LEU:HD11	1:C:70:ILE:HD12	1.90	0.53
1:A:240:LEU:HD13	1:B:239:ILE:HG12	1.91	0.53
1:B:70:ILE:HG22	1:B:71:TRP:N	2.24	0.53
1:B:119:PRO:O	1:B:193:TYR:HB3	2.09	0.53
1:B:219:SER:OG	1:B:222:ALA:HB3	2.09	0.53
1:C:62:VAL:HG13	1:C:93:VAL:O	2.08	0.53
1:C:226:LEU:CD2	1:D:224:VAL:HB	2.37	0.53
1:D:54:ASP:HB2	1:D:57:ARG:CB	2.37	0.53
1:D:118:TYR:CD1	1:D:245:LEU:HD11	2.43	0.53
1:D:274:VAL:C	1:D:276:HIS:N	2.66	0.53
1:E:215:PHE:CZ	1:E:298:PHE:CD1	2.96	0.53
1:A:23:LEU:CD2	1:A:38:VAL:HG21	2.38	0.53
1:A:215:PHE:CZ	1:A:298:PHE:CD1	2.96	0.53
1:B:86:ALA:HB2	1:B:105:PHE:CB	2.39	0.53
1:C:76:ARG:HH22	1:C:130:ILE:CD1	2.17	0.53
1:D:261:ILE:O	1:D:262:TYR:C	2.52	0.53
1:D:98:THR:O	1:D:98:THR:HG22	2.09	0.53
1:D:119:PRO:O	1:D:193:TYR:HB3	2.09	0.53
1:C:225:THR:HG21	1:D:225:THR:OG1	2.09	0.53
1:D:48:ASP:C	1:D:50:ARG:N	2.67	0.53
1:D:264:PHE:CE2	1:D:302:PHE:HB2	2.44	0.53
1:A:260:MET:HE2	1:A:309:LEU:HD22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:LYS:HE2	1:B:165:THR:HA	1.90	0.53
1:C:22:TYR:HA	1:C:149:GLY:HA2	1.91	0.53
1:C:27:TYR:CE1	1:D:81:GLU:CD	2.87	0.53
1:D:48:ASP:C	1:D:50:ARG:H	2.17	0.53
1:A:54:ASP:HB2	1:A:57:ARG:CB	2.39	0.52
1:B:215:PHE:O	1:B:291:THR:HG22	2.09	0.52
1:C:118:TYR:CE1	1:C:245:LEU:HD13	2.43	0.52
1:C:267:VAL:HG23	1:C:298:PHE:CZ	2.44	0.52
1:C:54:ASP:HB2	1:C:57:ARG:CB	2.38	0.52
1:C:147:LYS:C	1:C:149:GLY:N	2.68	0.52
1:D:221:GLU:OE2	1:E:221:GLU:CD	2.52	0.52
1:E:118:TYR:CE2	1:E:196:TYR:HE2	2.27	0.52
1:A:144:ASP:HA	1:A:147:LYS:HB3	1.90	0.52
1:B:249:PRO:HD2	1:B:250:TYR:CE1	2.44	0.52
1:C:140:VAL:HG22	1:C:181:SER:HB3	1.91	0.52
1:C:278:LEU:HD23	1:C:287:ALA:HA	1.90	0.52
1:D:23:LEU:CD2	1:D:38:VAL:HG21	2.39	0.52
1:D:146:GLU:HG3	1:E:176:GLU:CG	2.39	0.52
1:D:225:THR:HG21	1:E:224:VAL:CG2	2.33	0.52
1:E:47:LYS:HD3	1:E:49:ARG:HH21	1.73	0.52
1:E:118:TYR:CE1	1:E:245:LEU:HD13	2.44	0.52
1:A:221:GLU:OE2	1:B:221:GLU:CD	2.53	0.52
1:C:226:LEU:HD23	1:D:224:VAL:HG21	1.92	0.52
1:D:219:SER:OG	1:D:222:ALA:HB3	2.08	0.52
1:E:23:LEU:CD2	1:E:38:VAL:HG21	2.39	0.52
1:B:215:PHE:CZ	1:B:298:PHE:CD1	2.96	0.52
1:D:77:PHE:CE2	1:D:127:ILE:HG23	2.45	0.52
1:D:95:PRO:C	1:D:97:GLY:H	2.17	0.52
1:D:215:PHE:O	1:D:291:THR:HG22	2.09	0.52
1:E:147:LYS:HE2	1:E:165:THR:HA	1.91	0.52
1:E:234:HIS:CE1	1:E:261:ILE:CG2	2.92	0.52
1:A:210:ILE:HG23	1:B:269:VAL:HG11	1.92	0.52
1:D:260:MET:HE2	1:D:309:LEU:HD22	1.91	0.52
1:A:119:PRO:O	1:A:193:TYR:HB3	2.10	0.52
1:D:253:TYR:O	1:D:256:ALA:HB3	2.10	0.52
1:E:70:ILE:HG22	1:E:71:TRP:N	2.25	0.52
1:E:109:VAL:HG11	1:E:126:HIS:O	2.10	0.52
1:E:215:PHE:O	1:E:291:THR:HG22	2.09	0.52
1:A:305:ALA:O	1:A:309:LEU:HB2	2.09	0.51
1:B:153:ASP:O	1:B:154:VAL:C	2.53	0.51
1:B:222:ALA:O	1:B:226:LEU:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:140:VAL:HG22	1:E:181:SER:HB3	1.91	0.51
1:B:215:PHE:O	1:B:291:THR:CG2	2.58	0.51
1:C:109:VAL:HG11	1:C:126:HIS:O	2.11	0.51
1:D:123:GLN:HB2	1:D:189:ILE:HG13	1.92	0.51
1:E:212:TRP:CZ3	1:E:298:PHE:HB3	2.45	0.51
1:A:256:ALA:HB1	1:A:309:LEU:HD21	1.92	0.51
1:E:222:ALA:O	1:E:226:LEU:HB2	2.11	0.51
1:B:77:PHE:CE2	1:B:127:ILE:HG23	2.46	0.51
1:C:155:PHE:CD1	1:D:110:LEU:CD2	2.93	0.51
1:C:222:ALA:CB	1:D:221:GLU:OE1	2.59	0.51
1:E:23:LEU:HA	1:E:40:ALA:HB2	1.93	0.51
1:B:191:ARG:HG3	1:B:192:GLN:N	2.26	0.51
1:C:53:PHE:CD1	1:C:95:PRO:HA	2.45	0.51
1:D:249:PRO:HD2	1:D:250:TYR:CE1	2.46	0.51
1:E:153:ASP:O	1:E:154:VAL:C	2.53	0.51
1:A:9:PRO:HD3	1:A:71:TRP:CE3	2.45	0.51
1:B:81:GLU:HG3	1:B:108:ARG:HG3	1.93	0.51
1:B:264:PHE:CE2	1:B:302:PHE:HB2	2.45	0.51
1:A:215:PHE:O	1:A:291:THR:HG22	2.09	0.51
1:C:256:ALA:HB1	1:C:309:LEU:HD21	1.92	0.51
1:D:147:LYS:C	1:D:149:GLY:N	2.68	0.51
1:E:37:LYS:HG2	1:E:108:ARG:HB3	1.91	0.51
1:A:53:PHE:CD1	1:A:95:PRO:HA	2.46	0.51
1:A:147:LYS:O	1:A:147:LYS:CD	2.59	0.51
1:A:153:ASP:O	1:A:154:VAL:C	2.51	0.51
1:E:133:SER:HB2	1:E:137:ARG:NH1	2.25	0.51
1:A:62:VAL:HG13	1:A:93:VAL:O	2.10	0.51
1:B:147:LYS:O	1:B:147:LYS:CD	2.59	0.51
1:C:37:LYS:HG2	1:C:108:ARG:HB3	1.92	0.51
1:C:77:PHE:CE2	1:C:127:ILE:HG23	2.46	0.51
1:D:305:ALA:O	1:D:309:LEU:HB2	2.10	0.51
1:E:77:PHE:CE2	1:E:127:ILE:HG23	2.46	0.51
1:A:18:ASN:HB2	1:A:45:SER:OG	2.11	0.51
1:A:215:PHE:O	1:A:291:THR:CG2	2.59	0.51
1:A:260:MET:CE	1:A:309:LEU:HD22	2.41	0.51
1:B:44:LEU:HD12	1:B:101:TYR:CD2	2.46	0.51
1:B:119:PRO:HB3	1:B:196:TYR:CD2	2.46	0.51
1:D:119:PRO:HB3	1:D:196:TYR:CD2	2.46	0.51
1:D:215:PHE:O	1:D:291:THR:CG2	2.58	0.51
1:E:147:LYS:O	1:E:147:LYS:CD	2.59	0.51
1:A:119:PRO:HB3	1:A:196:TYR:CD2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:SER:CB	1:B:220:TYR:HE2	2.23	0.50
1:A:226:LEU:HD23	1:B:224:VAL:CG2	2.42	0.50
1:C:240:LEU:HD22	1:D:239:ILE:HD11	1.92	0.50
1:C:305:ALA:O	1:C:309:LEU:HB2	2.10	0.50
1:A:27:TYR:HB3	1:B:110:LEU:HD11	1.90	0.50
1:B:48:ASP:C	1:B:50:ARG:H	2.18	0.50
1:B:70:ILE:HG22	1:B:71:TRP:O	2.11	0.50
1:E:253:TYR:HA	1:E:313:PHE:CD2	2.46	0.50
1:B:197:ILE:CG2	1:B:202:LEU:HG	2.41	0.50
1:C:98:THR:O	1:C:98:THR:HG22	2.10	0.50
1:C:215:PHE:O	1:C:291:THR:CG2	2.59	0.50
1:B:48:ASP:O	1:B:50:ARG:N	2.44	0.50
1:D:253:TYR:HA	1:D:313:PHE:CD2	2.46	0.50
1:A:209:PHE:HB2	1:B:266:PHE:HE1	1.76	0.50
1:C:18:ASN:O	1:C:44:LEU:HA	2.12	0.50
1:D:42:LEU:HD23	1:D:103:GLU:OE1	2.11	0.50
1:E:44:LEU:HD12	1:E:101:TYR:CD2	2.47	0.50
1:E:249:PRO:HD2	1:E:250:TYR:CE1	2.46	0.50
1:C:123:GLN:HA	1:C:123:GLN:NE2	2.26	0.50
1:C:253:TYR:HA	1:C:313:PHE:CD2	2.47	0.50
1:A:22:TYR:HA	1:A:149:GLY:HA2	1.94	0.50
1:B:79:ASN:H	1:B:79:ASN:ND2	2.02	0.50
1:C:215:PHE:HB2	1:C:216:TRP:CE3	2.47	0.50
