



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:30 PM UTC

PDB ID : 2XQ9 / pdb_00002xq9
Title : Pentameric ligand gated ion channel GLIC mutant E221A in complex with tetraethylarsonium (TEAs)
Authors : Hilf, R.J.C.; Bertozzi, C.; Zimmermann, I.; Reiter, A.; Trauner, D.; Dutzler, R.
Deposited on : 2010-09-01
Resolution : 3.20 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

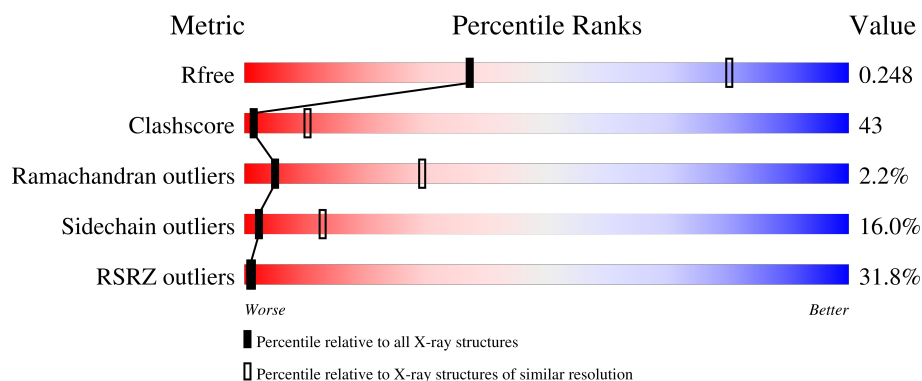
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	32% 35% 50% 12% ..
1	B	317	25% 34% 50% 12% ..
1	C	317	32% 34% 52% 10% ..
1	D	317	34% 32% 53% 11% ..
1	E	317	32% 37% 48% 12% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12601 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
			2520	1661	403	452	4			
1	B	310	Total	C	N	O	S	0	0	0
			2520	1661	403	452	4			
1	C	310	Total	C	N	O	S	0	0	0
			2520	1661	403	452	4			
1	D	310	Total	C	N	O	S	0	0	0
			2520	1661	403	452	4			
1	E	310	Total	C	N	O	S	0	0	0
			2520	1661	403	452	4			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	221	ASP	GLU	engineered mutation	UNP Q7NDN8
B	221	ASP	GLU	engineered mutation	UNP Q7NDN8
C	221	ASP	GLU	engineered mutation	UNP Q7NDN8
D	221	ASP	GLU	engineered mutation	UNP Q7NDN8
E	221	ASP	GLU	engineered mutation	UNP Q7NDN8

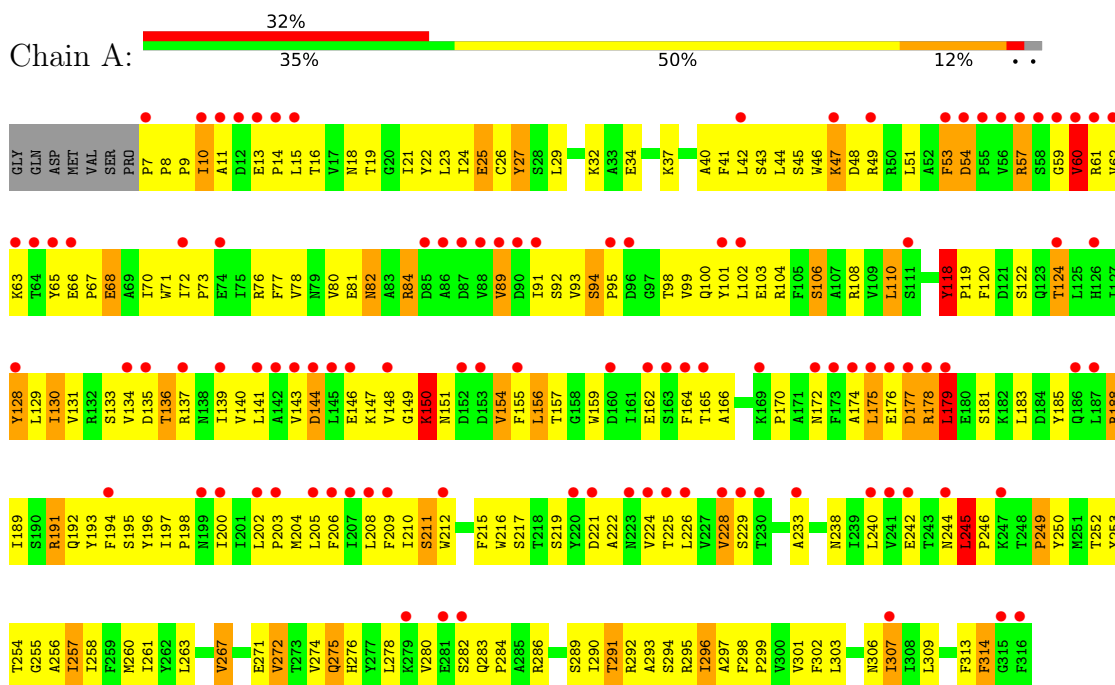
- Molecule 2 is ARSENIC (CCD ID: ARS) (formula: As).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	As	0	0
			1	1		

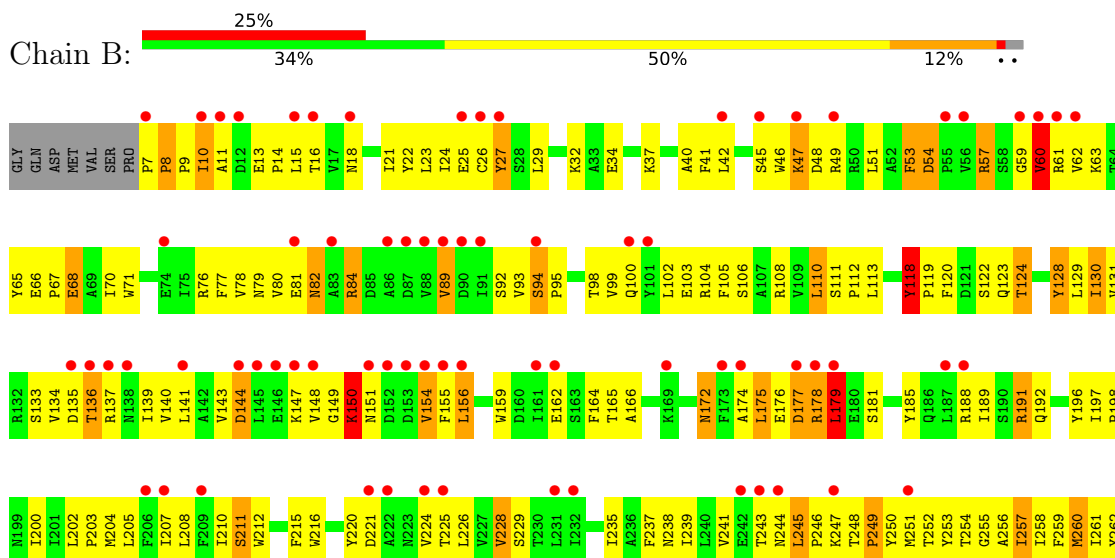
3 Residue-property plots [i](#)

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

• Molecule 1: GLR4197 PROTEIN

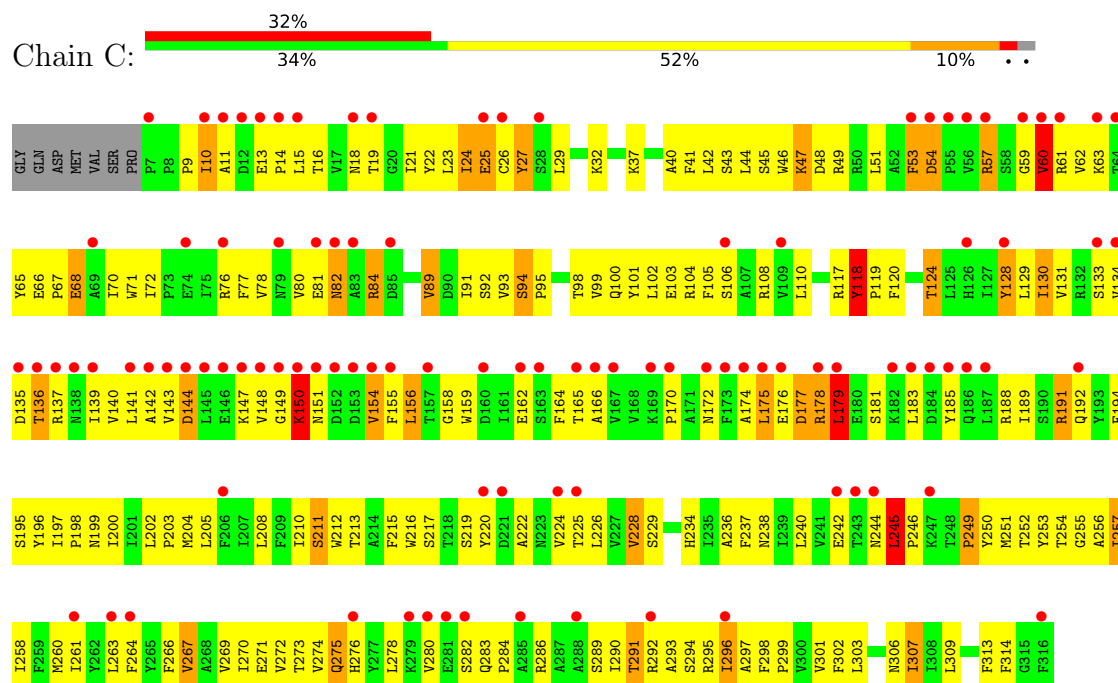


• Molecule 1: GLR4197 PROTEIN

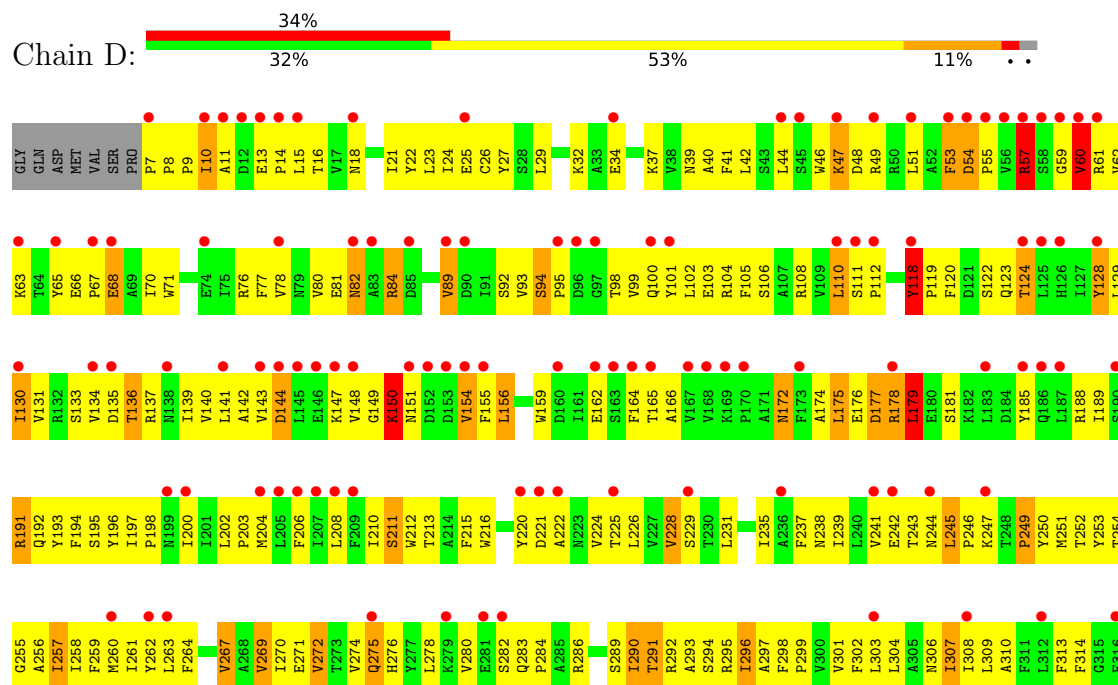




• Molecule 1: GLR4197 PROTEIN



• 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)	40.00 – 3.20 40.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.00-3.20) 99.9 (40.00-3.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.29 (at 3.06Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.252 , 0.257 (Not available) , 0.248	Depositor DCC
R_{free} test set	2805 reflections (4.22%)	wwPDB-VP
Wilson B-factor (Å ²)	78.8	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 89.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	12601	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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: ARS

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	0.61	0/2588	1.08	17/3534 (0.5%)
1	B	0.64	1/2588 (0.0%)	1.09	18/3534 (0.5%)
1	C	0.64	1/2588 (0.0%)	1.09	18/3534 (0.5%)
1	D	0.67	4/2588 (0.2%)	1.08	16/3534 (0.5%)
1	E	0.64	1/2588 (0.0%)	1.10	19/3534 (0.5%)
All	All	0.64	7/12940 (0.1%)	1.09	88/17670 (0.5%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	55	PRO	C-N	-6.27	1.26	1.33
1	B	172	ASN	C-N	5.89	1.41	1.33
1	D	57	ARG	C-N	-5.73	1.25	1.33
1	C	142	ALA	CA-CB	5.59	1.61	1.53
1	D	142	ALA	CA-CB	5.58	1.61	1.53
1	E	142	ALA	CA-CB	5.52	1.61	1.53
1	D	172	ASN	C-N	5.34	1.40	1.33