1:C:226:LEU:HD23	1:D:224:VAL:CG2	2.42	0.50
1:D:234:HIS:CE1	1:D:261:ILE:CG2	2.93	0.50
1:A:198:PRO:HG2	1:B:251:MET:HE1	1.92	0.50
1:A:253:TYR:HA	1:A:313:PHE:CD2	2.47	0.50
1:A:261:ILE:O	1:A:262:TYR:C	2.54	0.50
1:D:44:LEU:HD12	1:D:101:TYR:CD2	2.46	0.50
1:D:52:ALA:HA	1:D:95:PRO:O	2.11	0.50
1:D:256:ALA:HB1	1:D:309:LEU:HD21	1.94	0.50
1:A:76:ARG:HH22	1:A:130:ILE:CD1	2.16	0.50
1:A:267:VAL:HG23	1:A:298:PHE:CZ	2.46	0.50
1:D:197:ILE:CG2	1:D:202:LEU:HG	2.42	0.49
1:D:147:LYS:O	1:D:147:LYS:CD	2.59	0.49
1:D:198:PRO:HG2	1:E:251:MET:HE1	1.93	0.49
1:E:268:ALA:HA	1:E:298:PHE:HE1	1.77	0.49
1:C:179:LEU:C	1:C:179:LEU:HD12	2.38	0.49
1:C:253:TYR:O	1:C:256:ALA:HB3	2.12	0.49
1:D:78:VAL:HB	1:D:128:TYR:HB2	1.94	0.49
1:E:215:PHE:O	1:E:291:THR:CG2	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:SER:HB3	1:B:223:ASN:OD1	2.12	0.49
1:C:78:VAL:CG2	1:C:130:ILE:HG12	2.39	0.49
1:D:78:VAL:CG2	1:D:130:ILE:HG12	2.41	0.49
1:D:200:ILE:O	1:D:204:MET:HB2	2.11	0.49
1:A:179:LEU:C	1:A:179:LEU:HD12	2.38	0.49
1:C:238:ASN:HA	1:C:258:ILE:HD13	1.95	0.49
1:A:77:PHE:CE2	1:A:127:ILE:HG23	2.47	0.49
1:B:13:GLU:HB3	1:B:14:PRO:CD	2.42	0.49
1:C:27:TYR:CD1	1:D:81:GLU:OE2	2.65	0.49
1:D:147:LYS:HE2	1:D:165:THR:HA	1.94	0.49
1:E:127:ILE:HB	1:E:185:TYR:HB2	1.95	0.49
1:C:119:PRO:HB3	1:C:196:TYR:CD2	2.48	0.49
1:E:196:TYR:O	1:E:200:ILE:HB	2.13	0.49
1:A:240:LEU:HD22	1:B:239:ILE:HD11	1.94	0.49
1:A:283:GLN:H	1:A:284:PRO:HD3	1.78	0.49
1:B:179:LEU:HD12	1:B:179:LEU:C	2.38	0.49
1:C:119:PRO:O	1:C:193:TYR:HB3	2.13	0.49
1:C:147:LYS:O	1:C:147:LYS:CD	2.59	0.49
1:E:238:ASN:HA	1:E:258:ILE:HD13	1.93	0.49
1:B:42:LEU:HD23	1:B:103:GLU:OE1	2.13	0.49
1:B:47:LYS:HD2	1:B:49:ARG:HH21	1.77	0.49
1:C:53:PHE:CE2	1:C:63:LYS:HB3	2.47	0.49
1:E:76:ARG:HH22	1:E:130:ILE:CD1	2.18	0.49
1:E:217:SER:HB3	1:E:223:ASN:OD1	2.12	0.49
1:A:27:TYR:HB2	1:B:110:LEU:HD11	1.94	0.49
1:A:155:PHE:HE1	1:B:112:PRO:CA	2.26	0.49
1:B:212:TRP:CZ3	1:B:298:PHE:HB3	2.48	0.49
1:B:253:TYR:HA	1:B:313:PHE:CD2	2.48	0.49
1:D:217:SER:HB3	1:D:223:ASN:OD1	2.12	0.49
1:E:179:LEU:C	1:E:179:LEU:HD12	2.38	0.49
1:B:260:MET:CE	1:B:309:LEU:HD22	2.43	0.48
1:D:196:TYR:N	1:D:196:TYR:HD1	2.11	0.48
1:B:52:ALA:HA	1:B:95:PRO:O	2.14	0.48
1:B:70:ILE:N	1:B:70:ILE:HD13	2.27	0.48
1:C:207:ILE:HG13	1:C:208:LEU:N	2.28	0.48
1:C:217:SER:HB3	1:C:223:ASN:OD1	2.13	0.48
1:D:53:PHE:HE2	1:D:63:LYS:CB	2.26	0.48
1:D:196:TYR:N	1:D:196:TYR:CD1	2.80	0.48
1:B:48:ASP:C	1:B:50:ARG:N	2.68	0.48
1:B:95:PRO:C	1:B:97:GLY:H	2.21	0.48
1:B:119:PRO:HB3	1:B:196:TYR:HD2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:GLU:HG3	1:D:108:ARG:HG3	1.95	0.48
1:D:179:LEU:HD12	1:D:179:LEU:C	2.38	0.48
1:E:207:ILE:HG13	1:E:208:LEU:N	2.28	0.48
1:A:48:ASP:O	1:A:50:ARG:N	2.46	0.48
1:A:202:LEU:CD1	1:B:259:PHE:CZ	2.97	0.48
1:C:194:PHE:O	1:C:196:TYR:N	2.46	0.48
1:C:276:HIS:C	1:C:278:LEU:N	2.71	0.48
1:D:66:GLU:HG3	1:D:67:PRO:CD	2.40	0.48
1:E:226:LEU:HD22	1:E:226:LEU:HA	1.67	0.48
1:A:19:THR:HG22	1:A:44:LEU:CD2	2.44	0.48
1:A:137:ARG:HD3	1:A:137:ARG:HA	1.53	0.48
1:D:215:PHE:HB2	1:D:216:TRP:CE3	2.48	0.48
1:A:47:LYS:CD	1:A:49:ARG:HH21	2.27	0.48
1:A:123:GLN:HB2	1:A:189:ILE:HG13	1.96	0.48
1:C:133:SER:HB2	1:C:137:ARG:NH1	2.29	0.48
1:A:198:PRO:HA	1:B:259:PHE:CD1	2.49	0.48
1:B:238:ASN:HA	1:B:258:ILE:HD13	1.94	0.48
1:D:194:PHE:O	1:D:198:PRO:HD2	2.13	0.48
1:D:226:LEU:HD22	1:D:226:LEU:HA	1.63	0.48
1:D:296:ILE:HD13	1:D:296:ILE:HA	1.76	0.48
1:E:42:LEU:HD23	1:E:103:GLU:OE1	2.14	0.48
1:E:119:PRO:O	1:E:193:TYR:HB3	2.13	0.48
1:E:224:VAL:O	1:E:226:LEU:N	2.47	0.48
1:A:197:ILE:CG2	1:A:202:LEU:HG	2.44	0.48
1:A:215:PHE:HB2	1:A:216:TRP:CE3	2.49	0.48
1:A:264:PHE:CE2	1:A:302:PHE:HB2	2.49	0.48
1:B:215:PHE:HB2	1:B:216:TRP:CE3	2.48	0.48
1:E:70:ILE:HG22	1:E:71:TRP:O	2.13	0.48
1:B:37:LYS:HG2	1:B:108:ARG:HB3	1.96	0.48
1:A:70:ILE:HG22	1:A:71:TRP:O	2.14	0.48
1:A:147:LYS:C	1:A:149:GLY:N	2.68	0.48
1:B:200:ILE:O	1:B:204:MET:CB	2.62	0.48
1:B:276:HIS:C	1:B:278:LEU:N	2.71	0.48
1:C:70:ILE:HG22	1:C:71:TRP:N	2.29	0.48
1:C:197:ILE:HB	1:C:198:PRO:CD	2.37	0.48
1:C:260:MET:HE2	1:C:309:LEU:HD22	1.95	0.48
1:B:18:ASN:O	1:B:44:LEU:HA	2.13	0.47
1:B:79:ASN:HD22	1:B:79:ASN:N	2.01	0.47
1:D:261:ILE:HD13	1:D:302:PHE:HE1	1.79	0.47
1:E:261:ILE:HD13	1:E:302:PHE:HE1	1.79	0.47
1:B:261:ILE:HD13	1:B:302:PHE:HE1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:SER:HB2	1:C:37:LYS:HD2	1.97	0.47
1:C:274:VAL:C	1:C:276:HIS:N	2.66	0.47
1:A:119:PRO:HB3	1:A:196:TYR:HD2	1.79	0.47
1:A:224:VAL:O	1:A:226:LEU:N	2.47	0.47
1:A:226:LEU:HA	1:A:226:LEU:HD22	1.59	0.47
1:B:76:ARG:HH12	1:B:130:ILE:HD11	1.80	0.47
1:B:98:THR:HG22	1:B:98:THR:O	2.14	0.47
1:B:133:SER:HB2	1:B:137:ARG:NH1	2.29	0.47
1:B:278:LEU:HD21	1:B:286:ARG:HB3	1.96	0.47
1:C:268:ALA:HA	1:C:298:PHE:HE1	1.77	0.47
1:A:48:ASP:C	1:A:50:ARG:N	2.70	0.47
1:A:204:MET:HE2	1:A:204:MET:HB3	1.80	0.47
1:A:217:SER:HB3	1:A:223:ASN:OD1	2.14	0.47
1:A:225:THR:CG2	1:B:224:VAL:HG23	2.43	0.47
1:B:234:HIS:CE1	1:B:261:ILE:CG2	2.93	0.47
1:B:296:ILE:O	1:B:300:VAL:HG23	2.13	0.47
1:C:202:LEU:HD23	1:C:202:LEU:HA	1.56	0.47
1:D:62:VAL:HG13	1:D:93:VAL:O	2.14	0.47
1:D:68:GLU:CD	1:D:68:GLU:H	2.22	0.47
1:E:48:ASP:C	1:E:50:ARG:H	2.22	0.47
1:A:53:PHE:HE2	1:A:63:LYS:CB	2.26	0.47
1:A:53:PHE:O	1:A:54:ASP:C	2.58	0.47
1:A:221:GLU:OE2	1:B:221:GLU:OE2	2.33	0.47
1:A:276:HIS:C	1:A:278:LEU:N	2.71	0.47
1:B:22:TYR:HA	1:B:149:GLY:HA2	1.93	0.47
1:B:78:VAL:CG2	1:B:130:ILE:HG12	2.38	0.47
1:B:254:THR:HA	1:B:257:ILE:HG12	1.97	0.47