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	179	LEU	N-CA-C	-8.69	97.62	110.48
1	A	179	LEU	N-CA-C	-8.67	97.65	110.48
1	C	179	LEU	N-CA-C	-8.66	97.66	110.48
1	E	179	LEU	N-CA-C	-8.65	97.69	110.48
1	D	179	LEU	N-CA-C	-8.64	97.69	110.48
1	B	128	TYR	N-CA-C	8.12	123.74	112.93
1	C	128	TYR	N-CA-C	8.11	123.72	112.93
1	E	128	TYR	N-CA-C	8.11	123.71	112.93
1	A	128	TYR	N-CA-C	8.11	123.71	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	128	TYR	N-CA-C	8.09	123.69	112.93
1	A	135	ASP	N-CA-C	-7.17	105.45	114.56
1	C	135	ASP	N-CA-C	-7.17	105.45	114.56
1	D	135	ASP	N-CA-C	-7.16	105.46	114.56
1	E	135	ASP	N-CA-C	-7.16	105.47	114.56
1	B	178	ARG	N-CA-C	-7.15	95.58	110.80
1	B	135	ASP	N-CA-C	-7.14	105.49	114.56
1	E	178	ARG	N-CA-C	-7.13	95.60	110.80
1	A	178	ARG	N-CA-C	-7.13	95.61	110.80
1	D	178	ARG	N-CA-C	-7.12	95.64	110.80
1	C	178	ARG	N-CA-C	-7.11	95.65	110.80
1	C	177	ASP	N-CA-C	7.08	121.69	111.56
1	A	177	ASP	N-CA-C	7.05	121.65	111.56
1	B	118	TYR	CA-C-N	-7.04	112.37	119.56
1	B	118	TYR	C-N-CA	-7.04	112.37	119.56
1	E	177	ASP	N-CA-C	7.04	121.62	111.56
1	B	177	ASP	N-CA-C	7.03	121.61	111.56
1	D	177	ASP	N-CA-C	7.03	121.61	111.56
1	D	118	TYR	CA-C-N	-6.93	112.56	119.56
1	D	118	TYR	C-N-CA	-6.93	112.56	119.56
1	A	118	TYR	CA-C-N	-6.89	112.60	119.56
1	A	118	TYR	C-N-CA	-6.89	112.60	119.56
1	C	118	TYR	CA-C-N	-6.62	112.88	119.56
1	C	118	TYR	C-N-CA	-6.62	112.88	119.56
1	A	249	PRO	N-CA-C	-6.52	107.89	114.68
1	B	150	LYS	N-CA-C	-6.41	97.14	110.80
1	A	150	LYS	N-CA-C	-6.41	97.15	110.80
1	C	150	LYS	N-CA-C	-6.40	97.18	110.80
1	E	150	LYS	N-CA-C	-6.39	97.18	110.80
1	D	150	LYS	N-CA-C	-6.38	97.20	110.80
1	C	245	LEU	CA-C-N	6.28	126.64	119.92
1	C	245	LEU	C-N-CA	6.28	126.64	119.92
1	D	249	PRO	N-CA-C	-6.26	108.17	114.68
1	B	134	VAL	N-CA-C	6.14	122.12	109.34
1	A	134	VAL	N-CA-C	6.14	122.11	109.34
1	D	134	VAL	N-CA-C	6.13	122.09	109.34
1	E	134	VAL	N-CA-C	6.13	122.09	109.34
1	C	134	VAL	N-CA-C	6.12	122.07	109.34
1	E	118	TYR	CA-C-N	-6.08	113.36	119.56
1	E	118	TYR	C-N-CA	-6.08	113.36	119.56
1	C	249	PRO	N-CA-C	-5.92	108.52	114.68
1	E	249	PRO	N-CA-C	-5.83	108.61	114.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	150	LYS	N-CA-CB	5.81	120.30	110.49
1	E	245	LEU	CA-C-N	5.79	125.76	120.03
1	E	245	LEU	C-N-CA	5.79	125.76	120.03
1	C	150	LYS	N-CA-CB	5.78	120.26	110.49
1	D	150	LYS	N-CA-CB	5.78	120.26	110.49
1	A	150	LYS	N-CA-CB	5.78	120.26	110.49
1	C	236	ALA	N-CA-C	-5.77	105.08	111.71
1	B	150	LYS	N-CA-CB	5.75	120.21	110.49
1	B	8	PRO	O-C-N	5.62	123.79	121.15
1	A	245	LEU	CA-C-N	5.57	125.88	119.92
1	A	245	LEU	C-N-CA	5.57	125.88	119.92
1	A	27	TYR	N-CA-C	5.56	115.88	108.38
1	C	24	ILE	N-CA-C	-5.53	106.80	111.56
1	D	111	SER	CA-C-N	5.46	125.66	120.31
1	D	111	SER	C-N-CA	5.46	125.66	120.31
1	E	236	ALA	N-CA-C	-5.41	105.49	111.71
1	B	249	PRO	N-CA-C	-5.38	108.52	114.92
1	E	27	TYR	N-CA-C	5.36	115.61	108.38
1	E	111	SER	CA-C-N	5.29	125.76	120.52
1	E	111	SER	C-N-CA	5.29	125.76	120.52
1	C	27	TYR	N-CA-C	5.28	115.51	108.38
1	B	111	SER	CA-C-N	5.26	125.46	120.31
1	B	111	SER	C-N-CA	5.26	125.46	120.31
1	C	156	LEU	N-CA-C	5.24	117.58	111.02
1	A	156	LEU	N-CA-C	5.24	117.57	111.02
1	B	156	LEU	N-CA-C	5.24	117.56	111.02
1	E	156	LEU	N-CA-C	5.23	117.56	111.02
1	D	156	LEU	N-CA-C	5.22	117.55	111.02
1	D	272	VAL	N-CA-CB	5.18	116.94	110.47
1	A	272	VAL	N-CA-CB	5.17	116.93	110.47
1	B	134	VAL	CB-CA-C	-5.08	102.96	111.29
1	B	27	TYR	N-CA-C	5.08	115.24	108.38
1	C	134	VAL	CB-CA-C	-5.07	102.97	111.29
1	E	134	VAL	CB-CA-C	-5.06	102.98	111.29
1	D	134	VAL	CB-CA-C	-5.05	103.00	111.29
1	A	134	VAL	CB-CA-C	-5.05	103.01	111.29
1	B	260	MET	N-CA-C	-5.02	105.08	111.11

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	2520	0	2535	270	0
1	B	2520	0	2535	267	0
1	C	2520	0	2535	229	0
1	D	2520	0	2535	247	0
1	E	2520	0	2535	211	0
2	C	1	0	0	0	0
All	All	12601	0	12675	1086	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 43.

All (1086) 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:C:84:ARG:HG3	1:C:84:ARG:HH11	1.07	1.20
1:A:155:PHE:CE1	1:B:112:PRO:HB3	1.81	1.15
1:D:84:ARG:HG3	1:D:84:ARG:HH11	1.03	1.12
1:A:84:ARG:HH11	1:A:84:ARG:HG3	1.02	1.11
1:E:84:ARG:HG3	1:E:84:ARG:HH11	1.03	1.11
1:B:84:ARG:HG3	1:B:84:ARG:HH11	1.03	1.06
1:D:22:TYR:HA	1:D:149:GLY:HA3	1.37	1.06
1:C:22:TYR:HA	1:C:149:GLY:HA3	1.39	1.03
1:B:76:ARG:HH22	1:B:130:ILE:HD12	1.23	1.01
1:A:76:ARG:HH22	1:A:130:ILE:HD12	1.26	0.99
1:A:222:ALA:HB2	1:B:221:ASP:HA	1.40	0.99
1:B:22:TYR:HA	1:B:149:GLY:HA3	1.41	0.99
1:E:76:ARG:HH22	1:E:130:ILE:HD12	1.25	0.98
1:E:22:TYR:HA	1:E:149:GLY:HA3	1.43	0.98
1:A:22:TYR:HA	1:A:149:GLY:HA3	1.43	0.97
1:D:22:TYR:HA	1:D:149:GLY:CA	1.94	0.97
1:C:22:TYR:HA	1:C:149:GLY:CA	1.95	0.95
1:D:76:ARG:HH22	1:D:130:ILE:HD12	1.26	0.95
1:A:27:TYR:HB3	1:B:110:LEU:HD21	1.47	0.95
1:C:76:ARG:HH22	1:C:130:ILE:HD12	1.29	0.95
1:D:22:TYR:CD1	1:D:149:GLY:HA2	2.02	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:139:ILE:HG12	1:E:172:ASN:HD21	1.34	0.93
1:A:147:LYS:HE2	1:A:165:THR:HA	1.51	0.92
1:B:22:TYR:HA	1:B:149:GLY:CA	1.98	0.92
1:C:147:LYS:C	1:C:149:GLY:H	1.76	0.91
1:D:41:PHE:HE2	1:E:175:LEU:HD13	1.34	0.91
1:A:22:TYR:HA	1:A:149:GLY:CA	1.99	0.91
1:E:22:TYR:HA	1:E:149:GLY:CA	2.00	0.91
1:B:22:TYR:CD1	1:B:149:GLY:HA2	2.06	0.91
1:E:147:LYS:C	1:E:149:GLY:H	1.76	0.91
1:A:84:ARG:HG3	1:A:84:ARG:NH1	1.82	0.91
1:A:139:ILE:HG12	1:A:172:ASN:HD21	1.35	0.90
1:E:260:MET:HE3	1:E:309:LEU:HD22	1.54	0.90
1:E:267:VAL:HG23	1:E:298:PHE:CZ	2.06	0.90
1:A:147:LYS:C	1:A:149:GLY:H	1.76	0.90
1:D:51:LEU:HB3	1:D:93:VAL:HG11	1.54	0.90
1:C:267:VAL:HG23	1:C:298:PHE:CZ	2.07	0.89
1:D:260:MET:HE3	1:D:309:LEU:HD22	1.54	0.89
1:D:267:VAL:HG23	1:D:298:PHE:CZ	2.08	0.89
1:A:267:VAL:HG23	1:A:298:PHE:CZ	2.07	0.89
1:A:84:ARG:HH11	1:A:84:ARG:CG	1.86	0.89
1:C:147:LYS:HE2	1:C:165:THR:HA	1.53	0.88
1:A:51:LEU:HB3	1:A:93:VAL:HG11	1.54	0.88
1:B:260:MET:HE3	1:B:309:LEU:HD22	1.55	0.88
1:B:51:LEU:HB3	1:B:93:VAL:HG11	1.55	0.88
1:E:22:TYR:CD1	1:E:149:GLY:HA2	2.09	0.88
1:E:147:LYS:HE2	1:E:165:THR:HA	1.56	0.88
1:C:139:ILE:HG12	1:C:172:ASN:HD21	1.36	0.88
1:C:260:MET:HE3	1:C:309:LEU:HD22	1.56	0.88
1:B:267:VAL:HG23	1:B:298:PHE:CZ	2.10	0.87
1:D:147:LYS:C	1:D:149:GLY:H	1.76	0.87
1:C:199:ASN:HB3	1:D:242:GLU:CD	2.00	0.87
1:D:84:ARG:HH11	1:D:84:ARG:CG	1.86	0.87
1:E:51:LEU:HB3	1:E:93:VAL:HG11	1.55	0.87
1:C:22:TYR:CD1	1:C:149:GLY:HA2	2.09	0.87
1:E:84:ARG:HH11	1:E:84:ARG:CG	1.88	0.86
1:B:147:LYS:HE2	1:B:165:THR:HA	1.57	0.86
1:C:84:ARG:HG3	1:C:84:ARG:NH1	1.87	0.86
1:A:260:MET:HE3	1:A:309:LEU:HD22	1.56	0.86
1:D:139:ILE:HG12	1:D:172:ASN:HD21	1.41	0.86
1:B:84:ARG:HG3	1:B:84:ARG:NH1	1.83	0.85
1:C:51:LEU:HB3	1:C:93:VAL:HG11	1.55	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:ILE:HG23	1:E:269:VAL:HG11	1.56	0.85
1:B:84:ARG:HH11	1:B:84:ARG:CG	1.89	0.85
1:B:147:LYS:C	1:B:149:GLY:H	1.76	0.85
1:E:84:ARG:HG3	1:E:84:ARG:NH1	1.83	0.84
1:A:22:TYR:CD1	1:A:149:GLY:HA2	2.12	0.84
1:A:76:ARG:NH2	1:A:130:ILE:HD12	1.92	0.84
1:B:76:ARG:NH2	1:B:130:ILE:HD12	1.92	0.84
1:D:155:PHE:CE1	1:E:112:PRO:HB3	2.13	0.84
1:D:76:ARG:NH2	1:D:130:ILE:HD12	1.93	0.83
1:B:139:ILE:HG12	1:B:172:ASN:HD21	1.42	0.83
1:C:84:ARG:HH11	1:C:84:ARG:CG	1.90	0.82
1:D:84:ARG:HG3	1:D:84:ARG:NH1	1.83	0.82
1:D:147:LYS:HE2	1:D:165:THR:HA	1.61	0.82
1:E:76:ARG:NH2	1:E:130:ILE:HD12	1.93	0.82
1:A:210:ILE:HG23	1:B:269:VAL:HG21	1.62	0.81
1:B:13:GLU:HB3	1:B:14:PRO:HD2	1.63	0.81
1:C:13:GLU:HB3	1:C:14:PRO:HD2	1.62	0.81
1:A:198:PRO:CG	1:B:251:MET:HE1	2.10	0.81
1:D:297:ALA:O	1:D:301:VAL:HG23	1.81	0.80
1:E:257:ILE:HG22	1:E:309:LEU:HD23	1.61	0.80
1:C:76:ARG:NH2	1:C:130:ILE:HD12	1.96	0.80
1:C:197:ILE:HB	1:C:198:PRO:HD3	1.63	0.80
1:D:13:GLU:HB3	1:D:14:PRO:HD2	1.63	0.80
1:A:297:ALA:O	1:A:301:VAL:HG23	1.83	0.79
1:C:257:ILE:HG22	1:C:309:LEU:HD23	1.61	0.79
1:A:257:ILE:HG22	1:A:309:LEU:HD23	1.62	0.79
1:C:175:LEU:HD22	1:C:176:GLU:HG3	1.65	0.79
1:D:257:ILE:HG22	1:D:309:LEU:HD23	1.62	0.79
1:D:175:LEU:HD22	1:D:176:GLU:HG3	1.65	0.79
1:E:297:ALA:O	1:E:301:VAL:HG23	1.82	0.79
1:B:297:ALA:O	1:B:301:VAL:HG23	1.82	0.79
1:E:13:GLU:HB3	1:E:14:PRO:HD2	1.62	0.79
1:A:13:GLU:HB3	1:A:14:PRO:HD2	1.63	0.79
1:E:175:LEU:HD22	1:E:176:GLU:HG3	1.65	0.79
1:A:175:LEU:HD22	1:A:176:GLU:HG3	1.65	0.78
1:E:238:ASN:HA	1:E:258:ILE:HD11	1.65	0.78
1:A:229:SER:HB2	1:B:228:VAL:HG11	1.65	0.78
1:C:249:PRO:HD2	1:C:250:TYR:CD1	2.18	0.78
1:C:297:ALA:O	1:C:301:VAL:HG23	1.83	0.78
1:B:257:ILE:HG22	1:B:309:LEU:HD23	1.64	0.77
1:B:175:LEU:HD22	1:B:176:GLU:HG3	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ARG:CD	1:B:76:ARG:NH1	2.48	0.77
1:E:249:PRO:HD2	1:E:250:TYR:CD1	2.20	0.77
1:E:89:VAL:HG11	1:E:102:LEU:HD23	1.65	0.76
1:A:155:PHE:CE1	1:B:112:PRO:CB	2.66	0.76
1:D:192:GLN:NE2	1:E:249:PRO:HB3	2.00	0.76
1:B:249:PRO:HD2	1:B:250:TYR:CD1	2.21	0.76
1:E:197:ILE:HB	1:E:198:PRO:HD3	1.66	0.75
1:A:104:ARG:HD2	1:B:76:ARG:NH1	2.01	0.75
1:E:303:LEU:O	1:E:307:ILE:HD12	1.86	0.75
1:A:89:VAL:HG11	1:A:102:LEU:HD23	1.67	0.74
1:A:222:ALA:CB	1:B:221:ASP:HA	2.15	0.74
1:B:47:LYS:HD2	1:B:49:ARG:NH2	2.03	0.74
1:A:197:ILE:HB	1:A:198:PRO:HD3	1.69	0.74
1:B:238:ASN:HA	1:B:258:ILE:HD11	1.70	0.74
1:D:41:PHE:CE2	1:E:175:LEU:HD13	2.19	0.74
1:E:47:LYS:HD2	1:E:49:ARG:NH2	2.02	0.73
1:A:198:PRO:HG2	1:B:251:MET:HE1	1.69	0.73
1:C:78:VAL:HG22	1:C:130:ILE:HG12	1.71	0.73
1:C:147:LYS:C	1:C:149:GLY:N	2.46	0.73
1:E:278:LEU:HD13	1:E:286:ARG:HB3	1.70	0.73
1:A:240:LEU:HD22	1:B:239:ILE:HG12	1.69	0.73
1:A:249:PRO:HD2	1:A:250:TYR:CD1	2.23	0.73
1:E:147:LYS:C	1:E:149:GLY:N	2.46	0.73
1:D:47:LYS:HD2	1:D:49:ARG:NH2	2.04	0.73
1:B:89:VAL:HG11	1:B:102:LEU:HD23	1.69	0.72
1:D:238:ASN:HA	1:D:258:ILE:HD11	1.71	0.72
1:C:199:ASN:HB3	1:D:242:GLU:OE2	1.89	0.72
1:C:238:ASN:HA	1:C:258:ILE:HD11	1.70	0.72
1:B:191:ARG:HG3	1:B:192:GLN:N	2.02	0.72
1:A:27:TYR:CB	1:B:110:LEU:HD21	2.20	0.71
1:A:47:LYS:HD2	1:A:49:ARG:NH2	2.04	0.71
1:B:78:VAL:HG22	1:B:130:ILE:HG12	1.71	0.71
1:B:197:ILE:HB	1:B:198:PRO:HD3	1.70	0.71
1:C:177:ASP:O	1:C:178:ARG:HG3	1.90	0.71
1:D:177:ASP:O	1:D:178:ARG:HG3	1.90	0.71
1:D:197:ILE:HB	1:D:198:PRO:HD3	1.70	0.71
1:D:249:PRO:HD2	1:D:250:TYR:CD1	2.25	0.71
1:A:41:PHE:HE2	1:B:175:LEU:HD13	1.55	0.71
1:B:147:LYS:C	1:B:149:GLY:N	2.46	0.71
1:B:177:ASP:O	1:B:178:ARG:HG3	1.90	0.71
1:D:89:VAL:HG11	1:D:102:LEU:HD23	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:78:VAL:HG22	1:E:130:ILE:HG12	1.71	0.71
1:E:245:LEU:HD12	1:E:246:PRO:HD2	1.73	0.71
1:B:47:LYS:HD2	1:B:49:ARG:CZ	2.21	0.71
1:E:177:ASP:O	1:E:178:ARG:HG3	1.90	0.71
1:B:303:LEU:O	1:B:307:ILE:HD12	1.91	0.70
1:A:177:ASP:O	1:A:178:ARG:HG3	1.90	0.70
1:D:191:ARG:HG3	1:D:192:GLN:N	2.06	0.70
1:E:47:LYS:HD2	1:E:49:ARG:CZ	2.22	0.70
1:B:278:LEU:HD13	1:B:286:ARG:HB3	1.73	0.70
1:C:47:LYS:HD2	1:C:49:ARG:NH2	2.07	0.70
1:E:9:PRO:HD3	1:E:71:TRP:CE3	2.27	0.70
1:A:215:PHE:HZ	1:A:298:PHE:CE1	2.10	0.70
1:A:303:LEU:O	1:A:307:ILE:HD12	1.92	0.70
1:C:149:GLY:O	1:C:164:PHE:HD1	1.75	0.69
1:D:78:VAL:HG22	1:D:130:ILE:HG12	1.73	0.69
1:A:192:GLN:CD	1:B:249:PRO:HB3	2.17	0.69
1:C:303:LEU:O	1:C:307:ILE:HD12	1.91	0.69
1:D:278:LEU:HD13	1:D:286:ARG:HB3	1.74	0.69
1:A:78:VAL:HG22	1:A:130:ILE:HG12	1.74	0.69
1:A:238:ASN:HA	1:A:258:ILE:HD11	1.74	0.69
1:E:275:GLN:HG3	1:E:291:THR:OG1	1.93	0.69
1:E:149:GLY:O	1:E:164:PHE:HD1	1.76	0.69
1:E:275:GLN:O	1:E:275:GLN:HG2	1.93	0.69
1:A:229:SER:CB	1:B:228:VAL:HG11	2.23	0.69
1:C:275:GLN:O	1:C:275:GLN:HG2	1.93	0.69
1:B:13:GLU:HB3	1:B:14:PRO:CD	2.23	0.69
1:D:18:ASN:HB3	1:D:143:VAL:HG23	1.75	0.69
1:A:9:PRO:HD3	1:A:71:TRP:CE3	2.28	0.68
1:C:80:VAL:HG12	1:C:82:ASN:O	1.93	0.68
1:D:47:LYS:HD2	1:D:49:ARG:CZ	2.23	0.68
1:D:275:GLN:O	1:D:275:GLN:HG2	1.93	0.68
1:A:80:VAL:HG12	1:A:82:ASN:O	1.93	0.68
1:A:275:GLN:O	1:A:275:GLN:HG2	1.93	0.68
1:A:13:GLU:HB3	1:A:14:PRO:CD	2.23	0.68
1:A:210:ILE:CG2	1:B:269:VAL:HG21	2.24	0.68
1:B:9:PRO:HD3	1:B:71:TRP:CE3	2.29	0.68
1:B:275:GLN:HG2	1:B:275:GLN:O	1.93	0.68
1:E:80:VAL:HG12	1:E:82:ASN:O	1.93	0.68
1:B:80:VAL:HG12	1:B:82:ASN:O	1.93	0.68
1:B:215:PHE:HZ	1:B:298:PHE:CE1	2.11	0.68
1:C:191:ARG:HG3	1:C:192:GLN:N	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:13:GLU:HB3	1:E:14:PRO:CD	2.22	0.68
1:A:149:GLY:O	1:A:164:PHE:HD1	1.77	0.68
1:D:216:TRP:CH2	1:D:295:ARG:HB2	2.29	0.68
1:A:217:SER:OG	1:B:220:TYR:CE2	2.47	0.68
1:D:215:PHE:HZ	1:D:298:PHE:CE1	2.11	0.68
1:D:229:SER:CB	1:E:228:VAL:HG11	2.23	0.68
1:C:13:GLU:HB3	1:C:14:PRO:CD	2.22	0.68
1:C:60:VAL:HG23	1:C:61:ARG:N	2.09	0.68
1:D:80:VAL:HG12	1:D:82:ASN:O	1.93	0.68
1:D:275:GLN:HG3	1:D:291:THR:OG1	1.94	0.68
1:A:60:VAL:HG23	1:A:61:ARG:N	2.09	0.67
1:B:245:LEU:HD12	1:B:246:PRO:HD2	1.76	0.67
1:C:217:SER:HB2	1:D:220:TYR:CE2	2.28	0.67
1:D:60:VAL:HG23	1:D:61:ARG:N	2.09	0.67
1:E:60:VAL:HG23	1:E:61:ARG:N	2.09	0.67
1:C:89:VAL:HG11	1:C:102:LEU:HD23	1.75	0.67
1:D:13:GLU:HB3	1:D:14:PRO:CD	2.25	0.67
1:A:283:GLN:N	1:A:284:PRO:HD3	2.08	0.67
1:C:47:LYS:HD2	1:C:49:ARG:CZ	2.25	0.67
1:A:47:LYS:HD2	1:A:49:ARG:CZ	2.24	0.67
1:A:147:LYS:C	1:A:149:GLY:N	2.46	0.67
1:A:255:GLY:O	1:A:258:ILE:HG22	1.93	0.67
1:A:191:ARG:HG3	1:A:192:GLN:N	2.10	0.66
1:B:60:VAL:HG23	1:B:61:ARG:N	2.09	0.66
1:A:275:GLN:HG3	1:A:291:THR:OG1	1.95	0.66
1:B:216:TRP:CH2	1:B:295:ARG:HB2	2.31	0.66
1:C:215:PHE:HZ	1:C:298:PHE:CE1	2.13	0.66
1:C:245:LEU:HD12	1:C:246:PRO:HD2	1.77	0.66
1:D:303:LEU:O	1:D:307:ILE:HD12	1.96	0.66
1:E:216:TRP:CH2	1:E:295:ARG:HB2	2.30	0.66
1:C:275:GLN:HG3	1:C:291:THR:OG1	1.96	0.66
1:D:245:LEU:HD12	1:D:246:PRO:HD2	1.77	0.66
1:A:41:PHE:CE2	1:B:175:LEU:HD13	2.30	0.66
1:A:245:LEU:HD12	1:A:246:PRO:HD2	1.78	0.66
1:C:21:ILE:O	1:C:149:GLY:HA3	1.96	0.66
1:B:275:GLN:HG3	1:B:291:THR:OG1	1.95	0.66
1:E:18:ASN:HB3	1:E:143:VAL:HG23	1.78	0.66
1:A:217:SER:HB2	1:B:220:TYR:CE2	2.31	0.66
1:B:149:GLY:O	1:B:164:PHE:HD1	1.78	0.66
1:C:278:LEU:HD13	1:C:286:ARG:HB3	1.77	0.65
1:E:215:PHE:HZ	1:E:298:PHE:CE1	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:GLN:N	1:D:284:PRO:HD3	2.11	0.65
1:C:9:PRO:HD3	1:C:71:TRP:CE3	2.31	0.65
1:A:21:ILE:O	1:A:149:GLY:HA3	1.97	0.65
1:E:283:GLN:N	1:E:284:PRO:HD3	2.11	0.65
1:D:147:LYS:C	1:D:149:GLY:N	2.46	0.65
1:D:255:GLY:HA2	1:D:258:ILE:HG22	1.79	0.65
1:C:283:GLN:N	1:C:284:PRO:HD3	2.12	0.65
1:A:229:SER:CB	1:B:228:VAL:CG1	2.75	0.65
1:A:255:GLY:HA2	1:A:258:ILE:HG22	1.79	0.65
1:D:149:GLY:O	1:D:164:PHE:HD1	1.80	0.64
1:C:18:ASN:HB3	1:C:143:VAL:HG23	1.79	0.64
1:D:21:ILE:O	1:D:149:GLY:HA3	1.98	0.64
1:E:191:ARG:HG3	1:E:192:GLN:N	2.12	0.64
1:A:23:LEU:HA	1:A:40:ALA:HB2	1.79	0.64
1:A:216:TRP:CH2	1:A:295:ARG:HB2	2.32	0.64
1:B:24:ILE:HD13	1:B:104:ARG:HE	1.62	0.64
1:E:21:ILE:O	1:E:149:GLY:HA3	1.98	0.64
1:B:283:GLN:N	1:B:284:PRO:HD3	2.13	0.64
1:B:21:ILE:O	1:B:149:GLY:HA3	1.98	0.63
1:A:157:THR:CG2	1:B:34:GLU:OE2	2.46	0.63
1:A:278:LEU:HD13	1:A:286:ARG:HB3	1.78	0.63
1:A:192:GLN:NE2	1:B:249:PRO:HB3	2.14	0.63
1:A:37:LYS:HE3	1:A:108:ARG:HD2	1.80	0.62
1:B:255:GLY:HA2	1:B:258:ILE:HG22	1.80	0.62
1:E:255:GLY:HA2	1:E:258:ILE:HG22	1.80	0.62
1:A:18:ASN:HB3	1:A:143:VAL:HG23	1.80	0.62
1:A:24:ILE:HD13	1:A:104:ARG:HE	1.63	0.62
1:B:37:LYS:HE3	1:B:108:ARG:HD2	1.82	0.62
1:B:23:LEU:HA	1:B:40:ALA:HB2	1.80	0.62
1:D:37:LYS:HE3	1:D:108:ARG:HD2	1.80	0.62
1:C:202:LEU:HD12	1:D:259:PHE:CE1	2.34	0.62
1:E:291:THR:O	1:E:295:ARG:HG2	1.99	0.62
1:C:194:PHE:HZ	1:D:251:MET:HE2	1.64	0.62
1:C:216:TRP:CH2	1:C:295:ARG:HB2	2.35	0.62
1:C:11:ALA:HB3	1:C:136:THR:HG21	1.82	0.62
1:D:84:ARG:CG	1:D:84:ARG:NH1	2.53	0.62
1:A:27:TYR:CZ	1:A:37:LYS:HB3	2.35	0.61
1:A:217:SER:CB	1:B:220:TYR:CE2	2.83	0.61
1:B:11:ALA:HB3	1:B:136:THR:HG21	1.82	0.61
1:C:27:TYR:CE1	1:D:81:GLU:CD	2.78	0.61
1:A:11:ALA:HB3	1:A:136:THR:HG21	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:ALA:HB3	1:D:136:THR:HG21	1.82	0.61
1:A:225:THR:HG21	1:B:225:THR:OG1	2.01	0.61
1:A:255:GLY:C	1:A:258:ILE:HG22	2.26	0.61
1:C:271:GLU:HG3	1:C:294:SER:OG	2.00	0.61
1:C:274:VAL:C	1:C:276:HIS:H	2.09	0.61
1:E:37:LYS:HE3	1:E:108:ARG:HD2	1.83	0.61
1:E:84:ARG:CG	1:E:84:ARG:NH1	2.54	0.61
1:A:222:ALA:HB2	1:B:221:ASP:CA	2.23	0.61
1:D:23:LEU:HA	1:D:40:ALA:HB2	1.83	0.61
1:C:131:VAL:HG11	1:C:140:VAL:HG13	1.80	0.61
1:A:195:SER:HB3	1:B:248:THR:O	2.00	0.60
1:B:271:GLU:HG3	1:B:294:SER:OG	2.01	0.60
1:B:286:ARG:O	1:B:289:SER:HB3	2.01	0.60
1:A:128:TYR:O	1:A:129:LEU:HB2	2.01	0.60
1:A:217:SER:HB2	1:B:220:TYR:CZ	2.36	0.60
1:B:131:VAL:HG11	1:B:140:VAL:HG13	1.82	0.60
1:C:128:TYR:O	1:C:129:LEU:HB2	2.01	0.60
1:A:255:GLY:HA2	1:A:258:ILE:CG2	2.32	0.60
1:D:9:PRO:HD3	1:D:71:TRP:CE3	2.36	0.60
1:D:42:LEU:HB3	1:D:103:GLU:CG	2.32	0.60
1:B:257:ILE:O	1:B:261:ILE:HG12	2.01	0.60
1:E:11:ALA:HB3	1:E:136:THR:HG21	1.82	0.60
1:D:22:TYR:HA	1:D:149:GLY:HA2	1.84	0.60
1:D:286:ARG:O	1:D:289:SER:HB3	2.02	0.60
1:A:131:VAL:HG11	1:A:140:VAL:HG13	1.82	0.60
1:C:257:ILE:O	1:C:261:ILE:HG12	2.01	0.60
1:E:24:ILE:HD13	1:E:104:ARG:HE	1.66	0.60
1:E:271:GLU:HG3	1:E:294:SER:OG	2.02	0.60
1:D:128:TYR:O	1:D:129:LEU:HB2	2.01	0.60
1:D:192:GLN:CD	1:E:249:PRO:HB3	2.27	0.60
1:E:274:VAL:C	1:E:276:HIS:H	2.09	0.60
1:C:291:THR:O	1:C:295:ARG:HG2	2.02	0.60
1:D:198:PRO:CG	1:E:251:MET:HE1	2.32	0.60
1:D:257:ILE:O	1:D:261:ILE:HG12	2.01	0.60
1:E:128:TYR:O	1:E:129:LEU:HB2	2.01	0.60
1:E:257:ILE:O	1:E:261:ILE:HG12	2.01	0.60
1:D:198:PRO:HG2	1:E:251:MET:HE1	1.84	0.60
1:E:23:LEU:HA	1:E:40:ALA:HB2	1.84	0.60
1:D:274:VAL:C	1:D:276:HIS:H	2.09	0.59
1:A:257:ILE:O	1:A:261:ILE:HG12	2.02	0.59
1:B:18:ASN:HB3	1:B:143:VAL:HG23	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:TYR:O	1:B:129:LEU:HB2	2.01	0.59
1:B:274:VAL:C	1:B:276:HIS:H	2.09	0.59
1:D:131:VAL:HG11	1:D:140:VAL:HG13	1.84	0.59
1:D:24:ILE:HD13	1:D:104:ARG:HE	1.66	0.59
1:D:255:GLY:HA2	1:D:258:ILE:CG2	2.32	0.59
1:C:42:LEU:HB3	1:C:103:GLU:CG	2.32	0.59
1:C:118:TYR:HB3	1:C:119:PRO:HD3	1.83	0.59
1:E:89:VAL:CG1	1:E:102:LEU:HD23	2.32	0.59
1:E:53:PHE:CE1	1:E:95:PRO:HA	2.37	0.59
1:E:286:ARG:O	1:E:289:SER:HB3	2.02	0.59
1:A:202:LEU:HD12	1:B:259:PHE:CE1	2.37	0.59
1:A:271:GLU:HG3	1:A:294:SER:OG	2.03	0.59
1:B:42:LEU:HB3	1:B:103:GLU:CG	2.33	0.59
1:B:208:LEU:O	1:B:211:SER:HB3	2.03	0.59
1:C:222:ALA:HB2	1:D:221:ASP:HA	1.83	0.59
1:E:298:PHE:HB2	1:E:299:PRO:HD3	1.84	0.59
1:C:255:GLY:O	1:C:258:ILE:HG22	2.02	0.59
1:A:104:ARG:CD	1:B:76:ARG:HH11	2.14	0.58
1:B:255:GLY:HA2	1:B:258:ILE:CG2	2.34	0.58
1:E:42:LEU:HB3	1:E:103:GLU:CG	2.32	0.58
1:E:147:LYS:O	1:E:147:LYS:HG2	2.03	0.58
1:A:42:LEU:HB3	1:A:103:GLU:CG	2.33	0.58
1:A:119:PRO:HB3	1:A:196:TYR:HD2	1.69	0.58
1:C:24:ILE:HD13	1:C:104:ARG:HE	1.68	0.58
1:D:271:GLU:HG3	1:D:294:SER:OG	2.02	0.58
1:E:208:LEU:O	1:E:211:SER:HB3	2.03	0.58
1:E:238:ASN:HA	1:E:258:ILE:CD1	2.34	0.58
1:C:147:LYS:HG2	1:C:147:LYS:O	2.03	0.58
1:D:27:TYR:CZ	1:D:37:LYS:HB3	2.39	0.58
1:D:70:ILE:HG22	1:D:71:TRP:O	2.03	0.58
1:A:27:TYR:CE1	1:A:37:LYS:HB3	2.38	0.58
1:E:144:ASP:HA	1:E:147:LYS:HB3	1.86	0.58
1:A:157:THR:HG21	1:B:34:GLU:OE2	2.03	0.58
1:A:274:VAL:C	1:A:276:HIS:H	2.09	0.58
1:E:53:PHE:CD1	1:E:95:PRO:HA	2.39	0.58
1:A:147:LYS:O	1:A:147:LYS:HG2	2.03	0.58
1:B:84:ARG:NH1	1:B:84:ARG:CG	2.55	0.58
1:A:155:PHE:HE1	1:B:112:PRO:HB3	1.61	0.58
1:A:291:THR:O	1:A:295:ARG:HG2	2.04	0.58
1:C:22:TYR:HA	1:C:149:GLY:HA2	1.84	0.58
1:C:62:VAL:HG12	1:C:94:SER:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:LYS:HE2	1:C:165:THR:CA	2.30	0.58
1:E:118:TYR:HB3	1:E:119:PRO:HD3	1.85	0.58
1:A:217:SER:OG	1:B:220:TYR:HE2	1.86	0.58
1:D:53:PHE:CE1	1:D:95:PRO:HA	2.38	0.58
1:A:118:TYR:HB3	1:A:119:PRO:HD3	1.84	0.57
1:D:53:PHE:CD1	1:D:95:PRO:HA	2.39	0.57
1:D:68:GLU:CD	1:D:68:GLU:H	2.10	0.57
1:C:29:LEU:C	1:C:29:LEU:HD23	2.28	0.57
1:A:146:GLU:HG3	1:B:176:GLU:CG	2.35	0.57
1:C:65:TYR:CG	1:C:70:ILE:HD11	2.40	0.57
1:A:267:VAL:CG2	1:A:298:PHE:CZ	2.87	0.57
1:A:286:ARG:O	1:A:289:SER:HB3	2.03	0.57