1:B:270:ILE:HD13	1:B:270:ILE:HA	1.67	0.47
1:C:53:PHE:HE2	1:C:63:LYS:CB	2.26	0.47
1:C:222:ALA:O	1:C:226:LEU:HB2	2.14	0.47
1:C:270:ILE:HD13	1:C:270:ILE:HA	1.64	0.47
1:E:48:ASP:C	1:E:50:ARG:N	2.71	0.47
1:B:9:PRO:HD3	1:B:71:TRP:CE3	2.49	0.47
1:B:207:ILE:HG13	1:B:208:LEU:N	2.29	0.47
1:C:23:LEU:HA	1:C:40:ALA:HB2	1.95	0.47
1:C:46:TRP:HH2	1:C:72:ILE:HG23	1.79	0.47
1:C:123:GLN:HB2	1:C:189:ILE:HG13	1.97	0.47
1:C:278:LEU:HD21	1:C:286:ARG:HB3	1.96	0.47
1:D:67:PRO:HG3	1:D:91:ILE:HD11	1.95	0.47
1:D:261:ILE:CD1	1:D:302:PHE:HE1	2.27	0.47
1:E:123:GLN:NE2	1:E:123:GLN:HA	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:264:PHE:HE2	1:E:302:PHE:HB2	1.79	0.47
1:A:13:GLU:HB3	1:A:14:PRO:CD	2.45	0.47
1:A:70:ILE:HG22	1:A:71:TRP:N	2.29	0.47
1:B:67:PRO:HG3	1:B:91:ILE:HD11	1.95	0.47
1:B:123:GLN:HB2	1:B:189:ILE:HG13	1.95	0.47
1:B:196:TYR:N	1:B:196:TYR:CD1	2.83	0.47
1:D:89:VAL:CG1	1:E:132:ARG:HD3	2.45	0.47
1:D:119:PRO:HB3	1:D:196:TYR:HD2	1.78	0.47
1:D:238:ASN:HA	1:D:258:ILE:HD13	1.95	0.47
1:E:53:PHE:O	1:E:54:ASP:C	2.58	0.47
1:E:76:ARG:NH2	1:E:130:ILE:CD1	2.62	0.47
1:E:278:LEU:HD21	1:E:286:ARG:HB3	1.97	0.47
1:A:254:THR:HA	1:A:257:ILE:HG12	1.97	0.47
1:A:278:LEU:HD21	1:A:286:ARG:HB3	1.96	0.47
1:B:53:PHE:CE2	1:B:63:LYS:HB3	2.46	0.47
1:C:95:PRO:C	1:C:97:GLY:H	2.23	0.47
1:D:53:PHE:O	1:D:54:ASP:C	2.58	0.47
1:D:70:ILE:HG22	1:D:71:TRP:N	2.30	0.47
1:E:9:PRO:HD3	1:E:71:TRP:CE3	2.50	0.47
1:E:253:TYR:O	1:E:256:ALA:HB3	2.15	0.47
1:B:18:ASN:HB2	1:B:45:SER:OG	2.15	0.47
1:B:53:PHE:O	1:B:54:ASP:C	2.58	0.47
1:B:202:LEU:HD23	1:B:202:LEU:HA	1.65	0.47
1:D:191:ARG:HG3	1:D:192:GLN:N	2.29	0.47
1:D:278:LEU:HD21	1:D:286:ARG:HB3	1.96	0.47
1:E:53:PHE:CE2	1:E:63:LYS:HB3	2.46	0.47
1:A:70:ILE:HD13	1:A:70:ILE:N	2.29	0.47
1:C:21:ILE:HA	1:C:41:PHE:O	2.15	0.47
1:E:48:ASP:O	1:E:50:ARG:N	2.48	0.47
1:E:81:GLU:HG3	1:E:108:ARG:HG3	1.97	0.47
1:A:76:ARG:CZ	1:A:130:ILE:HD12	2.44	0.46
1:A:194:PHE:O	1:A:198:PRO:HD2	2.14	0.46
1:B:194:PHE:O	1:B:196:TYR:N	2.49	0.46
1:E:196:TYR:N	1:E:196:TYR:CD1	2.84	0.46
1:E:261:ILE:CD1	1:E:302:PHE:HE1	2.27	0.46
1:A:143:VAL:O	1:A:143:VAL:HG12	2.15	0.46
1:A:196:TYR:N	1:A:196:TYR:CD1	2.82	0.46
1:B:274:VAL:C	1:B:276:HIS:N	2.66	0.46
1:E:194:PHE:O	1:E:196:TYR:N	2.49	0.46
1:A:78:VAL:CG2	1:A:130:ILE:HG12	2.42	0.46
1:A:268:ALA:HA	1:A:298:PHE:HE1	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:TYR:O	1:A:281:GLU:HG3	2.16	0.46
1:C:261:ILE:HD13	1:C:302:PHE:HE1	1.80	0.46
1:E:95:PRO:C	1:E:97:GLY:H	2.23	0.46
1:E:137:ARG:HD3	1:E:137:ARG:HA	1.58	0.46
1:E:215:PHE:HB2	1:E:216:TRP:CE3	2.50	0.46
1:A:41:PHE:CZ	1:B:76:ARG:NH2	2.82	0.46
1:A:202:LEU:HD23	1:A:202:LEU:HA	1.62	0.46
1:A:249:PRO:HD2	1:A:250:TYR:CE1	2.50	0.46
1:C:13:GLU:HB3	1:C:14:PRO:CD	2.46	0.46
1:C:53:PHE:O	1:C:54:ASP:C	2.58	0.46
1:C:197:ILE:CB	1:C:198:PRO:HD3	2.36	0.46
1:C:249:PRO:HD2	1:C:250:TYR:CE1	2.51	0.46
1:C:252:THR:HB	1:C:255:GLY:H	1.79	0.46
1:D:76:ARG:HH12	1:D:130:ILE:HD11	1.79	0.46
1:D:207:ILE:HG13	1:D:208:LEU:N	2.31	0.46
1:D:260:MET:CE	1:D:309:LEU:HD22	2.45	0.46
1:D:277:TYR:O	1:D:281:GLU:HG3	2.16	0.46
1:E:256:ALA:HB1	1:E:309:LEU:HD21	1.96	0.46
1:A:196:TYR:N	1:A:196:TYR:HD1	2.14	0.46
1:A:202:LEU:HD12	1:B:259:PHE:HZ	1.78	0.46
1:B:268:ALA:HA	1:B:298:PHE:HE1	1.80	0.46
1:B:277:TYR:O	1:B:281:GLU:HG3	2.16	0.46
1:C:48:ASP:C	1:C:50:ARG:N	2.72	0.46
1:C:104:ARG:NH2	1:D:77:PHE:O	2.40	0.46
1:C:277:TYR:O	1:C:281:GLU:HG3	2.16	0.46
1:D:267:VAL:HG23	1:D:298:PHE:CZ	2.50	0.46
1:E:67:PRO:HG3	1:E:91:ILE:HD11	1.97	0.46
1:A:98:THR:O	1:A:98:THR:HG22	2.14	0.46
1:B:9:PRO:HB3	1:B:48:ASP:OD1	2.15	0.46
1:A:123:GLN:HA	1:A:123:GLN:NE2	2.31	0.46
1:C:48:ASP:O	1:C:50:ARG:N	2.48	0.46
1:D:119:PRO:HD3	1:D:254:THR:OG1	2.15	0.46
1:E:78:VAL:CG2	1:E:130:ILE:HG12	2.42	0.46
1:C:191:ARG:HG3	1:C:192:GLN:N	2.31	0.46
1:C:306:ASN:O	1:C:310:ALA:N	2.44	0.46
1:D:70:ILE:HG22	1:D:71:TRP:O	2.16	0.46
1:E:47:LYS:HD2	1:E:49:ARG:HH21	1.81	0.46
1:E:123:GLN:HB2	1:E:189:ILE:HG13	1.97	0.46
1:E:260:MET:CE	1:E:309:LEU:HD22	2.46	0.46
1:A:48:ASP:C	1:A:50:ARG:H	2.22	0.46
1:A:78:VAL:HB	1:A:128:TYR:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ARG:HA	1:B:137:ARG:HD3	1.59	0.46
1:B:196:TYR:N	1:B:196:TYR:HD1	2.13	0.46
1:C:254:THR:HA	1:C:257:ILE:HG12	1.98	0.46
1:D:84:ARG:NH1	1:D:84:ARG:CB	2.76	0.46
1:D:222:ALA:HA	1:D:225:THR:HB	1.97	0.46
1:E:202:LEU:HB2	1:E:203:PRO:HD3	1.97	0.46
1:D:13:GLU:HB3	1:D:14:PRO:CD	2.44	0.46
1:E:119:PRO:HB3	1:E:196:TYR:CD2	2.51	0.46
1:B:245:LEU:HD12	1:B:245:LEU:HA	1.83	0.45
1:C:48:ASP:C	1:C:50:ARG:H	2.24	0.45
1:C:70:ILE:HD13	1:C:70:ILE:N	2.31	0.45
1:D:30:ASP:HB3	1:D:33:ALA:HB3	1.98	0.45
1:D:77:PHE:CE2	1:D:127:ILE:CG2	2.99	0.45
1:A:155:PHE:HE1	1:B:112:PRO:CB	2.23	0.45
1:A:207:ILE:HG13	1:A:208:LEU:N	2.30	0.45
1:D:268:ALA:HA	1:D:298:PHE:HE1	1.80	0.45
1:D:275:GLN:HG3	1:D:291:THR:OG1	2.16	0.45
1:A:19:THR:HG22	1:A:44:LEU:HD23	1.99	0.45
1:A:88:VAL:HG12	1:A:89:VAL:N	2.31	0.45
1:A:202:LEU:CD1	1:B:259:PHE:HZ	2.30	0.45
1:A:243:THR:HG22	1:A:244:ASN:N	2.32	0.45
1:C:52:ALA:HA	1:C:95:PRO:O	2.16	0.45
1:C:196:TYR:O	1:C:200:ILE:HB	2.17	0.45
1:C:261:ILE:CD1	1:C:302:PHE:HE1	2.30	0.45
1:A:175:LEU:HA	1:A:175:LEU:HD12	1.67	0.45
1:B:28:SER:HB2	1:B:37:LYS:HD2	1.99	0.45
1:C:197:ILE:CG2	1:C:202:LEU:HG	2.47	0.45
1:E:77:PHE:CE2	1:E:127:ILE:CG2	3.00	0.45
1:E:252:THR:HB	1:E:255:GLY:H	1.82	0.45
1:E:261:ILE:O	1:E:262:TYR:C	2.59	0.45
1:E:270:ILE:HD13	1:E:270:ILE:HA	1.65	0.45
1:A:21:ILE:HA	1:A:41:PHE:O	2.17	0.45
1:A:28:SER:HB2	1:A:37:LYS:HD2	1.99	0.45
1:A:67:PRO:HG3	1:A:91:ILE:HD11	1.98	0.45
1:C:260:MET:CE	1:C:309:LEU:HD22	2.47	0.45
1:E:27:TYR:CE1	1:E:37:LYS:HB2	2.52	0.45
1:E:66:GLU:HG3	1:E:67:PRO:CD	2.41	0.45
1:E:76:ARG:CZ	1:E:130:ILE:HD12	2.45	0.45
1:E:243:THR:HG22	1:E:244:ASN:N	2.31	0.45
1:A:30:ASP:HB3	1:A:33:ALA:HB3	1.99	0.45
1:A:223:ASN:HD22	1:A:272:VAL:HG12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ILE:HB	1:B:185:TYR:HB2	1.99	0.45
1:B:256:ALA:HB1	1:B:309:LEU:HD21	1.97	0.45
1:C:47:LYS:HD2	1:C:49:ARG:HH21	1.82	0.45
1:C:212:TRP:CZ3	1:C:298:PHE:HB3	2.51	0.45
1:A:27:TYR:CB	1:B:110:LEU:CD1	2.90	0.45
1:A:53:PHE:CE2	1:A:63:LYS:HB3	2.47	0.45
1:A:240:LEU:HD22	1:B:239:ILE:CD1	2.47	0.45
1:E:52:ALA:HA	1:E:95:PRO:O	2.17	0.45
1:E:277:TYR:O	1:E:281:GLU:HG3	2.16	0.45
1:A:27:TYR:CE1	1:B:81:GLU:CD	2.95	0.45
1:A:191:ARG:HG3	1:A:192:GLN:N	2.31	0.45
1:E:298:PHE:CB	1:E:299:PRO:HD3	2.46	0.45
1:A:27:TYR:CD1	1:B:81:GLU:OE2	2.70	0.45
1:A:275:GLN:HG3	1:A:291:THR:OG1	2.17	0.45
1:C:119:PRO:HB3	1:C:196:TYR:HD2	1.82	0.45
1:D:229:SER:HB3	1:E:228:VAL:HG11	1.98	0.45
1:E:197:ILE:CG2	1:E:202:LEU:HG	2.47	0.45
1:A:89:VAL:CG1	1:B:132:ARG:HD3	2.47	0.44
1:B:78:VAL:HB	1:B:128:TYR:HB2	1.99	0.44
1:C:44:LEU:HD12	1:C:101:TYR:CE2	2.51	0.44
1:C:215:PHE:HB2	1:C:216:TRP:CZ3	2.52	0.44
1:C:216:TRP:HE3	1:C:216:TRP:H	1.65	0.44
1:D:104:ARG:HH22	1:E:78:VAL:CA	2.15	0.44
1:D:198:PRO:O	1:E:259:PHE:HD1	2.00	0.44
1:E:243:THR:HG22	1:E:244:ASN:HD22	1.82	0.44
1:A:194:PHE:CE2	1:B:250:TYR:O	2.63	0.44
1:C:70:ILE:HG22	1:C:71:TRP:O	2.17	0.44
1:C:79:ASN:OD1	1:C:109:VAL:HG12	2.18	0.44
1:D:53:PHE:CE2	1:D:63:LYS:HB3	2.49	0.44
1:D:254:THR:HA	1:D:257:ILE:HG12	1.99	0.44
1:E:18:ASN:O	1:E:44:LEU:HA	2.17	0.44
1:A:261:ILE:CD1	1:A:302:PHE:HE1	2.30	0.44
1:B:204:MET:HB3	1:B:204:MET:HE2	1.86	0.44
1:C:213:THR:HG22	1:C:226:LEU:CD1	2.48	0.44
1:D:22:TYR:HA	1:D:149:GLY:HA2	1.94	0.44
1:E:118:TYR:CD1	1:E:245:LEU:HD21	2.53	0.44
1:E:133:SER:HB3	1:E:137:ARG:HA	1.98	0.44
1:E:204:MET:HE2	1:E:204:MET:HB3	1.77	0.44
1:B:53:PHE:HE2	1:B:63:LYS:CB	2.27	0.44
1:E:21:ILE:HA	1:E:41:PHE:O	2.16	0.44
1:E:53:PHE:HE2	1:E:63:LYS:CB	2.29	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:VAL:HG11	1:A:126:HIS:O	2.17	0.44
1:A:127:ILE:HB	1:A:185:TYR:HB2	1.99	0.44
1:A:212:TRP:CZ3	1:A:298:PHE:HB3	2.52	0.44
1:A:217:SER:CB	1:B:220:TYR:CE2	3.00	0.44
1:B:125:LEU:HB2	1:B:187:LEU:HB3	2.00	0.44
1:B:309:LEU:O	1:B:310:ALA:C	2.61	0.44
1:C:9:PRO:HD3	1:C:71:TRP:CE3	2.52	0.44
1:C:76:ARG:CZ	1:C:130:ILE:HD12	2.46	0.44
1:C:196:TYR:N	1:C:196:TYR:CD1	2.86	0.44
1:E:197:ILE:CB	1:E:198:PRO:HD3	2.40	0.44
1:A:23:LEU:HA	1:A:40:ALA:CB	2.48	0.44
1:B:261:ILE:CD1	1:B:302:PHE:HE1	2.31	0.44
1:B:314:PHE:N	1:B:314:PHE:CD1	2.85	0.44
1:C:27:TYR:CE1	1:D:81:GLU:OE1	2.71	0.44
1:C:203:PRO:HB3	1:D:262:TYR:CZ	2.53	0.44
1:D:204:MET:HE2	1:D:204:MET:HB3	1.85	0.44
1:D:212:TRP:CZ3	1:D:298:PHE:HB3	2.52	0.44
1:A:270:ILE:HG22	1:A:271:GLU:N	2.31	0.44
1:C:240:LEU:HD22	1:D:239:ILE:CG1	2.48	0.44
1:C:274:VAL:O	1:C:278:LEU:HB3	2.18	0.44
1:D:210:ILE:CG2	1:E:269:VAL:HG11	2.37	0.44
1:E:9:PRO:HB3	1:E:48:ASP:OD1	2.18	0.44
1:E:274:VAL:O	1:E:278:LEU:HB3	2.18	0.44
1:A:290:ILE:HG22	1:A:291:THR:N	2.31	0.44
1:B:77:PHE:CE2	1:B:127:ILE:CG2	3.00	0.44
1:C:264:PHE:HE2	1:C:302:PHE:HB2	1.83	0.44
1:D:296:ILE:O	1:D:300:VAL:HG23	2.17	0.44
1:A:46:TRP:HH2	1:A:72:ILE:HG23	1.82	0.44
1:A:296:ILE:HD13	1:A:296:ILE:HA	1.78	0.44
1:B:150:LYS:HG3	1:B:154:VAL:HG21	2.00	0.44
1:B:274:VAL:O	1:B:278:LEU:HB3	2.18	0.44
1:D:150:LYS:HG3	1:D:154:VAL:HG21	2.00	0.44
1:E:13:GLU:HB3	1:E:14:PRO:CD	2.47	0.44
1:E:275:GLN:HG3	1:E:291:THR:OG1	2.18	0.44
1:E:309:LEU:O	1:E:310:ALA:C	2.61	0.44
1:A:52:ALA:HA	1:A:95:PRO:O	2.18	0.43
1:A:119:PRO:HD3	1:A:254:THR:OG1	2.18	0.43
1:A:133:SER:HB2	1:A:137:ARG:NH1	2.33	0.43
1:B:109:VAL:HG11	1:B:126:HIS:O	2.17	0.43
1:C:77:PHE:CE2	1:C:127:ILE:CG2	3.01	0.43
1:C:132:ARG:CA	1:C:180:GLU:HG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:ILE:O	1:C:204:MET:CB	2.64	0.43
1:D:9:PRO:HB3	1:D:48:ASP:OD1	2.18	0.43
1:D:49:ARG:HB3	1:D:49:ARG:NH1	2.33	0.43
1:E:150:LYS:HG3	1:E:154:VAL:HG21	2.00	0.43
1:E:194:PHE:O	1:E:198:PRO:HD2	2.17	0.43
1:E:200:ILE:O	1:E:204:MET:CB	2.66	0.43
1:E:216:TRP:HE3	1:E:216:TRP:H	1.66	0.43
1:A:150:LYS:HG3	1:A:154:VAL:HG21	2.00	0.43
1:A:197:ILE:CB	1:A:198:PRO:HD3	2.39	0.43
1:B:66:GLU:HG3	1:B:67:PRO:CD	2.41	0.43
1:B:76:ARG:NH1	1:B:130:ILE:HD11	2.33	0.43
1:B:271:GLU:O	1:B:272:VAL:C	2.60	0.43
1:C:150:LYS:HG3	1:C:154:VAL:HG21	2.00	0.43
1:C:195:SER:O	1:C:199:ASN:HB2	2.19	0.43
1:D:53:PHE:CE1	1:D:95:PRO:CA	3.01	0.43
1:D:76:ARG:NH1	1:D:130:ILE:HD11	2.33	0.43
1:E:53:PHE:CD1	1:E:53:PHE:C	2.97	0.43
1:A:81:GLU:HG3	1:A:108:ARG:HG3	2.00	0.43
1:A:155:PHE:CZ	1:B:112:PRO:CB	2.95	0.43
1:D:157:THR:HG21	1:E:34:GLU:OE1	2.18	0.43
1:B:132:ARG:NH2	1:B:178:ARG:HB2	2.33	0.43
1:C:23:LEU:HB2	1:C:150:LYS:HA	2.00	0.43
1:C:76:ARG:HH12	1:C:130:ILE:HD11	1.84	0.43
1:E:72:ILE:HA	1:E:73:PRO:HD3	1.87	0.43
1:E:196:TYR:N	1:E:196:TYR:HD1	2.16	0.43
1:E:223:ASN:HD22	1:E:272:VAL:HG12	1.83	0.43
1:A:27:TYR:CD2	1:B:110:LEU:HD13	2.54	0.43
1:A:200:ILE:CD1	1:A:240:LEU:HD23	2.45	0.43
1:A:233:ALA:HB2	1:B:232:ILE:HG12	2.01	0.43
1:B:224:VAL:O	1:B:228:VAL:HB	2.19	0.43
1:B:275:GLN:HG3	1:B:291:THR:OG1	2.18	0.43
1:C:81:GLU:HG3	1:C:108:ARG:HG3	1.99	0.43
1:C:275:GLN:HG3	1:C:291:THR:OG1	2.17	0.43
1:E:46:TRP:HH2	1:E:72:ILE:HG23	1.83	0.43
1:E:212:TRP:HB2	1:E:215:PHE:CE1	2.53	0.43
1:A:125:LEU:HB2	1:A:187:LEU:HB3	2.00	0.43