1:A:29:LEU:C	1:A:29:LEU:HD23	2.29	0.57
1:B:70:ILE:HG22	1:B:71:TRP:O	2.04	0.57
1:E:70:ILE:HG22	1:E:71:TRP:O	2.04	0.57
1:E:255:GLY:HA2	1:E:258:ILE:CG2	2.34	0.57
1:A:53:PHE:HE2	1:A:63:LYS:CB	2.18	0.57
1:A:146:GLU:HG3	1:B:176:GLU:HG2	1.86	0.57
1:A:215:PHE:CZ	1:A:298:PHE:CE1	2.92	0.57
1:A:276:HIS:O	1:A:280:VAL:HG22	2.05	0.57
1:C:53:PHE:CE1	1:C:95:PRO:HA	2.40	0.57
1:E:27:TYR:CZ	1:E:37:LYS:HB3	2.40	0.57
1:B:147:LYS:O	1:B:147:LYS:HG2	2.03	0.57
1:C:256:ALA:HB1	1:C:309:LEU:HD21	1.87	0.57
1:C:267:VAL:CG2	1:C:298:PHE:CZ	2.86	0.57
1:E:139:ILE:HG12	1:E:172:ASN:ND2	2.14	0.57
1:E:267:VAL:CG2	1:E:298:PHE:CZ	2.85	0.57
1:A:212:TRP:HB2	1:A:215:PHE:CE1	2.40	0.57
1:A:147:LYS:HE2	1:A:165:THR:CA	2.27	0.57
1:C:255:GLY:HA2	1:C:258:ILE:HG22	1.86	0.57
1:E:276:HIS:O	1:E:280:VAL:HG22	2.05	0.57
1:A:77:PHE:HB2	1:A:80:VAL:HG21	1.86	0.56
1:B:53:PHE:CE1	1:B:95:PRO:HA	2.40	0.56
1:B:274:VAL:C	1:B:276:HIS:N	2.62	0.56
1:D:147:LYS:O	1:D:147:LYS:HG2	2.03	0.56
1:E:29:LEU:C	1:E:29:LEU:HD23	2.30	0.56
1:A:104:ARG:NH2	1:B:78:VAL:HA	2.19	0.56
1:D:276:HIS:O	1:D:280:VAL:HG22	2.05	0.56
1:A:89:VAL:CG1	1:A:102:LEU:HD23	2.35	0.56
1:A:222:ALA:O	1:B:224:VAL:HG21	2.05	0.56
1:A:274:VAL:C	1:A:276:HIS:N	2.62	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:THR:O	1:B:295:ARG:HG2	2.04	0.56
1:C:27:TYR:CZ	1:C:37:LYS:HB3	2.40	0.56
1:D:291:THR:O	1:D:295:ARG:HG2	2.05	0.56
1:A:104:ARG:HD3	1:B:76:ARG:HH11	1.71	0.56
1:A:215:PHE:CZ	1:A:298:PHE:CD1	2.93	0.56
1:E:53:PHE:HE2	1:E:63:LYS:HB3	1.71	0.56
1:A:208:LEU:O	1:A:211:SER:HB3	2.05	0.56
1:C:155:PHE:HZ	1:D:34:GLU:OE2	1.87	0.56
1:B:298:PHE:HB2	1:B:299:PRO:HD3	1.87	0.56
1:D:42:LEU:HB3	1:D:103:GLU:HG2	1.88	0.56
1:D:53:PHE:HE2	1:D:63:LYS:CB	2.19	0.56
1:D:215:PHE:CZ	1:D:298:PHE:CE1	2.94	0.56
1:C:222:ALA:CB	1:D:221:ASP:HA	2.36	0.56
1:E:147:LYS:HE2	1:E:165:THR:CA	2.33	0.56
1:A:226:LEU:HD12	1:B:228:VAL:HG21	1.86	0.56
1:B:276:HIS:O	1:B:280:VAL:HG22	2.05	0.56
1:D:29:LEU:HD23	1:D:29:LEU:C	2.31	0.56
1:D:54:ASP:HB2	1:D:57:ARG:HG3	1.88	0.56
1:A:27:TYR:CE1	1:B:81:GLU:OE2	2.58	0.56
1:B:144:ASP:HA	1:B:147:LYS:HB3	1.88	0.56
1:C:217:SER:HB2	1:D:220:TYR:HE2	1.71	0.56
1:D:255:GLY:O	1:D:258:ILE:HG22	2.05	0.56
1:E:119:PRO:HB3	1:E:196:TYR:HD2	1.70	0.56
1:E:131:VAL:HG11	1:E:140:VAL:HG13	1.88	0.56
1:E:274:VAL:C	1:E:276:HIS:N	2.62	0.56
1:A:256:ALA:HB1	1:A:309:LEU:HD21	1.88	0.56
1:B:53:PHE:CD1	1:B:95:PRO:HA	2.40	0.56
1:B:256:ALA:HB1	1:B:309:LEU:HD21	1.88	0.56
1:C:276:HIS:O	1:C:280:VAL:HG22	2.05	0.56
1:D:48:ASP:CG	1:D:51:LEU:HD23	2.30	0.56
1:E:22:TYR:HB3	1:E:41:PHE:HB2	1.88	0.56
1:B:9:PRO:HD3	1:B:71:TRP:CD2	2.41	0.55
1:C:53:PHE:HE2	1:C:63:LYS:CB	2.18	0.55
1:D:22:TYR:CG	1:D:149:GLY:HA2	2.41	0.55
1:E:179:LEU:C	1:E:179:LEU:HD12	2.32	0.55
1:D:118:TYR:HB3	1:D:119:PRO:HD3	1.88	0.55
1:A:22:TYR:HB3	1:A:41:PHE:HB2	1.88	0.55
1:A:27:TYR:HB3	1:B:110:LEU:CD2	2.31	0.55
1:B:89:VAL:CG1	1:B:102:LEU:HD23	2.37	0.55
1:B:131:VAL:CG1	1:B:140:VAL:HG13	2.35	0.55
1:B:179:LEU:HD12	1:B:179:LEU:C	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:LEU:O	1:C:211:SER:HB3	2.06	0.55
1:E:53:PHE:HE2	1:E:63:LYS:CB	2.19	0.55
1:C:22:TYR:HB3	1:C:41:PHE:HB2	1.88	0.55
1:C:179:LEU:C	1:C:179:LEU:HD12	2.31	0.55
1:C:286:ARG:O	1:C:289:SER:HB3	2.06	0.55
1:D:212:TRP:HB2	1:D:215:PHE:CE1	2.40	0.55
1:A:62:VAL:HG12	1:A:94:SER:HA	1.88	0.55
1:A:139:ILE:HG12	1:A:172:ASN:ND2	2.15	0.55
1:A:202:LEU:CD1	1:B:259:PHE:CZ	2.90	0.55
1:B:68:GLU:CD	1:B:68:GLU:H	2.15	0.55
1:C:53:PHE:HE2	1:C:63:LYS:HB3	1.71	0.55
1:C:131:VAL:CG1	1:C:140:VAL:HG13	2.37	0.55
1:C:274:VAL:C	1:C:276:HIS:N	2.62	0.55
1:D:298:PHE:HB2	1:D:299:PRO:HD3	1.88	0.55
1:C:42:LEU:O	1:C:102:LEU:HD12	2.06	0.55
1:A:202:LEU:HD12	1:B:259:PHE:CZ	2.42	0.55
1:A:221:ASP:HB3	1:B:221:ASP:OD2	2.07	0.55
1:B:22:TYR:HA	1:B:149:GLY:HA2	1.87	0.55
1:B:53:PHE:HE2	1:B:63:LYS:CB	2.20	0.55
1:C:81:GLU:HG3	1:C:108:ARG:HD3	1.88	0.55
1:D:195:SER:HB3	1:E:248:THR:O	2.07	0.55
1:D:274:VAL:C	1:D:276:HIS:N	2.62	0.55
1:C:202:LEU:HD12	1:D:259:PHE:HE1	1.72	0.55
1:A:131:VAL:CG1	1:A:140:VAL:HG13	2.37	0.55
1:B:255:GLY:O	1:B:258:ILE:HG22	2.07	0.55
1:C:27:TYR:CE1	1:C:37:LYS:HB3	2.41	0.55
1:C:140:VAL:HG22	1:C:181:SER:OG	2.07	0.55
1:D:208:LEU:O	1:D:211:SER:HB3	2.06	0.55
1:D:215:PHE:CZ	1:D:298:PHE:CD1	2.95	0.55
1:D:256:ALA:HB1	1:D:309:LEU:HD21	1.89	0.55
1:A:174:ALA:HA	1:A:179:LEU:HA	1.90	0.54
1:C:215:PHE:CZ	1:C:298:PHE:CE1	2.96	0.54
1:D:42:LEU:O	1:D:102:LEU:HD12	2.06	0.54
1:B:174:ALA:HA	1:B:179:LEU:HA	1.89	0.54
1:C:77:PHE:HB2	1:C:80:VAL:HG21	1.90	0.54
1:C:298:PHE:HB2	1:C:299:PRO:HD3	1.89	0.54
1:A:89:VAL:HG23	1:B:76:ARG:HD3	1.89	0.54
1:C:37:LYS:HE3	1:C:108:ARG:HD2	1.89	0.54
1:C:174:ALA:HA	1:C:179:LEU:HA	1.90	0.54
1:C:212:TRP:HB2	1:C:215:PHE:CE1	2.41	0.54
1:D:179:LEU:HD12	1:D:179:LEU:C	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:PHE:CE1	1:A:95:PRO:HA	2.43	0.54
1:A:179:LEU:C	1:A:179:LEU:HD12	2.31	0.54
1:A:233:ALA:HB1	1:B:235:ILE:CD1	2.37	0.54
1:B:27:TYR:CZ	1:B:37:LYS:HB3	2.42	0.54
1:B:212:TRP:HB2	1:B:215:PHE:CE1	2.43	0.54
1:C:89:VAL:CG2	1:D:76:ARG:HD3	2.38	0.54
1:E:66:GLU:HG3	1:E:67:PRO:HD2	1.90	0.54
1:A:53:PHE:CD1	1:A:95:PRO:HA	2.43	0.54
1:B:215:PHE:CZ	1:B:298:PHE:CD1	2.95	0.54
1:C:53:PHE:CD1	1:C:95:PRO:HA	2.42	0.54
1:D:65:TYR:CG	1:D:70:ILE:HD11	2.43	0.54
1:D:255:GLY:C	1:D:258:ILE:HG22	2.32	0.54
1:E:62:VAL:HG12	1:E:94:SER:HA	1.89	0.54
1:A:53:PHE:HE2	1:A:63:LYS:HB3	1.72	0.54
1:D:131:VAL:CG1	1:D:140:VAL:HG13	2.38	0.54
1:A:22:TYR:HA	1:A:149:GLY:HA2	1.85	0.54
1:B:53:PHE:HE2	1:B:63:LYS:HB3	1.72	0.54
1:B:215:PHE:CZ	1:B:298:PHE:CE1	2.94	0.54
1:C:155:PHE:CZ	1:D:34:GLU:OE2	2.61	0.54
1:D:174:ALA:HA	1:D:179:LEU:HA	1.89	0.54
1:A:68:GLU:H	1:A:68:GLU:CD	2.15	0.54
1:A:255:GLY:CA	1:A:258:ILE:HG22	2.37	0.54
1:E:9:PRO:HD3	1:E:71:TRP:CD2	2.42	0.54
1:A:27:TYR:CB	1:B:110:LEU:CD2	2.86	0.54
1:A:133:SER:HB2	1:A:137:ARG:HH11	1.72	0.54
1:A:194:PHE:CZ	1:B:251:MET:HE2	2.42	0.54
1:C:210:ILE:HG22	1:C:226:LEU:HD11	1.90	0.54
1:B:42:LEU:O	1:B:102:LEU:HD12	2.08	0.54
1:B:147:LYS:HE2	1:B:165:THR:CA	2.34	0.53
1:D:53:PHE:HE2	1:D:63:LYS:HB3	1.73	0.53
1:A:179:LEU:HD12	1:A:179:LEU:O	2.08	0.53
1:B:267:VAL:CG2	1:B:298:PHE:CZ	2.89	0.53
1:C:179:LEU:HD12	1:C:179:LEU:O	2.08	0.53
1:E:54:ASP:HB2	1:E:57:ARG:HG3	1.90	0.53
1:C:70:ILE:HG22	1:C:71:TRP:O	2.09	0.53
1:E:174:ALA:HA	1:E:179:LEU:HA	1.90	0.53
1:E:212:TRP:HB2	1:E:215:PHE:CE1	2.43	0.53
1:A:42:LEU:O	1:A:102:LEU:HD12	2.07	0.53
1:A:70:ILE:HG22	1:A:71:TRP:O	2.08	0.53
1:C:54:ASP:HB2	1:C:57:ARG:HG3	1.90	0.53
1:C:139:ILE:HG12	1:C:172:ASN:ND2	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:LEU:HD12	1:D:179:LEU:O	2.08	0.53
1:E:22:TYR:HA	1:E:149:GLY:HA2	1.86	0.53
1:C:53:PHE:CD1	1:C:53:PHE:O	2.62	0.53
1:C:119:PRO:HB3	1:C:196:TYR:HD2	1.72	0.53
1:B:53:PHE:CD1	1:B:53:PHE:O	2.62	0.53
1:B:179:LEU:HD12	1:B:179:LEU:O	2.08	0.53
1:D:84:ARG:H	1:D:84:ARG:HD3	1.73	0.53
1:A:159:TRP:CE3	1:A:189:ILE:HD12	2.44	0.53
1:B:48:ASP:CG	1:B:51:LEU:HD23	2.34	0.53
1:A:204:MET:HE1	1:A:258:ILE:HA	1.89	0.53
1:A:210:ILE:HG22	1:A:226:LEU:HD11	1.91	0.53
1:B:42:LEU:HB3	1:B:103:GLU:HG2	1.91	0.53
1:E:255:GLY:O	1:E:258:ILE:HG22	2.09	0.53
1:B:137:ARG:HH12	1:B:178:ARG:HA	1.73	0.53
1:D:210:ILE:HG22	1:D:226:LEU:HD11	1.90	0.53
1:E:53:PHE:CD1	1:E:53:PHE:O	2.62	0.53
1:E:77:PHE:HB2	1:E:80:VAL:HG21	1.90	0.53
1:A:53:PHE:HD1	1:A:53:PHE:O	1.92	0.52
1:A:229:SER:HB3	1:B:228:VAL:CG1	2.39	0.52
1:C:25:GLU:HG3	1:D:110:LEU:HD23	1.90	0.52
1:C:53:PHE:O	1:C:53:PHE:HD1	1.93	0.52
1:C:215:PHE:CZ	1:C:298:PHE:CD1	2.97	0.52
1:D:53:PHE:CD1	1:D:53:PHE:O	2.62	0.52
1:B:76:ARG:HH12	1:B:130:ILE:HD11	1.74	0.52
1:C:68:GLU:H	1:C:68:GLU:CD	2.16	0.52
1:D:89:VAL:CG1	1:D:102:LEU:HD23	2.39	0.52
1:A:27:TYR:CG	1:B:110:LEU:CD2	2.91	0.52
1:B:62:VAL:HG12	1:B:94:SER:HA	1.91	0.52
1:B:119:PRO:HB3	1:B:196:TYR:HD2	1.74	0.52
1:C:23:LEU:HA	1:C:40:ALA:HB2	1.89	0.52
1:C:271:GLU:O	1:C:272:VAL:C	2.51	0.52
1:D:18:ASN:HB3	1:D:143:VAL:CG2	2.39	0.52
1:E:68:GLU:CD	1:E:68:GLU:H	2.17	0.52
1:B:53:PHE:O	1:B:53:PHE:HD1	1.92	0.52
1:C:255:GLY:HA2	1:C:258:ILE:CG2	2.39	0.52
1:E:84:ARG:H	1:E:84:ARG:HD3	1.74	0.52
1:E:131:VAL:CG1	1:E:140:VAL:HG13	2.40	0.52
1:A:27:TYR:OH	1:B:81:GLU:HA	2.09	0.52
1:A:53:PHE:CD1	1:A:53:PHE:O	2.62	0.52
1:E:15:LEU:HD11	1:E:46:TRP:HB2	1.92	0.52
1:A:9:PRO:HD3	1:A:71:TRP:CD2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:LEU:HB2	1:B:156:LEU:HD11	1.92	0.52
1:B:255:GLY:C	1:B:258:ILE:HG22	2.34	0.52
1:E:179:LEU:HD12	1:E:179:LEU:O	2.08	0.52
1:A:298:PHE:HB2	1:A:299:PRO:HD3	1.91	0.52
1:B:54:ASP:HB2	1:B:57:ARG:HG3	1.91	0.52
1:D:27:TYR:CE1	1:D:37:LYS:HB3	2.44	0.52
1:D:66:GLU:HG3	1:D:67:PRO:HD2	1.92	0.52
1:E:65:TYR:CG	1:E:70:ILE:HD11	2.45	0.52
1:E:256:ALA:HB1	1:E:309:LEU:HD21	1.92	0.52
1:A:54:ASP:HB2	1:A:57:ARG:HG3	1.91	0.52
1:C:29:LEU:HB2	1:C:156:LEU:HD11	1.91	0.52
1:C:133:SER:HB2	1:C:137:ARG:HH11	1.74	0.52
1:D:15:LEU:HD11	1:D:46:TRP:HB2	1.92	0.52
1:D:216:TRP:CZ2	1:D:295:ARG:HB2	2.45	0.52
1:A:137:ARG:HH12	1:A:178:ARG:HA	1.74	0.51
1:B:66:GLU:HG3	1:B:67:PRO:HD2	1.91	0.51
1:B:204:MET:HE1	1:B:258:ILE:HA	1.92	0.51
1:C:48:ASP:CG	1:C:51:LEU:HD23	2.34	0.51
1:A:66:GLU:HG3	1:A:67:PRO:HD2	1.92	0.51
1:C:255:GLY:C	1:C:258:ILE:HG22	2.35	0.51
1:D:119:PRO:HB3	1:D:196:TYR:HD2	1.75	0.51
1:D:255:GLY:CA	1:D:258:ILE:HG22	2.39	0.51
1:A:65:TYR:CG	1:A:70:ILE:HD11	2.45	0.51
1:A:84:ARG:NH1	1:A:84:ARG:CG	2.52	0.51
1:B:29:LEU:HD23	1:B:29:LEU:C	2.34	0.51
1:E:42:LEU:O	1:E:102:LEU:HD12	2.10	0.51
1:A:48:ASP:CG	1:A:51:LEU:HD23	2.34	0.51
1:B:150:LYS:HG3	1:B:154:VAL:HG21	1.93	0.51
1:C:89:VAL:CG1	1:C:102:LEU:HD23	2.39	0.51
1:D:137:ARG:HH12	1:D:178:ARG:HA	1.74	0.51
1:E:27:TYR:CE1	1:E:37:LYS:HB3	2.45	0.51
1:E:255:GLY:C	1:E:258:ILE:HG22	2.35	0.51
1:A:209:PHE:HB2	1:B:266:PHE:CE1	2.45	0.51
1:A:215:PHE:CE1	1:A:298:PHE:CD1	2.99	0.51
1:B:77:PHE:HB2	1:B:80:VAL:HG21	1.91	0.51
1:C:84:ARG:H	1:C:84:ARG:HD3	1.75	0.51
1:D:62:VAL:HG12	1:D:94:SER:HA	1.91	0.51
1:E:48:ASP:CG	1:E:51:LEU:HD23	2.35	0.51
1:A:27:TYR:CE1	1:B:81:GLU:CD	2.88	0.51
1:A:27:TYR:CD1	1:B:81:GLU:OE2	2.63	0.51
1:B:65:TYR:CG	1:B:70:ILE:HD11	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:PRO:HD3	1:C:71:TRP:CD2	2.46	0.51
1:E:133:SER:HB2	1:E:137:ARG:HH11	1.75	0.51
1:A:150:LYS:HG3	1:A:154:VAL:HG21	1.93	0.51
1:B:118:TYR:HB3	1:B:119:PRO:HD3	1.92	0.51
1:E:81:GLU:HG3	1:E:108:ARG:HD3	1.93	0.51
1:E:140:VAL:HG22	1:E:181:SER:OG	2.11	0.51
1:C:22:TYR:CG	1:C:149:GLY:HA2	2.45	0.51
1:D:150:LYS:HG3	1:D:154:VAL:HG21	1.92	0.51
1:A:18:ASN:HB3	1:A:143:VAL:CG2	2.41	0.51
1:C:170:PRO:HA	1:C:183:LEU:HD23	1.93	0.51
1:D:133:SER:HB2	1:D:137:ARG:HH11	1.75	0.51
1:E:215:PHE:CZ	1:E:298:PHE:CD1	2.99	0.51
1:B:133:SER:HB2	1:B:137:ARG:HH11	1.75	0.51
1:C:42:LEU:HB3	1:C:103:GLU:HG2	1.93	0.51
1:E:53:PHE:O	1:E:53:PHE:HD1	1.93	0.51
1:B:144:ASP:OD1	1:B:144:ASP:N	2.42	0.50
1:C:150:LYS:HG3	1:C:154:VAL:HG21	1.93	0.50
1:D:53:PHE:O	1:D:53:PHE:HD1	1.92	0.50
1:D:77:PHE:HB2	1:D:80:VAL:HG21	1.93	0.50
1:C:237:PHE:HE1	1:D:235:ILE:HD13	1.74	0.50
1:A:140:VAL:HG22	1:A:181:SER:OG	2.10	0.50
1:A:196:TYR:HE1	1:B:247:LYS:HD2	1.76	0.50
1:A:253:TYR:HD1	1:A:313:PHE:CD1	2.29	0.50
1:B:139:ILE:HG12	1:B:172:ASN:ND2	2.21	0.50
1:D:267:VAL:CG2	1:D:298:PHE:CZ	2.87	0.50
1:E:18:ASN:HB3	1:E:143:VAL:CG2	2.42	0.50
1:B:22:TYR:HB3	1:B:41:PHE:HB2	1.92	0.50
1:B:255:GLY:CA	1:B:258:ILE:HG22	2.41	0.50
1:C:27:TYR:HB3	1:D:110:LEU:HD21	1.93	0.50
1:C:144:ASP:HA	1:C:147:LYS:HB3	1.93	0.50
1:C:197:ILE:CB	1:C:198:PRO:HD3	2.38	0.50
1:D:144:ASP:OD1	1:D:144:ASP:N	2.43	0.50
1:A:144:ASP:OD1	1:A:144:ASP:N	2.43	0.50
1:C:66:GLU:HG3	1:C:67:PRO:HD2	1.93	0.50
1:D:204:MET:HE1	1:D:258:ILE:HA	1.93	0.50
1:D:215:PHE:CE1	1:D:298:PHE:CD1	3.00	0.50
1:A:15:LEU:HD11	1:A:46:TRP:HB2	1.93	0.50
1:B:238:ASN:HA	1:B:258:ILE:CD1	2.40	0.50
1:C:18:ASN:HB3	1:C:143:VAL:CG2	2.42	0.50
1:C:194:PHE:CZ	1:D:251:MET:HE2	2.47	0.50
1:E:137:ARG:HH12	1:E:178:ARG:HA	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:150:LYS:HG3	1:E:154:VAL:HG21	1.93	0.50
1:E:210:ILE:HG22	1:E:226:LEU:HD11	1.94	0.50
1:B:84:ARG:H	1:B:84:ARG:HD3	1.77	0.50
1:B:18:ASN:HB3	1:B:143:VAL:CG2	2.42	0.49
1:A:271:GLU:O	1:A:272:VAL:C	2.55	0.49
1:D:139:ILE:HG12	1:D:172:ASN:ND2	2.21	0.49
1:E:29:LEU:HB2	1:E:156:LEU:HD11	1.93	0.49
1:E:175:LEU:CD2	1:E:176:GLU:HG3	2.39	0.49
1:A:216:TRP:CZ2	1:A:295:ARG:HB2	2.48	0.49
1:C:15:LEU:HD11	1:C:46:TRP:HB2	1.93	0.49
1:B:210:ILE:HG22	1:B:226:LEU:HD11	1.94	0.49
1:E:271:GLU:O	1:E:272:VAL:C	2.55	0.49
1:A:24:ILE:CG2	1:B:78:VAL:HG13	2.42	0.49
1:B:78:VAL:CG2	1:B:130:ILE:HG12	2.41	0.49
1:C:210:ILE:HD12	1:D:231:LEU:CD2	2.43	0.49
1:E:216:TRP:CZ2	1:E:295:ARG:HB2	2.47	0.49
1:A:34:GLU:OE2	1:E:155:PHE:HZ	1.95	0.49
1:D:175:LEU:CD2	1:D:176:GLU:HG3	2.39	0.49
1:D:210:ILE:HG12	1:E:266:PHE:CD1	2.47	0.49
1:C:137:ARG:HH12	1:C:178:ARG:HA	1.76	0.49
1:E:202:LEU:HB2	1:E:203:PRO:HD3	1.94	0.49
1:A:196:TYR:CE1	1:B:247:LYS:HD2	2.47	0.49
1:A:314:PHE:CD1	1:A:314:PHE:N	2.80	0.49
1:B:22:TYR:CG	1:B:149:GLY:HA2	2.48	0.49
1:B:271:GLU:O	1:B:272:VAL:C	2.55	0.49
1:B:215:PHE:CE1	1:B:298:PHE:CD1	3.01	0.49
1:E:51:LEU:HD11	1:E:70:ILE:HD12	1.95	0.49
1:A:18:ASN:HB2	1:A:45:SER:HB2	1.94	0.49
1:B:290:ILE:O	1:B:293:ALA:N	2.43	0.49
1:E:204:MET:HE1	1:E:258:ILE:HA	1.95	0.49
1:E:215:PHE:CZ	1:E:298:PHE:CE1	2.97	0.49
1:D:92:SER:HB2	1:D:100:GLN:HB2	1.95	0.48
1:D:144:ASP:HA	1:D:147:LYS:HB3	1.95	0.48
1:A:157:THR:HG22	1:B:34:GLU:OE2	2.13	0.48
1:A:175:LEU:CD2	1:A:176:GLU:HG3	2.39	0.48
1:B:159:TRP:CE3	1:B:189:ILE:HD12	2.49	0.48
1:C:27:TYR:CE1	1:D:81:GLU:OE1	2.66	0.48
1:C:84:ARG:NH1	1:C:84:ARG:CG	2.56	0.48
1:C:149:GLY:O	1:C:164:PHE:CD1	2.62	0.48
1:C:238:ASN:HA	1:C:258:ILE:CD1	2.40	0.48
1:E:47:LYS:HB3	1:E:47:LYS:HE2	1.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:TYR:CG	1:A:149:GLY:HA2	2.48	0.48
1:A:51:LEU:HD11	1:A:70:ILE:HD12	1.94	0.48
1:B:27:TYR:N	1:B:27:TYR:CD2	2.82	0.48
1:B:147:LYS:O	1:B:147:LYS:CG	2.61	0.48
1:C:151:ASN:O	1:C:154:VAL:HG22	2.14	0.48
1:B:237:PHE:O	1:B:238:ASN:C	2.57	0.48
1:D:151:ASN:O	1:D:154:VAL:HG22	2.14	0.48
1:E:202:LEU:O	1:E:203:PRO:C	2.55	0.48
1:A:84:ARG:H	1:A:84:ARG:HD3	1.78	0.48
1:A:206:PHE:HD1	1:B:262:TYR:HB3	1.77	0.48
1:C:51:LEU:HD11	1:C:70:ILE:HD12	1.95	0.48
1:C:314:PHE:CD1	1:C:314:PHE:N	2.80	0.48
1:C:175:LEU:CD2	1:C:176:GLU:HG3	2.39	0.48
1:D:9:PRO:HD3	1:D:71:TRP:CD2	2.49	0.48
1:E:42:LEU:HB3	1:E:103:GLU:HG2	1.94	0.48
1:A:202:LEU:O	1:A:203:PRO:C	2.56	0.48
1:D:159:TRP:CE3	1:D:189:ILE:HD12	2.48	0.48
1:E:151:ASN:O	1:E:154:VAL:HG22	2.14	0.48
1:D:22:TYR:HB3	1:D:41:PHE:HB2	1.96	0.48
1:B:15:LEU:HD11	1:B:46:TRP:HB2	1.94	0.48
1:B:216:TRP:CZ2	1:B:295:ARG:HB2	2.47	0.48
1:C:80:VAL:CG1	1:C:82:ASN:O	2.62	0.48
1:C:204:MET:HE1	1:C:258:ILE:HA	1.95	0.48
1:E:290:ILE:O	1:E:293:ALA:N	2.47	0.48
1:A:42:LEU:HB3	1:A:103:GLU:HG2	1.95	0.48
1:A:225:THR:CG2	1:B:225:THR:HA	2.43	0.48
1:B:27:TYR:CE1	1:B:37:LYS:HB3	2.48	0.48
1:B:215:PHE:HB3	1:B:295:ARG:HB3	1.96	0.48
1:C:147:LYS:O	1:C:147:LYS:CG	2.61	0.48
1:C:202:LEU:O	1:C:203:PRO:C	2.55	0.48
1:D:228:VAL:HG12	1:D:229:SER:N	2.27	0.48
1:E:147:LYS:O	1:E:147:LYS:CG	2.61	0.48
1:E:255:GLY:CA	1:E:258:ILE:HG22	2.42	0.48
1:A:224:VAL:HG23	1:A:225:THR:N	2.29	0.47
1:C:222:ALA:HB2	1:D:221:ASP:CG	2.39	0.47
1:D:147:LYS:O	1:D:147:LYS:CG	2.61	0.47
1:D:166:ALA:HB2	1:D:185:TYR:CD2	2.49	0.47
1:D:238:ASN:HA	1:D:258:ILE:CD1	2.43	0.47
1:D:76:ARG:O	1:D:129:LEU:HA	2.14	0.47
1:E:27:TYR:N	1:E:27:TYR:CD2	2.82	0.47
1:E:253:TYR:HD1	1:E:313:PHE:CD1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:VAL:HG12	1:A:94:SER:O	2.14	0.47
1:A:144:ASP:HA	1:A:147:LYS:HB3	1.97	0.47
1:B:296:ILE:HD13	1:B:296:ILE:HA	1.80	0.47
1:D:54:ASP:HB2	1:D:57:ARG:CG	2.44	0.47
1:E:76:ARG:HH12	1:E:130:ILE:HD11	1.79	0.47
1:A:147:LYS:O	1:A:147:LYS:CG	2.61	0.47
1:C:253:TYR:HD1	1:C:313:PHE:CD1	2.32	0.47