1:A:225:THR:HG22	1:A:225:THR:O	2.18	0.43
1:B:76:ARG:CZ	1:B:130:ILE:HD12	2.40	0.43
1:B:232:ILE:O	1:B:235:ILE:HB	2.19	0.43
1:C:119:PRO:HD3	1:C:254:THR:OG1	2.19	0.43
1:D:194:PHE:O	1:D:196:TYR:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:ILE:HD13	1:D:201:ILE:HA	1.86	0.43
1:D:298:PHE:CB	1:D:299:PRO:HD3	2.48	0.43
1:E:283:GLN:H	1:E:284:PRO:HD3	1.82	0.43
1:A:95:PRO:C	1:A:97:GLY:H	2.27	0.43
1:A:274:VAL:O	1:A:278:LEU:HB3	2.18	0.43
1:B:212:TRP:HB2	1:B:215:PHE:CE1	2.53	0.43
1:B:283:GLN:C	1:B:285:ALA:N	2.76	0.43
1:C:88:VAL:HG12	1:C:89:VAL:N	2.34	0.43
1:C:194:PHE:O	1:C:198:PRO:HD2	2.19	0.43
1:E:225:THR:HG22	1:E:225:THR:O	2.18	0.43
1:A:44:LEU:HD12	1:A:101:TYR:CE2	2.54	0.43
1:A:192:GLN:OE1	1:B:249:PRO:HB3	2.19	0.43
1:A:194:PHE:O	1:A:196:TYR:N	2.51	0.43
1:A:261:ILE:HD13	1:A:302:PHE:HE1	1.83	0.43
1:A:298:PHE:CB	1:A:299:PRO:HD3	2.49	0.43
1:C:53:PHE:CD1	1:C:53:PHE:C	2.97	0.43
1:C:226:LEU:HA	1:C:226:LEU:HD22	1.64	0.43
1:C:283:GLN:H	1:C:284:PRO:HD3	1.80	0.43
1:D:28:SER:HB2	1:D:37:LYS:HD2	2.01	0.43
1:D:274:VAL:O	1:D:278:LEU:HB3	2.18	0.43
1:D:276:HIS:C	1:D:278:LEU:N	2.71	0.43
1:D:296:ILE:HG22	1:D:297:ALA:N	2.33	0.43
1:A:48:ASP:HB3	1:A:51:LEU:CD2	2.49	0.43
1:A:314:PHE:CD1	1:A:314:PHE:N	2.87	0.43
1:C:72:ILE:HG22	1:C:73:PRO:HD2	2.00	0.43
1:D:127:ILE:HB	1:D:185:TYR:HB2	2.01	0.43
1:D:155:PHE:CZ	1:E:112:PRO:HB3	2.50	0.43
1:E:76:ARG:HH12	1:E:130:ILE:HD11	1.84	0.43
1:A:53:PHE:CD1	1:A:53:PHE:C	2.97	0.43
1:B:215:PHE:HB2	1:B:216:TRP:CZ3	2.54	0.43
1:C:118:TYR:CD1	1:C:245:LEU:HD21	2.53	0.43
1:C:127:ILE:HB	1:C:185:TYR:HB2	2.01	0.43
1:C:193:TYR:CD2	1:C:193:TYR:C	2.96	0.43
1:C:194:PHE:CE2	1:D:250:TYR:O	2.70	0.43
1:C:243:THR:HG22	1:C:244:ASN:HD22	1.84	0.43
1:D:27:TYR:CE1	1:D:37:LYS:HB2	2.54	0.43
1:E:179:LEU:HD12	1:E:179:LEU:O	2.19	0.43
1:E:270:ILE:HG22	1:E:271:GLU:N	2.34	0.43
1:A:192:GLN:CG	1:B:249:PRO:HB3	2.49	0.42
1:A:202:LEU:HB2	1:A:203:PRO:HD3	2.01	0.42
1:B:23:LEU:HA	1:B:40:ALA:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:PRO:HD3	1:B:254:THR:OG1	2.19	0.42
1:C:66:GLU:HG3	1:C:67:PRO:CD	2.45	0.42
1:C:243:THR:HG22	1:C:244:ASN:N	2.34	0.42
1:E:193:TYR:CD2	1:E:193:TYR:C	2.97	0.42
1:A:193:TYR:CD2	1:A:193:TYR:C	2.98	0.42
1:A:238:ASN:HA	1:A:258:ILE:HD13	1.97	0.42
1:A:247:LYS:HA	1:A:247:LYS:HD3	1.80	0.42
1:B:27:TYR:CE1	1:B:37:LYS:HB2	2.54	0.42
1:B:30:ASP:HB3	1:B:33:ALA:HB3	2.01	0.42
1:B:225:THR:O	1:B:225:THR:HG22	2.18	0.42
1:C:68:GLU:H	1:C:68:GLU:CD	2.26	0.42
1:C:261:ILE:O	1:C:262:TYR:C	2.62	0.42
1:E:22:TYR:HA	1:E:149:GLY:HA2	1.95	0.42
1:E:119:PRO:HD3	1:E:254:THR:OG1	2.19	0.42
1:A:76:ARG:HH12	1:A:130:ILE:HD11	1.84	0.42
1:A:179:LEU:HD12	1:A:179:LEU:O	2.19	0.42
1:A:259:PHE:CD2	1:A:259:PHE:C	2.96	0.42
1:C:67:PRO:HG3	1:C:91:ILE:HD11	2.00	0.42
1:C:212:TRP:HB2	1:C:215:PHE:CE1	2.54	0.42
1:C:298:PHE:CB	1:C:299:PRO:HD3	2.48	0.42
1:E:133:SER:HB2	1:E:137:ARG:HH11	1.82	0.42
1:E:291:THR:O	1:E:295:ARG:HG3	2.19	0.42
1:A:155:PHE:HE1	1:B:112:PRO:HB3	1.63	0.42
1:A:212:TRP:HB2	1:A:215:PHE:CE1	2.54	0.42
1:B:232:ILE:HA	1:B:235:ILE:HD12	2.01	0.42
1:B:243:THR:HG22	1:B:244:ASN:HD22	1.84	0.42
1:C:133:SER:HB3	1:C:137:ARG:HA	2.01	0.42
1:C:210:ILE:HG21	1:D:228:VAL:HG22	2.00	0.42
1:C:225:THR:O	1:C:225:THR:HG22	2.18	0.42
1:D:286:ARG:O	1:D:289:SER:N	2.45	0.42
1:E:143:VAL:O	1:E:143:VAL:HG12	2.20	0.42
1:E:191:ARG:HG3	1:E:192:GLN:N	2.34	0.42
1:E:276:HIS:C	1:E:278:LEU:N	2.71	0.42
1:A:159:TRP:CE3	1:A:189:ILE:HD12	2.55	0.42
1:B:202:LEU:HB2	1:B:203:PRO:HD3	2.01	0.42
1:C:183:LEU:HD23	1:C:183:LEU:HA	1.88	0.42
1:E:28:SER:HB2	1:E:37:LYS:HD2	2.02	0.42
1:E:53:PHE:CD1	1:E:53:PHE:O	2.72	0.42
1:E:197:ILE:HB	1:E:198:PRO:CD	2.40	0.42
1:E:267:VAL:HG23	1:E:298:PHE:CZ	2.54	0.42
1:A:53:PHE:CD1	1:A:53:PHE:O	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:LEU:HD22	1:B:226:LEU:HA	1.74	0.42
1:D:225:THR:HG22	1:D:225:THR:O	2.19	0.42
1:E:243:THR:CG2	1:E:244:ASN:N	2.81	0.42
1:A:240:LEU:HD13	1:B:239:ILE:HG13	2.00	0.42
1:C:53:PHE:CD1	1:C:53:PHE:O	2.72	0.42
1:C:156:LEU:HD12	1:C:156:LEU:HA	1.73	0.42
1:D:53:PHE:CD1	1:D:53:PHE:C	2.97	0.42
1:D:78:VAL:HB	1:D:128:TYR:CB	2.48	0.42
1:D:212:TRP:HB2	1:D:215:PHE:CE1	2.55	0.42
1:B:7:PRO:O	1:B:50:ARG:NH1	2.50	0.42
1:B:13:GLU:OE1	1:B:14:PRO:HD3	2.20	0.42
1:B:21:ILE:HA	1:B:41:PHE:O	2.20	0.42
1:B:197:ILE:CB	1:B:198:PRO:HD3	2.44	0.42
1:C:30:ASP:HB3	1:C:33:ALA:HB3	2.01	0.42
1:C:201:ILE:HD13	1:C:201:ILE:HA	1.91	0.42
1:D:53:PHE:CD1	1:D:53:PHE:O	2.72	0.42
1:D:143:VAL:O	1:D:143:VAL:HG12	2.19	0.42
1:D:243:THR:HG22	1:D:244:ASN:N	2.35	0.42
1:E:254:THR:HA	1:E:257:ILE:HG12	2.01	0.42
1:A:23:LEU:HB2	1:A:150:LYS:HA	2.01	0.42
1:B:53:PHE:CD1	1:B:53:PHE:O	2.72	0.42
1:B:68:GLU:CD	1:B:68:GLU:H	2.28	0.42
1:B:179:LEU:HD12	1:B:179:LEU:O	2.19	0.42
1:D:21:ILE:HA	1:D:41:PHE:O	2.20	0.42
1:A:27:TYR:CE1	1:A:37:LYS:HB2	2.55	0.42
1:A:42:LEU:HB3	1:A:103:GLU:HG3	2.02	0.42
1:A:213:THR:HG22	1:A:226:LEU:CD1	2.49	0.42
1:B:270:ILE:HG22	1:B:271:GLU:N	2.35	0.42
1:C:132:ARG:HH22	1:C:176:GLU:HB2	1.85	0.42
1:C:133:SER:HB2	1:C:137:ARG:HH11	1.85	0.42
1:C:271:GLU:O	1:C:272:VAL:C	2.62	0.42
1:C:314:PHE:CD1	1:C:314:PHE:N	2.87	0.42
1:D:72:ILE:HA	1:D:73:PRO:HD3	1.91	0.42
1:D:77:PHE:HE2	1:D:127:ILE:CG2	2.33	0.42
1:D:179:LEU:HD12	1:D:179:LEU:O	2.19	0.42
1:D:202:LEU:HB2	1:D:203:PRO:HD3	2.02	0.42
1:A:202:LEU:O	1:A:203:PRO:C	2.60	0.41
1:A:233:ALA:HB1	1:B:235:ILE:HD13	2.02	0.41
1:D:76:ARG:CZ	1:D:130:ILE:HD12	2.43	0.41
1:D:95:PRO:O	1:D:97:GLY:N	2.53	0.41