1:E:166:ALA:HB2	1:E:185:TYR:CD2	2.50	0.47
1:A:7:PRO:O	1:A:71:TRP:HB2	2.15	0.47
1:A:151:ASN:O	1:A:154:VAL:HG22	2.14	0.47
1:C:54:ASP:HB2	1:C:57:ARG:CG	2.45	0.47
1:A:194:PHE:HZ	1:B:251:MET:HE2	1.80	0.47
1:B:80:VAL:CG1	1:B:82:ASN:O	2.62	0.47
1:C:65:TYR:CD2	1:C:70:ILE:HD11	2.50	0.47
1:C:215:PHE:CE1	1:C:298:PHE:CD1	3.02	0.47
1:D:61:ARG:O	1:D:95:PRO:HG3	2.15	0.47
1:E:159:TRP:CE3	1:E:189:ILE:HD12	2.49	0.47
1:E:261:ILE:HD13	1:E:302:PHE:HE1	1.80	0.47
1:B:151:ASN:O	1:B:154:VAL:HG22	2.14	0.47
1:B:166:ALA:HB2	1:B:185:TYR:CD2	2.50	0.47
1:B:200:ILE:O	1:B:204:MET:HB2	2.14	0.47
1:C:18:ASN:HB2	1:C:45:SER:HB2	1.97	0.47
1:C:44:LEU:HD12	1:C:101:TYR:CD2	2.50	0.47
1:D:140:VAL:HG22	1:D:181:SER:OG	2.15	0.47
1:E:76:ARG:O	1:E:129:LEU:HA	2.15	0.47
1:A:206:PHE:CD1	1:B:262:TYR:HB3	2.49	0.47
1:A:283:GLN:N	1:A:284:PRO:CD	2.77	0.47
1:E:215:PHE:CE1	1:E:298:PHE:CD1	3.03	0.47
1:A:44:LEU:HD12	1:A:101:TYR:CD2	2.50	0.46
1:A:166:ALA:HB2	1:A:185:TYR:CD2	2.50	0.46
1:A:225:THR:HG21	1:B:225:THR:HA	1.96	0.46
1:D:40:ALA:HB3	1:D:105:PHE:CE1	2.51	0.46
1:A:149:GLY:O	1:A:164:PHE:CD1	2.63	0.46
1:C:215:PHE:HB3	1:C:295:ARG:HB3	1.96	0.46
1:D:253:TYR:HD1	1:D:313:PHE:CD1	2.33	0.46
1:E:53:PHE:CE2	1:E:63:LYS:HB3	2.50	0.46
1:A:253:TYR:HA	1:A:313:PHE:CZ	2.50	0.46
1:B:76:ARG:O	1:B:129:LEU:HA	2.16	0.46
1:C:261:ILE:HD13	1:C:302:PHE:HE1	1.78	0.46
1:D:47:LYS:HE2	1:D:47:LYS:HB3	1.61	0.46
1:E:149:GLY:O	1:E:164:PHE:CD1	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:SER:OG	1:B:82:ASN:HA	2.15	0.46
1:A:217:SER:HB2	1:B:220:TYR:OH	2.16	0.46
1:A:229:SER:HB3	1:B:228:VAL:HG13	1.97	0.46
1:C:78:VAL:CG2	1:C:130:ILE:HG12	2.45	0.46
1:A:27:TYR:CD2	1:A:27:TYR:N	2.83	0.46
1:A:81:GLU:HG3	1:A:108:ARG:HD3	1.98	0.46
1:A:170:PRO:HA	1:A:183:LEU:HD23	1.96	0.46
1:C:53:PHE:CE2	1:C:63:LYS:HB3	2.51	0.46
1:C:216:TRP:CZ2	1:C:295:ARG:HB2	2.50	0.46
1:D:193:TYR:O	1:D:194:PHE:C	2.59	0.46
1:D:215:PHE:HB3	1:D:295:ARG:HB3	1.98	0.46
1:E:267:VAL:HG23	1:E:298:PHE:HZ	1.72	0.46
1:B:228:VAL:HG12	1:B:229:SER:N	2.30	0.46
1:D:271:GLU:O	1:D:272:VAL:C	2.58	0.46
1:A:25:GLU:HG2	1:B:79:ASN:HA	1.98	0.46
1:A:47:LYS:HB3	1:A:47:LYS:HE2	1.66	0.46
1:C:144:ASP:OD1	1:C:144:ASP:N	2.45	0.46
1:E:98:THR:O	1:E:98:THR:HG22	2.14	0.46
1:B:93:VAL:HG12	1:B:94:SER:O	2.16	0.46
1:A:110:LEU:HD23	1:E:25:GLU:HG3	1.98	0.46
1:E:228:VAL:HG12	1:E:229:SER:N	2.29	0.46
1:B:202:LEU:O	1:B:203:PRO:C	2.55	0.46
1:B:280:VAL:C	1:B:282:SER:H	2.24	0.46
1:C:27:TYR:CD1	1:D:81:GLU:OE2	2.68	0.46
1:C:224:VAL:HG23	1:C:225:THR:N	2.31	0.46
1:C:234:HIS:CD2	1:C:261:ILE:HG21	2.51	0.46
1:D:80:VAL:CG1	1:D:82:ASN:O	2.62	0.46
1:D:229:SER:CB	1:E:228:VAL:CG1	2.94	0.46
1:C:280:VAL:C	1:C:282:SER:H	2.25	0.45
1:D:68:GLU:CD	1:D:68:GLU:N	2.74	0.45
1:D:261:ILE:HD13	1:D:302:PHE:HE1	1.80	0.45
1:E:54:ASP:HB2	1:E:57:ARG:CG	2.47	0.45
1:A:29:LEU:HB2	1:A:156:LEU:HD11	1.98	0.45
1:B:261:ILE:HD13	1:B:302:PHE:HE1	1.81	0.45
1:D:290:ILE:O	1:D:293:ALA:N	2.50	0.45
1:E:44:LEU:HD12	1:E:101:TYR:CD2	2.51	0.45
1:E:304:LEU:O	1:E:308:ILE:HG12	2.16	0.45
1:A:78:VAL:CG2	1:A:130:ILE:HG12	2.46	0.45
1:B:8:PRO:HA	1:B:71:TRP:CD1	2.51	0.45
1:B:81:GLU:HG3	1:B:108:ARG:HD3	1.97	0.45
1:D:27:TYR:N	1:D:27:TYR:CD2	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:ARG:HH12	1:D:130:ILE:HD11	1.81	0.45
1:D:93:VAL:HG12	1:D:94:SER:O	2.17	0.45
1:E:93:VAL:HG12	1:E:94:SER:O	2.16	0.45
1:A:80:VAL:CG1	1:A:82:ASN:O	2.62	0.45
1:B:54:ASP:HB2	1:B:57:ARG:CG	2.46	0.45
1:C:255:GLY:CA	1:C:258:ILE:HG22	2.46	0.45
1:D:147:LYS:HE2	1:D:165:THR:CA	2.37	0.45
1:D:280:VAL:C	1:D:282:SER:H	2.25	0.45
1:A:8:PRO:HA	1:A:71:TRP:CG	2.52	0.45
1:A:280:VAL:C	1:A:282:SER:H	2.25	0.45
1:D:81:GLU:HG3	1:D:108:ARG:HD3	1.98	0.45
1:D:253:TYR:O	1:D:256:ALA:HB3	2.17	0.45
1:E:314:PHE:CD1	1:E:314:PHE:N	2.84	0.45
1:C:240:LEU:HD22	1:D:239:ILE:HG12	1.98	0.45
1:D:222:ALA:CB	1:E:220:TYR:CD2	3.00	0.45
1:D:296:ILE:HD13	1:D:296:ILE:HA	1.80	0.45
1:A:34:GLU:OE2	1:E:155:PHE:CZ	2.69	0.45
1:B:140:VAL:HG22	1:B:181:SER:OG	2.16	0.45
1:D:261:ILE:O	1:D:262:TYR:C	2.60	0.45
1:D:304:LEU:O	1:D:308:ILE:HG12	2.16	0.45
1:A:53:PHE:CE2	1:A:63:LYS:HB3	2.51	0.45
1:A:261:ILE:HD13	1:A:302:PHE:HE1	1.81	0.45
1:B:314:PHE:N	1:B:314:PHE:CD1	2.84	0.45
1:C:93:VAL:HG12	1:C:94:SER:O	2.17	0.45
1:C:296:ILE:HD13	1:C:296:ILE:HA	1.81	0.45
1:D:149:GLY:O	1:D:164:PHE:CD1	2.66	0.45
1:D:202:LEU:O	1:D:203:PRO:C	2.60	0.45
1:E:80:VAL:CG1	1:E:82:ASN:O	2.62	0.45
1:E:309:LEU:O	1:E:310:ALA:C	2.60	0.45
1:B:51:LEU:HD11	1:B:70:ILE:HD12	1.98	0.44
1:C:92:SER:HB2	1:C:100:GLN:HB2	1.99	0.44
1:C:200:ILE:O	1:C:204:MET:HB2	2.17	0.44
1:D:229:SER:HB3	1:E:228:VAL:CG1	2.46	0.44
1:D:309:LEU:HD12	1:D:309:LEU:HA	1.78	0.44
1:B:120:PHE:HB2	1:B:314:PHE:CE2	2.52	0.44
1:B:175:LEU:CD2	1:B:176:GLU:HG3	2.39	0.44
1:C:76:ARG:HH12	1:C:130:ILE:HD11	1.82	0.44
1:D:283:GLN:N	1:D:284:PRO:CD	2.79	0.44
1:E:200:ILE:O	1:E:204:MET:HB2	2.17	0.44
1:E:280:VAL:C	1:E:282:SER:H	2.25	0.44
1:C:196:TYR:CE1	1:D:247:LYS:HE3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:THR:HB	1:D:188:ARG:NE	2.33	0.44
1:D:206:PHE:CE1	1:E:263:LEU:CD1	3.00	0.44
1:A:76:ARG:HH12	1:A:130:ILE:HD11	1.82	0.44
1:A:224:VAL:O	1:A:225:THR:C	2.59	0.44
1:C:196:TYR:HE1	1:D:247:LYS:CD	2.30	0.44
1:C:217:SER:CB	1:D:220:TYR:HE2	2.29	0.44
1:D:202:LEU:HB2	1:D:203:PRO:HD3	1.99	0.44
1:E:215:PHE:HB3	1:E:295:ARG:HB3	1.98	0.44
1:A:202:LEU:CD1	1:B:259:PHE:CE1	3.01	0.44
1:A:202:LEU:HD13	1:B:259:PHE:HZ	1.83	0.44
1:A:228:VAL:HG12	1:A:229:SER:N	2.31	0.44
1:B:53:PHE:CE2	1:B:63:LYS:HB3	2.51	0.44
1:C:76:ARG:O	1:C:129:LEU:HA	2.17	0.44
1:D:309:LEU:O	1:D:310:ALA:C	2.60	0.44
1:A:54:ASP:HB2	1:A:57:ARG:CG	2.47	0.44
1:A:206:PHE:CE1	1:B:263:LEU:CD1	3.00	0.44
1:B:283:GLN:N	1:B:284:PRO:CD	2.81	0.44
1:D:51:LEU:HD11	1:D:70:ILE:HD12	1.99	0.44
1:E:42:LEU:HB3	1:E:103:GLU:HG3	2.00	0.44
1:A:77:PHE:CB	1:A:80:VAL:HG21	2.47	0.44
1:A:200:ILE:O	1:A:204:MET:HB2	2.17	0.44
1:B:253:TYR:HD1	1:B:313:PHE:CD1	2.35	0.44
1:A:124:THR:HB	1:A:188:ARG:NE	2.33	0.44
1:C:159:TRP:CE3	1:C:189:ILE:HD12	2.53	0.44
1:D:120:PHE:HB2	1:D:314:PHE:CE2	2.53	0.44
1:A:11:ALA:HB3	1:A:136:THR:CG2	2.48	0.44
1:C:166:ALA:HB2	1:C:185:TYR:CD2	2.53	0.44
1:D:314:PHE:CD1	1:D:314:PHE:N	2.85	0.44
1:A:120:PHE:HB2	1:A:314:PHE:CE2	2.53	0.43
1:B:47:LYS:HB3	1:B:47:LYS:HE2	1.64	0.43
1:C:202:LEU:CD1	1:D:259:PHE:CE1	3.01	0.43
1:D:11:ALA:HB3	1:D:136:THR:CG2	2.48	0.43
1:A:27:TYR:CZ	1:B:81:GLU:HA	2.53	0.43
1:B:215:PHE:HZ	1:B:298:PHE:CD1	2.36	0.43
1:C:213:THR:OG1	1:C:226:LEU:HD21	2.18	0.43
1:C:226:LEU:CD1	1:D:228:VAL:HG21	2.48	0.43
1:C:228:VAL:HG12	1:C:229:SER:N	2.33	0.43
1:D:210:ILE:HG12	1:E:266:PHE:CE1	2.53	0.43
1:D:104:ARG:CD	1:E:76:ARG:NH1	2.82	0.43
1:D:210:ILE:CG1	1:E:266:PHE:CD1	3.01	0.43
1:E:78:VAL:CG2	1:E:130:ILE:HG12	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:197:ILE:CB	1:E:198:PRO:HD3	2.41	0.43
1:A:202:LEU:HB2	1:A:203:PRO:HD3	2.00	0.43
1:C:283:GLN:N	1:C:284:PRO:CD	2.80	0.43
1:D:53:PHE:CE2	1:D:63:LYS:HB3	2.52	0.43
1:A:219:SER:OG	1:A:222:ALA:HB3	2.19	0.43
1:B:197:ILE:CB	1:B:198:PRO:HD3	2.45	0.43
1:C:40:ALA:HB3	1:C:105:PHE:CE1	2.53	0.43
1:D:237:PHE:O	1:D:238:ASN:C	2.59	0.43
1:E:253:TYR:HA	1:E:313:PHE:CZ	2.54	0.43
1:B:224:VAL:O	1:B:225:THR:C	2.60	0.43
1:D:156:LEU:HD12	1:D:156:LEU:HA	1.78	0.43
1:A:205:LEU:O	1:A:208:LEU:HB3	2.19	0.43
1:A:314:PHE:HD1	1:A:314:PHE:H	1.67	0.43
1:B:18:ASN:HB2	1:B:45:SER:HB2	2.00	0.43
1:C:47:LYS:HE2	1:C:47:LYS:HB3	1.62	0.43
1:C:155:PHE:CE1	1:D:112:PRO:HB3	2.53	0.43
1:C:175:LEU:HA	1:C:175:LEU:HD23	1.80	0.43
1:E:124:THR:HB	1:E:188:ARG:NE	2.33	0.43
1:E:204:MET:O	1:E:207:ILE:HG12	2.18	0.43
1:A:215:PHE:HB3	1:A:295:ARG:HB3	1.99	0.43
1:A:253:TYR:O	1:A:256:ALA:HB3	2.19	0.43
1:D:155:PHE:HE1	1:E:112:PRO:HB3	1.73	0.43
1:A:76:ARG:O	1:A:129:LEU:HA	2.18	0.43
1:B:210:ILE:HG12	1:C:266:PHE:CE1	2.54	0.43
1:A:155:PHE:CD1	1:B:112:PRO:HB3	2.43	0.43
1:A:194:PHE:HZ	1:B:251:MET:HB2	1.82	0.43
1:B:202:LEU:HB2	1:B:203:PRO:HD3	2.00	0.43
1:C:271:GLU:OE2	1:C:272:VAL:N	2.52	0.43
1:E:8:PRO:HA	1:E:71:TRP:CG	2.54	0.43
1:E:65:TYR:CD2	1:E:70:ILE:HD11	2.54	0.43
1:A:209:PHE:HB2	1:B:266:PHE:HE1	1.83	0.42
1:B:123:GLN:NE2	1:B:123:GLN:HA	2.34	0.42
1:C:237:PHE:CZ	1:D:235:ILE:HG23	2.53	0.42
1:E:9:PRO:HB3	1:E:48:ASP:CG	2.43	0.42
1:A:202:LEU:HD13	1:B:259:PHE:CZ	2.54	0.42
1:B:309:LEU:O	1:B:310:ALA:C	2.62	0.42
1:C:27:TYR:CD2	1:C:27:TYR:N	2.87	0.42
1:C:267:VAL:HG23	1:C:298:PHE:HZ	1.76	0.42
1:D:44:LEU:HD12	1:D:101:TYR:CD2	2.54	0.42
1:A:42:LEU:HB3	1:A:103:GLU:HG3	2.02	0.42
1:A:65:TYR:CD2	1:A:70:ILE:HD11	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ARG:HA	1:A:137:ARG:HD3	1.70	0.42
1:B:290:ILE:O	1:B:291:THR:C	2.62	0.42
1:D:8:PRO:HA	1:D:71:TRP:CD1	2.54	0.42
1:D:290:ILE:O	1:D:291:THR:C	2.62	0.42
1:D:293:ALA:O	1:D:294:SER:C	2.62	0.42
1:E:124:THR:HB	1:E:188:ARG:HE	1.84	0.42
1:E:213:THR:C	1:E:215:PHE:H	2.26	0.42
1:A:210:ILE:O	1:A:211:SER:C	2.63	0.42
1:B:124:THR:HB	1:B:188:ARG:NE	2.35	0.42
1:D:77:PHE:CB	1:D:80:VAL:HG21	2.49	0.42
1:D:269:VAL:O	1:D:270:ILE:C	2.63	0.42
1:A:290:ILE:O	1:A:293:ALA:N	2.51	0.42
1:B:8:PRO:HA	1:B:71:TRP:CG	2.54	0.42
1:C:11:ALA:HB3	1:C:136:THR:CG2	2.48	0.42
1:C:253:TYR:O	1:C:256:ALA:HB3	2.19	0.42
1:C:269:VAL:O	1:C:270:ILE:C	2.61	0.42
1:C:309:LEU:HD12	1:C:309:LEU:HA	1.82	0.42
1:E:251:MET:HE2	1:E:251:MET:HB2	1.87	0.42
1:E:283:GLN:N	1:E:284:PRO:CD	2.80	0.42
1:D:253:TYR:HA	1:D:313:PHE:CZ	2.55	0.42
1:A:210:ILE:HG23	1:B:269:VAL:HG11	2.00	0.42
1:A:238:ASN:HA	1:A:258:ILE:CD1	2.45	0.42
1:A:271:GLU:OE2	1:A:272:VAL:N	2.53	0.42
1:A:309:LEU:HD12	1:A:309:LEU:HA	1.83	0.42
1:B:40:ALA:HB3	1:B:105:PHE:CE1	2.54	0.42
1:C:77:PHE:CB	1:C:80:VAL:HG21	2.49	0.42
1:C:219:SER:OG	1:C:222:ALA:HB3	2.20	0.42
1:C:314:PHE:HD1	1:C:314:PHE:H	1.67	0.42
1:E:224:VAL:HG23	1:E:225:THR:N	2.35	0.42
1:A:59:GLY:C	1:A:60:VAL:CG1	2.93	0.42
1:B:210:ILE:O	1:B:211:SER:C	2.62	0.42
1:C:253:TYR:HA	1:C:313:PHE:CZ	2.55	0.42
1:D:27:TYR:HB3	1:E:110:LEU:HD21	2.00	0.42
1:D:213:THR:OG1	1:D:226:LEU:HD21	2.20	0.42
1:D:271:GLU:OE2	1:D:272:VAL:N	2.52	0.42
1:E:296:ILE:HD13	1:E:296:ILE:HA	1.82	0.42
1:C:120:PHE:HB2	1:C:314:PHE:CE2	2.55	0.42
1:D:59:GLY:C	1:D:60:VAL:CG1	2.93	0.42
1:D:155:PHE:C	1:D:155:PHE:CD2	2.98	0.42
1:B:149:GLY:O	1:B:164:PHE:CD1	2.66	0.42
1:C:251:MET:HE2	1:C:251:MET:HB2	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:ILE:O	1:D:211:SER:C	2.63	0.42
1:E:120:PHE:HB2	1:E:314:PHE:CE2	2.55	0.42
1:E:309:LEU:HD12	1:E:309:LEU:HA	1.83	0.42
1:A:8:PRO:HA	1:A:71:TRP:CD1	2.55	0.41
1:B:11:ALA:HB3	1:B:136:THR:CG2	2.48	0.41
1:B:253:TYR:O	1:B:256:ALA:HB3	2.19	0.41
1:C:91:ILE:HA	1:C:100:GLN:O	2.19	0.41
1:E:11:ALA:HB3	1:E:136:THR:CG2	2.48	0.41
1:E:290:ILE:O	1:E:291:THR:C	2.62	0.41
1:A:53:PHE:HE2	1:A:63:LYS:HB2	1.85	0.41
1:A:196:TYR:N	1:A:196:TYR:CD1	2.88	0.41
1:B:9:PRO:HB3	1:B:48:ASP:CG	2.45	0.41
1:B:179:LEU:C	1:B:179:LEU:CD1	2.93	0.41
1:C:9:PRO:HB3	1:C:48:ASP:CG	2.44	0.41
1:C:183:LEU:HD23	1:C:183:LEU:HA	1.87	0.41
1:C:202:LEU:HB2	1:C:203:PRO:HD3	2.02	0.41
1:E:40:ALA:HB3	1:E:105:PHE:CE1	2.56	0.41
1:E:59:GLY:C	1:E:60:VAL:CG1	2.93	0.41
1:E:205:LEU:O	1:E:208:LEU:HB3	2.21	0.41
1:B:205:LEU:O	1:B:208:LEU:HB3	2.20	0.41
1:C:225:THR:HG21	1:D:225:THR:OG1	2.21	0.41
1:C:264:PHE:CE2	1:C:302:PHE:HB2	2.55	0.41
1:C:290:ILE:O	1:C:293:ALA:N	2.53	0.41
1:D:124:THR:HB	1:D:188:ARG:HE	1.85	0.41
1:E:18:ASN:HB2	1:E:45:SER:HB2	2.02	0.41
1:E:144:ASP:OD1	1:E:144:ASP:N	2.47	0.41
1:A:124:THR:HB	1:A:188:ARG:HE	1.84	0.41
1:A:155:PHE:C	1:A:155:PHE:CD2	2.98	0.41
1:B:34:GLU:OE1	1:B:113:LEU:N	2.51	0.41
1:B:65:TYR:CD2	1:B:70:ILE:HD11	2.55	0.41
1:B:269:VAL:O	1:B:270:ILE:C	2.62	0.41
1:B:271:GLU:OE2	1:B:272:VAL:N	2.54	0.41
1:B:293:ALA:O	1:B:294:SER:C	2.63	0.41
1:C:89:VAL:HG23	1:D:76:ARG:HD3	2.01	0.41
1:D:8:PRO:HA	1:D:71:TRP:CG	2.55	0.41
1:D:274:VAL:O	1:D:276:HIS:N	2.54	0.41
1:E:155:PHE:C	1:E:155:PHE:CD2	2.98	0.41
1:E:260:MET:CE	1:E:309:LEU:HD22	2.39	0.41
1:E:274:VAL:O	1:E:276:HIS:N	2.54	0.41
1:A:19:THR:HA	1:A:43:SER:O	2.21	0.41
1:B:59:GLY:C	1:B:60:VAL:CG1	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:ARG:O	1:C:118:TYR:C	2.64	0.41
1:C:242:GLU:O	1:C:242:GLU:HG2	2.21	0.41
1:C:274:VAL:O	1:C:276:HIS:N	2.54	0.41
1:D:29:LEU:HB2	1:D:156:LEU:HD11	2.02	0.41
1:D:200:ILE:O	1:D:204:MET:HB2	2.19	0.41
1:D:264:PHE:CE2	1:D:302:PHE:HB2	2.56	0.41
1:E:179:LEU:C	1:E:179:LEU:CD1	2.94	0.41
1:B:92:SER:HB2	1:B:100:GLN:HB2	2.03	0.41
1:B:150:LYS:CG	1:B:154:VAL:HG21	2.51	0.41
1:C:27:TYR:HB3	1:D:110:LEU:CD2	2.50	0.41
1:C:46:TRP:CH2	1:C:72:ILE:HG23	2.56	0.41
1:C:59:GLY:C	1:C:60:VAL:CG1	2.93	0.41
1:D:241:VAL:C	1:D:243:THR:H	2.27	0.41
1:E:150:LYS:CG	1:E:154:VAL:HG21	2.51	0.41
1:A:9:PRO:HB3	1:A:48:ASP:CG	2.45	0.41
1:A:242:GLU:O	1:A:242:GLU:HG2	2.21	0.41
1:A:242:GLU:OE2	1:E:199:ASN:HB3	2.20	0.41
1:C:155:PHE:C	1:C:155:PHE:CD2	2.98	0.41
1:D:123:GLN:NE2	1:D:123:GLN:HA	2.35	0.41
1:D:224:VAL:HG23	1:D:225:THR:N	2.36	0.41
1:B:224:VAL:C	1:B:226:LEU:N	2.78	0.41
1:C:158:GLY:HA2	1:C:192:GLN:NE2	2.36	0.41
1:C:290:ILE:O	1:C:291:THR:C	2.63	0.41
1:D:179:LEU:C	1:D:179:LEU:CD1	2.93	0.41
1:E:213:THR:OG1	1:E:226:LEU:HD21	2.21	0.41
1:A:68:GLU:CD	1:A:68:GLU:N	2.79	0.41
1:A:91:ILE:HA	1:A:100:GLN:O	2.20	0.41
1:A:150:LYS:CG	1:A:154:VAL:HG21	2.51	0.41
1:A:224:VAL:CG2	1:A:225:THR:N	2.83	0.41
1:A:274:VAL:O	1:A:276:HIS:N	2.53	0.41
1:B:155:PHE:C	1:B:155:PHE:CD2	2.98	0.41
1:D:7:PRO:O	1:D:71:TRP:HB2	2.21	0.41
1:D:39:ASN:HD21	1:D:104:ARG:NH2	2.18	0.41
1:D:242:GLU:O	1:D:242:GLU:HG2	2.21	0.41
1:E:210:ILE:O	1:E:211:SER:C	2.64	0.41
1:A:92:SER:HB2	1:A:100:GLN:HB2	2.01	0.41
1:B:175:LEU:HD23	1:B:175:LEU:HA	1.80	0.41
1:B:241:VAL:C	1:B:243:THR:H	2.29	0.41
1:B:304:LEU:O	1:B:308:ILE:HG12	2.21	0.41
1:E:216:TRP:CE2	1:E:295:ARG:HD3	2.56	0.41
1:A:110:LEU:HD12	1:A:110:LEU:C	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:PHE:HE1	1:B:112:PRO:CB	2.24	0.40
1:B:7:PRO:O	1:B:71:TRP:HB2	2.21	0.40
1:C:202:LEU:CD1	1:D:259:PHE:HE1	2.33	0.40
1:E:293:ALA:O	1:E:294:SER:C	2.64	0.40
1:A:22:TYR:C	1:A:40:ALA:HB1	2.47	0.40
1:B:204:MET:O	1:B:207:ILE:HG12	2.22	0.40
1:C:19:THR:HA	1:C:43:SER:O	2.22	0.40
1:C:150:LYS:CG	1:C:154:VAL:HG21	2.51	0.40
1:C:217:SER:CB	1:D:220:TYR:CE2	3.00	0.40
1:C:220:TYR:HE1	1:C:273:THR:HA	1.86	0.40
1:C:224:VAL:O	1:C:225:THR:C	2.63	0.40
1:D:53:PHE:HE2	1:D:63:LYS:HB2	1.85	0.40
1:D:137:ARG:HD3	1:D:137:ARG:HA	1.73	0.40
1:D:215:PHE:O	1:D:291:THR:HG22	2.22	0.40
1:E:183:LEU:HD23	1:E:183:LEU:HA	1.76	0.40
1:E:224:VAL:O	1:E:225:THR:C	2.62	0.40
1:A:193:TYR:O	1:A:194:PHE:C	2.65	0.40
1:B:216:TRP:CE2	1:B:295:ARG:HD3	2.56	0.40
1:C:179:LEU:C	1:C:179:LEU:CD1	2.93	0.40
1:C:213:THR:C	1:C:215:PHE:H	2.27	0.40
1:D:65:TYR:CD2	1:D:70:ILE:HD11	2.56	0.40
1:D:110:LEU:HD12	1:D:110:LEU:C	2.45	0.40
1:E:7:PRO:O	1:E:71:TRP:HB2	2.22	0.40
1:B:120:PHE:HB2	1:B:314:PHE:CZ	2.57	0.40
1:B:253:TYR:HA	1:B:313:PHE:CZ	2.56	0.40
1:B:274:VAL:O	1:B:276:HIS:N	2.54	0.40
1:C:124:THR:HB	1:C:188:ARG:NE	2.36	0.40
1:C:195:SER:OG	1:D:247:LYS:HB3	2.21	0.40
1:C:205:LEU:O	1:C:208:LEU:HB3	2.20	0.40
1:C:210:ILE:CD1	1:D:231:LEU:HD22	2.52	0.40
1:D:150:LYS:CG	1:D:154:VAL:HG21	2.51	0.40
1:E:77:PHE:CB	1:E:80:VAL:HG21	2.52	0.40
1:E:242:GLU:HG2	1:E:242:GLU:O	2.21	0.40
1:A:72:ILE:CG2	1:A:73:PRO:HD2	2.51	0.40
1:A:296:ILE:HD13	1:A:296:ILE:HA	1.81	0.40
1:B:68:GLU:CD	1:B:68:GLU:N	2.78	0.40
1:B:251:MET:HE2	1:B:251:MET:HB2	1.92	0.40
1:B:282:SER:C	1:B:284:PRO:HD3	2.47	0.40
1:C:57:ARG:H	1:C:57:ARG:HG2	1.69	0.40
1:E:271:GLU:OE2	1:E:272:VAL:N	2.54	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%)	245 (80%)	57 (18%)	6 (2%)	6	33
1	B	308/317 (97%)	246 (80%)	55 (18%)	7 (2%)	5	29
1	C	308/317 (97%)	242 (79%)	60 (20%)	6 (2%)	6	33
1	D	308/317 (97%)	247 (80%)	54 (18%)	7 (2%)	5	29
1	E	308/317 (97%)	245 (80%)	55 (18%)	8 (3%)	4	26
All	All	1540/1585 (97%)	1225 (80%)	281 (18%)	34 (2%)	5	29