1:D:159:TRP:CE3	1:D:189:ILE:HD12	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:ASP:HB3	1:E:33:ALA:HB3	2.02	0.41
1:E:283:GLN:C	1:E:285:ALA:N	2.76	0.41
1:A:47:LYS:HD3	1:A:49:ARG:HH21	1.85	0.41
1:A:68:GLU:CD	1:A:68:GLU:H	2.26	0.41
1:B:46:TRP:HH2	1:B:72:ILE:HG23	1.86	0.41
1:B:49:ARG:HB3	1:B:49:ARG:NH1	2.35	0.41
1:B:53:PHE:CD1	1:B:53:PHE:C	2.97	0.41
1:D:232:ILE:HA	1:D:235:ILE:HD12	2.01	0.41
1:E:222:ALA:HA	1:E:225:THR:HB	2.02	0.41
1:B:34:GLU:OE2	1:B:113:LEU:N	2.49	0.41
1:B:78:VAL:HB	1:B:128:TYR:CB	2.51	0.41
1:B:243:THR:HG22	1:B:244:ASN:N	2.35	0.41
1:C:27:TYR:CD1	1:D:81:GLU:CD	2.98	0.41
1:C:179:LEU:HD12	1:C:179:LEU:O	2.19	0.41
1:C:232:ILE:HA	1:C:235:ILE:HD12	2.02	0.41
1:D:77:PHE:HE2	1:D:127:ILE:HG23	1.85	0.41
1:D:223:ASN:HD22	1:D:272:VAL:HG12	1.85	0.41
1:E:42:LEU:HB3	1:E:103:GLU:HG3	2.01	0.41
1:A:166:ALA:HB2	1:A:185:TYR:CD2	2.55	0.41
1:A:201:ILE:HD13	1:A:201:ILE:HA	1.88	0.41
1:A:232:ILE:CG2	1:A:233:ALA:N	2.81	0.41
1:B:222:ALA:HA	1:B:225:THR:HB	2.02	0.41
1:B:298:PHE:CB	1:B:299:PRO:HD3	2.50	0.41
1:C:270:ILE:HG22	1:C:271:GLU:N	2.35	0.41
1:D:232:ILE:O	1:D:235:ILE:HB	2.21	0.41
1:D:264:PHE:HE2	1:D:302:PHE:HB2	1.84	0.41
1:E:300:VAL:O	1:E:304:LEU:HB2	2.20	0.41
1:A:41:PHE:CE2	1:B:175:LEU:HD23	2.46	0.41
1:A:79:ASN:H	1:A:79:ASN:ND2	2.10	0.41
1:A:88:VAL:CG1	1:A:89:VAL:N	2.83	0.41
1:A:232:ILE:HA	1:A:235:ILE:HD12	2.02	0.41
1:B:175:LEU:HD12	1:B:175:LEU:HA	1.67	0.41
1:C:194:PHE:O	1:C:197:ILE:N	2.43	0.41
1:D:41:PHE:CE2	1:E:175:LEU:HD23	2.36	0.41
1:E:296:ILE:HG22	1:E:297:ALA:N	2.35	0.41
1:A:77:PHE:CE2	1:A:127:ILE:CG2	3.03	0.41
1:A:78:VAL:HB	1:A:128:TYR:CB	2.51	0.41
1:B:202:LEU:O	1:B:203:PRO:C	2.64	0.41
1:C:224:VAL:O	1:C:226:LEU:N	2.53	0.41
1:D:109:VAL:HG11	1:D:126:HIS:O	2.20	0.41
1:D:215:PHE:HB2	1:D:216:TRP:CZ3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:THR:HB	1:D:255:GLY:H	1.85	0.41
1:E:314:PHE:N	1:E:314:PHE:CD1	2.89	0.41
1:A:133:SER:HB3	1:A:137:ARG:HA	2.01	0.41
1:B:72:ILE:HA	1:B:73:PRO:HD3	1.85	0.41
1:B:183:LEU:HD23	1:B:183:LEU:HA	1.83	0.41
1:B:194:PHE:O	1:B:198:PRO:HD2	2.21	0.41
1:B:224:VAL:O	1:B:226:LEU:N	2.53	0.41
1:D:132:ARG:NH2	1:D:178:ARG:HB2	2.35	0.41
1:E:119:PRO:HB3	1:E:196:TYR:HD2	1.84	0.41
1:E:296:ILE:HD13	1:E:296:ILE:HA	1.83	0.41
1:A:216:TRP:HE3	1:A:216:TRP:H	1.68	0.41
1:A:240:LEU:HD22	1:B:239:ILE:HG13	2.02	0.41
1:E:213:THR:C	1:E:215:PHE:H	2.28	0.41
1:E:221:GLU:O	1:E:221:GLU:OE1	2.39	0.41
1:A:9:PRO:HB3	1:A:48:ASP:OD1	2.20	0.41
1:A:140:VAL:HG22	1:A:181:SER:CB	2.51	0.41
1:A:157:THR:HG21	1:B:34:GLU:CG	2.49	0.41
1:A:200:ILE:O	1:A:204:MET:CB	2.68	0.41
1:A:226:LEU:HD22	1:B:228:VAL:HG21	2.01	0.41
1:A:286:ARG:O	1:A:287:ALA:C	2.64	0.41
1:B:25:GLU:HB2	1:B:39:ASN:HB3	2.03	0.41
1:B:278:LEU:HD23	1:B:287:ALA:CA	2.51	0.41
1:B:314:PHE:N	1:B:314:PHE:HD1	2.19	0.41
1:C:10:ILE:H	1:C:10:ILE:HG13	1.70	0.41
1:C:72:ILE:HA	1:C:73:PRO:HD3	1.85	0.41
1:C:137:ARG:HA	1:C:137:ARG:HD3	1.54	0.41
1:C:159:TRP:CE3	1:C:189:ILE:HD12	2.56	0.41
1:C:222:ALA:HA	1:C:225:THR:HB	2.02	0.41
1:D:132:ARG:CA	1:D:180:GLU:HG2	2.48	0.41
1:D:278:LEU:HD23	1:D:287:ALA:CA	2.51	0.41
1:D:303:LEU:HD23	1:D:303:LEU:C	2.45	0.41
1:E:72:ILE:HG22	1:E:73:PRO:HD2	2.03	0.41
1:E:79:ASN:H	1:E:79:ASN:ND2	2.08	0.41
1:A:48:ASP:HB3	1:A:51:LEU:HD21	2.02	0.41
1:A:76:ARG:NH1	1:A:130:ILE:HD11	2.35	0.41
1:A:147:LYS:CE	1:A:165:THR:HA	2.51	0.41
1:B:44:LEU:HD12	1:B:101:TYR:CE2	2.56	0.41
1:B:48:ASP:HB3	1:B:51:LEU:HD21	2.03	0.41
1:B:261:ILE:O	1:B:262:TYR:C	2.63	0.41
1:D:229:SER:CB	1:E:228:VAL:HG11	2.51	0.41
1:A:132:ARG:NH2	1:A:178:ARG:HB2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:VAL:O	1:B:301:VAL:HG12	2.21	0.40
1:C:78:VAL:HB	1:C:128:TYR:HB2	2.03	0.40
1:C:130:ILE:CG2	1:C:182:LYS:HB2	2.51	0.40
1:D:41:PHE:HD1	1:D:41:PHE:HA	1.80	0.40
1:D:47:LYS:HD2	1:D:49:ARG:HH21	1.84	0.40
1:D:125:LEU:HB2	1:D:187:LEU:HB3	2.03	0.40
1:A:72:ILE:HG22	1:A:73:PRO:HD2	2.03	0.40
1:B:269:VAL:O	1:B:273:THR:HB	2.21	0.40
1:C:18:ASN:HB2	1:C:45:SER:OG	2.21	0.40
1:C:27:TYR:CE1	1:C:37:LYS:HB2	2.56	0.40
1:C:76:ARG:NH1	1:C:130:ILE:HD11	2.36	0.40
1:D:9:PRO:HD3	1:D:71:TRP:CE3	2.57	0.40
1:D:166:ALA:HB2	1:D:185:TYR:CD2	2.56	0.40
1:D:283:GLN:C	1:D:285:ALA:N	2.78	0.40
1:D:314:PHE:CD1	1:D:314:PHE:N	2.89	0.40
1:E:76:ARG:NH1	1:E:130:ILE:HD11	2.36	0.40
1:E:202:LEU:HA	1:E:202:LEU:HD23	1.59	0.40
1:E:209:PHE:O	1:E:210:ILE:C	2.64	0.40
1:E:215:PHE:HB2	1:E:216:TRP:CZ3	2.56	0.40
1:E:247:LYS:HD3	1:E:247:LYS:HA	1.89	0.40
1:E:271:GLU:O	1:E:272:VAL:C	2.63	0.40
1:A:215:PHE:HB2	1:A:216:TRP:CZ3	2.55	0.40
1:A:309:LEU:O	1:A:310:ALA:C	2.65	0.40
1:B:77:PHE:HE2	1:B:127:ILE:HG23	1.87	0.40
1:C:23:LEU:HD23	1:C:38:VAL:HG21	2.02	0.40
1:C:202:LEU:HB2	1:C:203:PRO:HD3	2.02	0.40
1:C:213:THR:C	1:C:215:PHE:H	2.30	0.40
1:C:283:GLN:C	1:C:285:ALA:N	2.79	0.40
1:D:147:LYS:C	1:D:147:LYS:HD3	2.47	0.40
1:A:94:SER:HB3	1:A:98:THR:HB	2.02	0.40
1:C:218:THR:HA	1:C:275:GLN:HE22	1.86	0.40
1:E:147:LYS:C	1:E:147:LYS:HD3	2.47	0.40
1:E:175:LEU:HA	1:E:175:LEU:HD12	1.67	0.40
1:A:27:TYR:OH	1:B:81:GLU:HA	2.22	0.40
1:C:204:MET:HB3	1:C:204:MET:HE2	1.82	0.40
1:D:133:SER:HB2	1:D:137:ARG:NH1	2.37	0.40
1:D:243:THR:CG2	1:D:244:ASN:N	2.83	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	308/317 (97%)	244 (79%)	55 (18%)	9 (3%)	3	26
1	B	308/317 (97%)	245 (80%)	55 (18%)	8 (3%)	4	28
1	C	308/317 (97%)	246 (80%)	51 (17%)	11 (4%)	2	23
1	D	308/317 (97%)	248 (80%)	51 (17%)	9 (3%)	3	26
1	E	308/317 (97%)	243 (79%)	54 (18%)	11 (4%)	2	23
All	All	1540/1585 (97%)	1226 (80%)	266 (17%)	48 (3%)	3	26

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	194	PHE
1	B	118	TYR
1	B	194	PHE
1	C	118	TYR
1	C	194	PHE
1	D	118	TYR
1	D	194	PHE
1	E	118	TYR
1	E	194	PHE
1	A	118	TYR
1	A	150	LYS
1	B	150	LYS
1	C	150	LYS
1	D	49	ARG
1	D	150	LYS
1	E	150	LYS
1	A	49	ARG
1	A	225	THR
1	A	275	GLN
1	A	277	TYR
1	B	49	ARG

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Mol	Chain	Res	Type
1	B	225	THR
1	B	275	GLN
1	B	277	TYR
1	C	49	ARG
1	C	195	SER
1	C	225	THR
1	C	275	GLN
1	C	277	TYR
1	D	275	GLN
1	D	277	TYR
1	E	195	SER
1	E	225	THR
1	E	275	GLN
1	E	277	TYR
1	A	148	VAL
1	B	148	VAL
1	C	148	VAL
1	D	148	VAL
1	D	225	THR
1	E	49	ARG
1	E	148	VAL
1	E	214	ALA
1	C	131	VAL
1	C	214	ALA
1	E	131	VAL
1	D	131	VAL
1	A	131	VAL

5.3.2 Protein sidechains ⓘ

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	278/284 (98%)	222 (80%)	56 (20%)	1	8
1	B	278/284 (98%)	223 (80%)	55 (20%)	1	9
1	C	278/284 (98%)	223 (80%)	55 (20%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	278/284 (98%)	221 (80%)	57 (20%)	1	8
1	E	278/284 (98%)	223 (80%)	55 (20%)	1	9
All	All	1390/1420 (98%)	1112 (80%)	278 (20%)	1	9

All (278) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASP
1	A	26	CYS
1	A	51	LEU
1	A	53	PHE
1	A	64	THR
1	A	68	GLU
1	A	72	ILE
1	A	79	ASN
1	A	84	ARG
1	A	89	VAL
1	A	98	THR
1	A	100	GLN
1	A	110	LEU
1	A	113	LEU
1	A	122	SER
1	A	124	THR
1	A	129	LEU
1	A	130	ILE
1	A	140	VAL
1	A	141	LEU
1	A	143	VAL
1	A	150	LYS
1	A	151	ASN
1	A	154	VAL
1	A	156	LEU
1	A	157	THR
1	A	162	GLU
1	A	177	ASP
1	A	179	LEU
1	A	195	SER
1	A	201	ILE
1	A	202	LEU
1	A	211	SER
1	A	213	THR

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Mol	Chain	Res	Type
1	A	218	THR
1	A	221	GLU
1	A	226	LEU
1	A	227	VAL
1	A	232	ILE
1	A	239	ILE
1	A	243	THR
1	A	252	THR
1	A	254	THR
1	A	258	ILE
1	A	260	MET
1	A	263	LEU
1	A	269	VAL
1	A	270	ILE
1	A	273	THR
1	A	274	VAL
1	A	282	SER
1	A	292	ARG
1	A	296	ILE
1	A	304	LEU
1	A	306	ASN
1	A	307	ILE
1	B	12	ASP
1	B	26	CYS
1	B	51	LEU
1	B	53	PHE
1	B	64	THR
1	B	68	GLU
1	B	72	ILE
1	B	79	ASN
1	B	84	ARG
1	B	89	VAL
1	B	98	THR
1	B	100	GLN
1	B	110	LEU
1	B	113	LEU
1	B	122	SER
1	B	124	THR
1	B	129	LEU
1	B	130	ILE
1	B	140	VAL
1	B	141	LEU

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Mol	Chain	Res	Type
1	B	143	VAL
1	B	150	LYS
1	B	151	ASN
1	B	154	VAL
1	B	156	LEU
1	B	157	THR
1	B	162	GLU
1	B	177	ASP
1	B	179	LEU
1	B	195	SER
1	B	201	ILE
1	B	211	SER
1	B	213	THR
1	B	218	THR
1	B	221	GLU
1	B	226	LEU
1	B	227	VAL
1	B	232	ILE
1	B	239	ILE
1	B	243	THR
1	B	252	THR
1	B	254	THR
1	B	258	ILE
1	B	260	MET
1	B	263	LEU
1	B	269	VAL
1	B	270	ILE
1	B	273	THR
1	B	274	VAL
1	B	282	SER
1	B	292	ARG
1	B	296	ILE
1	B	304	LEU
1	B	306	ASN
1	B	307	ILE
1	C	12	ASP
1	C	26	CYS
1	C	51	LEU
1	C	53	PHE
1	C	64	THR
1	C	68	GLU
1	C	72	ILE

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Mol	Chain	Res	Type
1	C	79	ASN
1	C	84	ARG
1	C	89	VAL
1	C	98	THR
1	C	100	GLN
1	C	110	LEU
1	C	113	LEU
1	C	122	SER
1	C	124	THR
1	C	129	LEU
1	C	130	ILE
1	C	140	VAL
1	C	141	LEU
1	C	143	VAL
1	C	150	LYS
1	C	151	ASN
1	C	154	VAL
1	C	156	LEU
1	C	157	THR
1	C	177	ASP
1	C	179	LEU
1	C	195	SER
1	C	201	ILE
1	C	202	LEU
1	C	211	SER
1	C	213	THR
1	C	218	THR
1	C	221	GLU
1	C	226	LEU
1	C	227	VAL
1	C	232	ILE
1	C	239	ILE
1	C	243	THR
1	C	252	THR
1	C	254	THR
1	C	258	ILE
1	C	260	MET
1	C	263	LEU
1	C	269	VAL
1	C	270	ILE
1	C	273	THR
1	C	274	VAL

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Mol	Chain	Res	Type
1	C	282	SER
1	C	292	ARG
1	C	296	ILE
1	C	304	LEU
1	C	306	ASN
1	C	307	ILE
1	D	12	ASP
1	D	26	CYS
1	D	51	LEU
1	D	53	PHE
1	D	64	THR
1	D	68	GLU
1	D	72	ILE
1	D	79	ASN
1	D	84	ARG
1	D	89	VAL
1	D	98	THR
1	D	100	GLN
1	D	110	LEU
1	D	113	LEU
1	D	122	SER
1	D	124	THR
1	D	129	LEU
1	D	130	ILE
1	D	140	VAL
1	D	141	LEU
1	D	143	VAL
1	D	150	LYS
1	D	151	ASN
1	D	154	VAL
1	D	156	LEU
1	D	157	THR
1	D	162	GLU
1	D	177	ASP
1	D	179	LEU
1	D	195	SER
1	D	201	ILE
1	D	202	LEU
1	D	211	SER
1	D	213	THR
1	D	218	THR
1	D	221	GLU

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Mol	Chain	Res	Type
1	D	226	LEU
1	D	227	VAL
1	D	232	ILE
1	D	239	ILE
1	D	243	THR
1	D	252	THR
1	D	254	THR
1	D	258	ILE
1	D	260	MET
1	D	263	LEU
1	D	269	VAL
1	D	270	ILE
1	D	273	THR
1	D	274	VAL
1	D	282	SER
1	D	292	ARG
1	D	296	ILE
1	D	304	LEU
1	D	306	ASN
1	D	307	ILE
1	D	309	LEU
1	E	12	ASP
1	E	26	CYS
1	E	51	LEU
1	E	53	PHE
1	E	64	THR
1	E	68	GLU
1	E	72	ILE
1	E	79	ASN
1	E	84	ARG
1	E	89	VAL
1	E	98	THR
1	E	100	GLN
1	E	110	LEU
1	E	113	LEU
1	E	122	SER
1	E	124	THR
1	E	129	LEU
1	E	130	ILE
1	E	140	VAL
1	E	141	LEU
1	E	143	VAL