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	TYR
1	B	118	TYR
1	C	118	TYR
1	D	118	TYR
1	E	118	TYR
1	A	150	LYS
1	A	275	GLN
1	B	150	LYS
1	B	275	GLN
1	C	150	LYS
1	C	275	GLN
1	D	150	LYS
1	D	275	GLN
1	E	150	LYS
1	E	275	GLN
1	A	148	VAL
1	B	148	VAL
1	C	148	VAL
1	D	148	VAL
1	E	148	VAL
1	A	10	ILE

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Mol	Chain	Res	Type
1	B	10	ILE
1	B	290	ILE
1	C	10	ILE
1	D	10	ILE
1	E	10	ILE
1	A	60	VAL
1	B	60	VAL
1	C	60	VAL
1	D	60	VAL
1	E	60	VAL
1	E	290	ILE
1	E	13	GLU
1	D	290	ILE

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%)	232 (84%)	46 (16%)	2	12
1	B	278/284 (98%)	234 (84%)	44 (16%)	2	13
1	C	278/284 (98%)	235 (84%)	43 (16%)	2	14
1	D	278/284 (98%)	233 (84%)	45 (16%)	2	12
1	E	278/284 (98%)	234 (84%)	44 (16%)	2	13
All	All	1390/1420 (98%)	1168 (84%)	222 (16%)	2	13