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Mol	Chain	Res	Type
1	E	150	LYS
1	E	151	ASN
1	E	154	VAL
1	E	156	LEU
1	E	157	THR
1	E	162	GLU
1	E	177	ASP
1	E	179	LEU
1	E	195	SER
1	E	201	ILE
1	E	202	LEU
1	E	211	SER
1	E	213	THR
1	E	218	THR
1	E	221	GLU
1	E	226	LEU
1	E	227	VAL
1	E	232	ILE
1	E	239	ILE
1	E	243	THR
1	E	252	THR
1	E	254	THR
1	E	258	ILE
1	E	260	MET
1	E	263	LEU
1	E	269	VAL
1	E	270	ILE
1	E	273	THR
1	E	274	VAL
1	E	282	SER
1	E	292	ARG
1	E	296	ILE
1	E	304	LEU
1	E	306	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	100	GLN
1	A	151	ASN
1	A	172	ASN

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Mol	Chain	Res	Type
1	A	238	ASN
1	A	244	ASN
1	A	275	GLN
1	B	79	ASN
1	B	100	GLN
1	B	151	ASN
1	B	172	ASN
1	B	244	ASN
1	B	275	GLN
1	C	79	ASN
1	C	100	GLN
1	C	151	ASN
1	C	172	ASN
1	C	199	ASN
1	C	238	ASN
1	C	244	ASN
1	C	275	GLN
1	D	79	ASN
1	D	100	GLN
1	D	151	ASN
1	D	172	ASN
1	D	244	ASN
1	D	275	GLN
1	E	18	ASN
1	E	79	ASN
1	E	100	GLN
1	E	151	ASN
1	E	172	ASN
1	E	199	ASN
1	E	244	ASN
1	E	275	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	310/317 (97%)	1.05	58 (18%) 3 4	57, 98, 154, 227	0
1	B	310/317 (97%)	0.96	47 (15%) 5 7	59, 98, 154, 227	0
1	C	310/317 (97%)	0.79	40 (12%) 7 9	58, 98, 154, 227	0
1	D	310/317 (97%)	0.93	44 (14%) 6 8	59, 98, 154, 227	0
1	E	310/317 (97%)	0.97	45 (14%) 6 8	58, 99, 154, 227	0
All	All	1550/1585 (97%)	0.94	234 (15%) 5 7	57, 98, 154, 227	0

All (234) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	60	VAL	9.1
1	D	153	ASP	8.6
1	B	148	VAL	7.4
1	D	152	ASP	7.1
1	B	152	ASP	6.5
1	A	59	GLY	6.3
1	A	58	SER	5.8
1	C	144	ASP	5.8
1	A	61	ARG	5.8
1	E	147	LYS	5.7
1	B	60	VAL	5.3
1	C	60	VAL	5.1
1	A	88	VAL	4.9
1	E	144	ASP	4.9
1	E	100	GLN	4.9
1	B	292	ARG	4.8
1	D	148	VAL	4.7
1	A	62	VAL	4.7
1	B	144	ASP	4.6
1	E	60	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	64	THR	4.5
1	B	11	ALA	4.2
1	B	47	LYS	4.2
1	E	61	ARG	4.1
1	C	176	GLU	4.0
1	A	13	GLU	4.0
1	A	66	GLU	4.0
1	E	146	GLU	3.9
1	A	53	PHE	3.9
1	B	136	THR	3.9
1	E	242	GLU	3.9
1	B	153	ASP	3.9
1	E	88	VAL	3.9
1	A	153	ASP	3.9
1	B	74	GLU	3.8
1	A	244	ASN	3.8
1	A	11	ALA	3.8
1	A	206	PHE	3.8
1	B	96	ASP	3.8
1	A	10	ILE	3.7
1	C	114	ASP	3.7
1	D	60	VAL	3.6
1	A	144	ASP	3.6
1	B	88	VAL	3.6
1	A	139	ILE	3.5
1	E	315	GLY	3.5
1	C	285	ALA	3.5
1	D	83	ALA	3.5
1	B	117	ARG	3.5
1	B	49	ARG	3.4
1	A	126	HIS	3.4
1	E	148	VAL	3.4
1	B	61	ARG	3.4
1	D	11	ALA	3.4
1	C	138	ASN	3.4
1	A	74	GLU	3.3
1	E	128	TYR	3.3
1	B	15	LEU	3.3
1	C	11	ALA	3.3
1	A	79	ASN	3.3
1	C	151	ASN	3.3
1	A	110	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	59	GLY	3.2
1	D	117	ARG	3.2
1	E	59	GLY	3.1
1	B	122	SER	3.1
1	E	262	TYR	3.1
1	B	145	LEU	3.1
1	B	86	ALA	3.1
1	D	57	ARG	3.0
1	E	47	LYS	3.0
1	B	26	CYS	3.0
1	D	221	GLU	3.0
1	D	154	VAL	3.0
1	C	242	GLU	2.9
1	B	216	TRP	2.9
1	D	187	LEU	2.9
1	A	186	GLN	2.9
1	C	85	ASP	2.9
1	B	231	LEU	2.9
1	D	18	ASN	2.9
1	D	10	ILE	2.9
1	C	116	ARG	2.9
1	A	148	VAL	2.9
1	C	83	ALA	2.9
1	B	87	ASP	2.8
1	E	221	GLU	2.9
1	A	134	VAL	2.8
1	D	100	GLN	2.8
1	A	177	ASP	2.8
1	C	316	PHE	2.8
1	C	136	THR	2.8
1	A	285	ALA	2.8
1	A	63	LYS	2.8
1	A	179	LEU	2.7
1	C	135	ASP	2.7
1	D	277	TYR	2.7
1	D	304	LEU	2.7
1	B	101	TYR	2.7
1	B	7	PRO	2.7
1	C	55	PRO	2.7
1	D	52	ALA	2.7
1	E	63	LYS	2.7
1	D	55	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	128	TYR	2.6
1	E	243	THR	2.6
1	A	208	LEU	2.6
1	D	82	ASN	2.6
1	C	139	ILE	2.6
1	D	275	GLN	2.6
1	B	277	TYR	2.6
1	E	115	PHE	2.6
1	E	56	VAL	2.6
1	D	56	VAL	2.6
1	C	118	TYR	2.5
1	E	139	ILE	2.5
1	E	277	TYR	2.5
1	D	7	PRO	2.5
1	A	128	TYR	2.5
1	A	15	LEU	2.5
1	D	61	ARG	2.5
1	D	126	HIS	2.5
1	A	173	PHE	2.5
1	A	209	PHE	2.5
1	C	244	ASN	2.5
1	D	85	ASP	2.5
1	D	145	LEU	2.5
1	A	56	VAL	2.5
1	C	147	LYS	2.4
1	A	14	PRO	2.4
1	A	55	PRO	2.4
1	A	12	ASP	2.4
1	A	279	LYS	2.4
1	B	316	PHE	2.4
1	E	209	PHE	2.4
1	B	27	TYR	2.4
1	C	174	ALA	2.4
1	E	166	ALA	2.4
1	A	47	LYS	2.4
1	A	316	PHE	2.4
1	B	10	ILE	2.4
1	E	101	TYR	2.4
1	A	95	PRO	2.4
1	A	172	ASN	2.4
1	C	7	PRO	2.4
1	D	138	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	78	VAL	2.4
1	A	91	ILE	2.4
1	B	187	LEU	2.4
1	E	222	ALA	2.4
1	E	282	SER	2.4
1	B	154	VAL	2.4
1	B	162	GLU	2.4
1	E	62	VAL	2.3
1	A	54	ASP	2.3
1	B	81	GLU	2.3
1	D	186	GLN	2.3
1	D	63	LYS	2.3
1	B	186	GLN	2.3
1	C	10	ILE	2.3
1	B	213	THR	2.3
1	A	87	ASP	2.3
1	B	12	ASP	2.3
1	C	146	GLU	2.3
1	D	167	VAL	2.3
1	C	141	LEU	2.3
1	B	174	ALA	2.3
1	A	68	GLU	2.3
1	B	90	ASP	2.3
1	D	134	VAL	2.3
1	C	173	PHE	2.3
1	E	174	ALA	2.3
1	E	217	SER	2.3
1	D	59	GLY	2.3
1	E	96	ASP	2.3
1	D	234	HIS	2.2
1	A	174	ALA	2.2
1	B	97	GLY	2.2
1	C	292	ARG	2.2
1	D	199	ASN	2.2
1	B	100	GLN	2.2
1	D	151	ASN	2.2
1	E	173	PHE	2.2
1	D	204	MET	2.2
1	C	157	THR	2.2
1	C	18	ASN	2.2
1	D	276	HIS	2.2
1	A	229	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	49	ARG	2.2
1	E	55	PRO	2.2
1	B	314	PHE	2.2
1	C	177	ASP	2.2
1	C	233	ALA	2.2
1	E	285	ALA	2.2
1	A	143	VAL	2.2
1	D	62	VAL	2.2
1	C	13	GLU	2.2
1	A	136	THR	2.2
1	E	244	ASN	2.2
1	C	168	VAL	2.1
1	A	221	GLU	2.1
1	C	162	GLU	2.1
1	A	138	ASN	2.1
1	D	310	ALA	2.1
1	E	91	ILE	2.1
1	D	220	TYR	2.1
1	A	7	PRO	2.1
1	E	136	THR	2.1
1	B	315	GLY	2.1
1	A	124	THR	2.1
1	B	263	LEU	2.1
1	B	188	ARG	2.1
1	E	11	ALA	2.1
1	E	83	ALA	2.1
1	D	195	SER	2.1
1	D	266	PHE	2.1
1	C	152	ASP	2.1
1	B	137	ARG	2.1
1	C	277	TYR	2.0
1	C	153	ASP	2.0
1	D	242	GLU	2.0
1	E	117	ARG	2.0
1	E	280	VAL	2.0
1	A	203	PRO	2.0
1	E	276	HIS	2.0
1	C	121	ASP	2.0
1	E	87	ASP	2.0
1	E	135	ASP	2.0
1	A	117	ARG	2.0
1	E	149	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	14	PRO	2.0
1	B	126	HIS	2.0
1	B	242	GLU	2.0
1	E	85	ASP	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SB	E	1316	1/1	0.93	0.09	151,151,151,151	0

6.5 Other polymers [i](#)

There are no such residues in this entry.