All (222) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	16	THR
1	A	25	GLU
1	A	26	CYS
1	A	32	LYS
1	A	47	LYS

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Mol	Chain	Res	Type
1	A	53	PHE
1	A	54	ASP
1	A	57	ARG
1	A	60	VAL
1	A	68	GLU
1	A	82	ASN
1	A	84	ARG
1	A	89	VAL
1	A	94	SER
1	A	98	THR
1	A	99	VAL
1	A	106	SER
1	A	110	LEU
1	A	122	SER
1	A	124	THR
1	A	130	ILE
1	A	136	THR
1	A	141	LEU
1	A	144	ASP
1	A	154	VAL
1	A	162	GLU
1	A	175	LEU
1	A	179	LEU
1	A	188	ARG
1	A	191	ARG
1	A	211	SER
1	A	228	VAL
1	A	244	ASN
1	A	245	LEU
1	A	252	THR
1	A	254	THR
1	A	257	ILE
1	A	263	LEU
1	A	267	VAL
1	A	291	THR
1	A	292	ARG
1	A	296	ILE
1	A	306	ASN
1	A	307	ILE
1	A	314	PHE
1	B	10	ILE
1	B	16	THR

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Mol	Chain	Res	Type
1	B	25	GLU
1	B	26	CYS
1	B	32	LYS
1	B	47	LYS
1	B	53	PHE
1	B	54	ASP
1	B	57	ARG
1	B	60	VAL
1	B	68	GLU
1	B	82	ASN
1	B	84	ARG
1	B	89	VAL
1	B	94	SER
1	B	98	THR
1	B	99	VAL
1	B	106	SER
1	B	110	LEU
1	B	122	SER
1	B	124	THR
1	B	130	ILE
1	B	136	THR
1	B	141	LEU
1	B	144	ASP
1	B	154	VAL
1	B	162	GLU
1	B	175	LEU
1	B	179	LEU
1	B	191	ARG
1	B	211	SER
1	B	228	VAL
1	B	244	ASN
1	B	245	LEU
1	B	252	THR
1	B	254	THR
1	B	257	ILE
1	B	263	LEU
1	B	267	VAL
1	B	291	THR
1	B	292	ARG
1	B	296	ILE
1	B	306	ASN
1	B	307	ILE

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Mol	Chain	Res	Type
1	C	10	ILE
1	C	16	THR
1	C	25	GLU
1	C	26	CYS
1	C	32	LYS
1	C	47	LYS
1	C	53	PHE
1	C	54	ASP
1	C	57	ARG
1	C	60	VAL
1	C	68	GLU
1	C	82	ASN
1	C	84	ARG
1	C	89	VAL
1	C	94	SER
1	C	98	THR
1	C	99	VAL
1	C	106	SER
1	C	110	LEU
1	C	124	THR
1	C	130	ILE
1	C	136	THR
1	C	141	LEU
1	C	144	ASP
1	C	154	VAL
1	C	162	GLU
1	C	175	LEU
1	C	179	LEU
1	C	191	ARG
1	C	211	SER
1	C	228	VAL
1	C	244	ASN
1	C	245	LEU
1	C	252	THR
1	C	254	THR
1	C	257	ILE
1	C	263	LEU
1	C	267	VAL
1	C	291	THR
1	C	292	ARG
1	C	296	ILE
1	C	306	ASN

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Mol	Chain	Res	Type
1	C	307	ILE
1	D	10	ILE
1	D	16	THR
1	D	25	GLU
1	D	26	CYS
1	D	32	LYS
1	D	47	LYS
1	D	53	PHE
1	D	54	ASP
1	D	57	ARG
1	D	60	VAL
1	D	68	GLU
1	D	82	ASN
1	D	84	ARG
1	D	89	VAL
1	D	94	SER
1	D	98	THR
1	D	99	VAL
1	D	106	SER
1	D	110	LEU
1	D	122	SER
1	D	124	THR
1	D	130	ILE
1	D	136	THR
1	D	141	LEU
1	D	144	ASP
1	D	154	VAL
1	D	162	GLU
1	D	175	LEU
1	D	179	LEU
1	D	191	ARG
1	D	211	SER
1	D	228	VAL
1	D	244	ASN
1	D	245	LEU
1	D	252	THR
1	D	254	THR
1	D	257	ILE
1	D	263	LEU
1	D	267	VAL
1	D	269	VAL
1	D	291	THR

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Mol	Chain	Res	Type
1	D	292	ARG
1	D	296	ILE
1	D	306	ASN
1	D	307	ILE
1	E	10	ILE
1	E	16	THR
1	E	25	GLU
1	E	26	CYS
1	E	32	LYS
1	E	47	LYS
1	E	53	PHE
1	E	54	ASP
1	E	57	ARG
1	E	60	VAL
1	E	68	GLU
1	E	82	ASN
1	E	84	ARG
1	E	89	VAL
1	E	94	SER
1	E	98	THR
1	E	99	VAL
1	E	106	SER
1	E	110	LEU
1	E	122	SER
1	E	124	THR
1	E	130	ILE
1	E	136	THR
1	E	141	LEU
1	E	144	ASP
1	E	154	VAL
1	E	162	GLU
1	E	175	LEU
1	E	179	LEU
1	E	191	ARG
1	E	211	SER
1	E	228	VAL
1	E	244	ASN
1	E	245	LEU
1	E	252	THR
1	E	254	THR
1	E	257	ILE
1	E	263	LEU

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Mol	Chain	Res	Type
1	E	267	VAL
1	E	291	THR
1	E	292	ARG
1	E	296	ILE
1	E	306	ASN
1	E	307	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	123	GLN
1	A	172	ASN
1	A	192	GLN
1	A	275	GLN
1	A	283	GLN
1	A	306	ASN
1	B	123	GLN
1	B	138	ASN
1	B	172	ASN
1	B	192	GLN
1	B	275	GLN
1	B	283	GLN
1	B	306	ASN
1	C	123	GLN
1	C	172	ASN
1	C	192	GLN
1	C	275	GLN
1	C	306	ASN
1	D	39	ASN
1	D	123	GLN
1	D	138	ASN
1	D	172	ASN
1	D	192	GLN
1	D	275	GLN
1	D	283	GLN
1	D	306	ASN
1	E	39	ASN
1	E	123	GLN
1	E	172	ASN
1	E	192	GLN
1	E	275	GLN

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Mol	Chain	Res	Type
1	E	306	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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%)	1.67	103 (33%) 1 1	55, 91, 140, 207	0
1	B	310/317 (97%)	1.47	80 (25%) 1 2	59, 91, 140, 207	0
1	C	310/317 (97%)	1.63	101 (32%) 1 1	57, 91, 140, 207	0
1	D	310/317 (97%)	1.79	109 (35%) 1 1	56, 91, 140, 207	0
1	E	310/317 (97%)	1.53	100 (32%) 1 1	56, 91, 140, 207	0
All	All	1550/1585 (97%)	1.62	493 (31%) 1 1	55, 91, 140, 207	0

All (493) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	153	ASP	15.8
1	A	59	GLY	14.1
1	B	153	ASP	11.9
1	B	152	ASP	11.0
1	A	60	VAL	9.5
1	E	144	ASP	9.1
1	A	153	ASP	8.5
1	C	153	ASP	8.2
1	E	59	GLY	8.2
1	B	148	VAL	7.9
1	D	60	VAL	7.7
1	E	126	HIS	7.5
1	A	144	ASP	7.5
1	D	59	GLY	7.1
1	A	206	PHE	7.1
1	B	242	GLU	7.1
1	C	59	GLY	6.8
1	B	60	VAL	6.7
1	A	221	ASP	6.6
1	E	60	VAL	6.5

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Mol	Chain	Res	Type	RSRZ
1	E	147	LYS	6.3
1	E	184	ASP	6.3
1	C	279	LYS	6.3
1	A	74	GLU	6.2
1	B	59	GLY	6.1
1	E	128	TYR	6.0
1	D	148	VAL	5.9
1	A	224	VAL	5.8
1	B	88	VAL	5.7
1	A	173	PHE	5.7
1	C	184	ASP	5.7
1	D	263	LEU	5.6
1	B	155	PHE	5.6
1	B	144	ASP	5.6
1	D	152	ASP	5.6
1	B	100	GLN	5.6
1	C	85	ASP	5.5
1	D	85	ASP	5.5
1	D	151	ASN	5.4
1	D	187	LEU	5.4
1	E	146	GLU	5.3
1	C	173	PHE	5.2
1	A	58	SER	5.2
1	D	111	SER	5.2
1	A	13	GLU	5.2
1	D	55	PRO	5.2
1	C	144	ASP	5.1
1	D	282	SER	5.1
1	B	101	TYR	5.1
1	A	209	PHE	5.0
1	C	128	TYR	5.0
1	E	222	ALA	5.0
1	A	148	VAL	5.0
1	B	222	ALA	5.0
1	D	7	PRO	4.9
1	D	146	GLU	4.9
1	B	61	ARG	4.9
1	B	47	LYS	4.9
1	C	155	PHE	4.8
1	D	10	ILE	4.7
1	D	112	PRO	4.7
1	B	11	ALA	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	173	PHE	4.7
1	C	126	HIS	4.7
1	D	82	ASN	4.7
1	A	63	LYS	4.7
1	A	64	THR	4.7
1	E	186	GLN	4.6
1	E	155	PHE	4.6
1	C	176	GLU	4.5
1	C	186	GLN	4.5
1	B	316	PHE	4.5
1	B	225	THR	4.5
1	A	203	PRO	4.5
1	E	148	VAL	4.5
1	E	282	SER	4.5
1	C	151	ASN	4.5
1	B	74	GLU	4.5
1	C	146	GLU	4.5
1	B	154	VAL	4.5
1	A	172	ASN	4.4
1	E	173	PHE	4.4
1	E	61	ARG	4.4
1	D	83	ALA	4.4
1	E	225	THR	4.4
1	D	124	THR	4.4
1	D	225	THR	4.4
1	C	244	ASN	4.4
1	B	146	GLU	4.3
1	B	282	SER	4.3
1	C	13	GLU	4.3
1	A	207	ILE	4.3
1	E	281	GLU	4.3
1	C	147	LYS	4.3
1	C	163	SER	4.3
1	D	155	PHE	4.3
1	B	7	PRO	4.2
1	D	128	TYR	4.2
1	A	316	PHE	4.2
1	C	14	PRO	4.2
1	E	47	LYS	4.2
1	E	139	ILE	4.1
1	B	174	ALA	4.1
1	E	174	ALA	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	134	VAL	4.1
1	C	55	PRO	4.0
1	C	224	VAL	4.0
1	D	221	ASP	4.0
1	A	65	TYR	4.0
1	C	165	THR	4.0
1	A	11	ALA	4.0
1	A	66	GLU	4.0
1	C	83	ALA	4.0
1	E	11	ALA	4.0
1	D	53	PHE	4.0
1	A	225	THR	4.0
1	A	208	LEU	4.0
1	B	49	ARG	3.9
1	C	25	GLU	3.9
1	D	144	ASP	3.9
1	C	148	VAL	3.9
1	D	61	ARG	3.9
1	D	13	GLU	3.9
1	D	242	GLU	3.9
1	E	209	PHE	3.8
1	C	221	ASP	3.8
1	A	212	TRP	3.8
1	A	220	TYR	3.8
1	A	155	PHE	3.8
1	B	187	LEU	3.8
1	D	126	HIS	3.8
1	A	143	VAL	3.8
1	A	244	ASN	3.8
1	E	279	LYS	3.8
1	D	316	PHE	3.8
1	A	89	VAL	3.8
1	C	134	VAL	3.8
1	C	169	LYS	3.8
1	C	316	PHE	3.8
1	C	243	THR	3.8
1	D	206	PHE	3.7
1	C	60	VAL	3.7
1	D	56	VAL	3.7
1	A	139	ILE	3.7
1	A	126	HIS	3.7
1	A	145	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	10	ILE	3.7
1	C	79	ASN	3.7
1	B	279	LYS	3.7
1	D	173	PHE	3.7
1	B	12	ASP	3.7
1	B	90	ASP	3.7
1	B	221	ASP	3.6
1	E	176	GLU	3.6
1	A	7	PRO	3.6
1	E	7	PRO	3.6
1	C	137	ARG	3.6
1	C	280	VAL	3.6
1	E	145	LEU	3.6
1	C	61	ARG	3.6
1	D	74	GLU	3.6
1	C	172	ASN	3.6
1	E	153	ASP	3.6
1	D	100	GLN	3.5
1	A	14	PRO	3.5
1	C	183	LEU	3.5
1	C	7	PRO	3.5
1	C	11	ALA	3.5
1	A	176	GLU	3.5
1	C	185	TYR	3.5
1	C	133	SER	3.5
1	C	139	ILE	3.5
1	A	101	TYR	3.5
1	A	12	ASP	3.5
1	A	187	LEU	3.5
1	C	18	ASN	3.5
1	A	87	ASP	3.5
1	E	135	ASP	3.5
1	E	242	GLU	3.4
1	A	169	LYS	3.4
1	A	177	ASP	3.4
1	E	152	ASP	3.4
1	E	221	ASP	3.4
1	D	135	ASP	3.4
1	D	97	GLY	3.4
1	C	225	THR	3.4
1	B	91	ILE	3.4
1	D	169	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	224	VAL	3.4
1	A	163	SER	3.4
1	A	90	ASP	3.4
1	D	207	ILE	3.4
1	A	165	THR	3.4
1	A	62	VAL	3.3
1	E	13	GLU	3.3
1	E	134	VAL	3.3
1	D	54	ASP	3.3
1	A	186	GLN	3.3
1	B	178	ARG	3.3
1	C	174	ALA	3.3
1	C	135	ASP	3.3
1	D	160	ASP	3.3
1	D	125	LEU	3.3
1	B	45	SER	3.3
1	B	266	PHE	3.3
1	A	152	ASP	3.3
1	B	56	VAL	3.3
1	E	88	VAL	3.3
1	B	162	GLU	3.3
1	C	74	GLU	3.3
1	C	149	GLY	3.3
1	D	186	GLN	3.2
1	C	178	ARG	3.2
1	C	109	VAL	3.2
1	E	243	THR	3.2
1	A	88	VAL	3.2
1	D	11	ALA	3.2
1	D	163	SER	3.2
1	D	145	LEU	3.1
1	D	241	VAL	3.1
1	E	56	VAL	3.1
1	E	82	ASN	3.1
1	E	154	VAL	3.1
1	E	10	ILE	3.1
1	C	154	VAL	3.1
1	C	282	SER	3.1
1	A	281	GLU	3.1
1	D	12	ASP	3.1
1	E	316	PHE	3.1
1	B	151	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	243	THR	3.1
1	D	47	LYS	3.1
1	D	49	ARG	3.0
1	B	136	THR	3.0
1	E	89	VAL	3.0
1	E	169	LYS	3.0
1	A	194	PHE	3.0
1	B	10	ILE	3.0
1	E	14	PRO	3.0
1	C	12	ASP	3.0
1	A	47	LYS	3.0
1	A	199	ASN	3.0
1	D	244	ASN	3.0
1	D	51	LEU	3.0
1	C	69	ALA	3.0
1	E	177	ASP	3.0
1	C	82	ASN	3.0
1	D	281	GLU	2.9
1	A	174	ALA	2.9
1	E	143	VAL	2.9
1	A	54	ASP	2.9
1	B	18	ASN	2.9
1	D	58	SER	2.9
1	A	141	LEU	2.9
1	D	78	VAL	2.9
1	A	49	ARG	2.9
1	A	10	ILE	2.9
1	B	145	LEU	2.9
1	B	188	ARG	2.9
1	A	240	LEU	2.8
1	B	315	GLY	2.8
1	A	230	THR	2.8
1	A	178	ARG	2.8
1	E	63	LYS	2.8
1	B	141	LEU	2.8
1	B	161	ILE	2.8
1	B	263	LEU	2.8
1	C	142	ALA	2.8
1	A	56	VAL	2.8
1	C	167	VAL	2.8
1	C	15	LEU	2.8
1	E	18	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	222	ALA	2.8
1	A	137	ARG	2.8
1	D	279	LYS	2.8
1	C	54	ASP	2.8
1	D	143	VAL	2.8
1	E	133	SER	2.8
1	E	124	THR	2.8
1	E	12	ASP	2.7
1	E	49	ARG	2.7
1	B	89	VAL	2.7
1	A	55	PRO	2.7
1	A	111	SER	2.7
1	E	136	THR	2.7
1	E	96	ASP	2.7
1	D	18	ASN	2.7
1	E	223	ASN	2.7
1	D	141	LEU	2.7
1	D	303	LEU	2.7
1	D	229	SER	2.7
1	A	279	LYS	2.7
1	A	134	VAL	2.7
1	E	8	PRO	2.7
1	C	19	THR	2.7
1	C	166	ALA	2.7
1	E	65	TYR	2.7
1	E	142	ALA	2.7
1	C	143	VAL	2.7
1	C	138	ASN	2.7
1	E	187	LEU	2.7
1	B	81	GLU	2.7
1	C	56	VAL	2.7
1	D	89	VAL	2.7
1	B	135	ASP	2.7
1	E	151	ASN	2.7
1	E	178	ARG	2.6
1	E	188	ARG	2.6
1	A	202	LEU	2.6
1	C	179	LEU	2.6
1	D	90	ASP	2.6
1	B	169	LYS	2.6
1	E	79	ASN	2.6
1	E	212	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	232	ILE	2.6
1	D	57	ARG	2.6
1	B	87	ASP	2.6
1	C	28	SER	2.6
1	D	45	SER	2.6
1	D	65	TYR	2.6
1	D	101	TYR	2.6
1	C	152	ASP	2.6
1	A	223	ASN	2.6
1	A	102	LEU	2.6
1	C	141	LEU	2.6
1	D	208	LEU	2.6
1	A	142	ALA	2.6
1	A	241	VAL	2.6
1	A	247	LYS	2.6
1	E	286	ARG	2.6
1	C	175	LEU	2.6
1	E	15	LEU	2.6
1	A	91	ILE	2.5
1	E	270	ILE	2.5
1	B	27	TYR	2.5
1	A	315	GLY	2.5
1	A	242	GLU	2.5
1	B	16	THR	2.5
1	A	175	LEU	2.5
1	A	85	ASP	2.5
1	E	87	ASP	2.5
1	C	206	PHE	2.5
1	E	168	VAL	2.5
1	C	285	ALA	2.5
1	D	34	GLU	2.5
1	A	53	PHE	2.5
1	C	157	THR	2.5
1	B	231	LEU	2.5
1	D	205	LEU	2.5
1	D	247	LYS	2.5
1	D	167	VAL	2.5
1	C	26	CYS	2.5
1	A	162	GLU	2.5
1	C	281	GLU	2.5
1	C	187	LEU	2.5
1	B	62	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	100	GLN	2.5
1	A	233	ALA	2.4
1	D	209	PHE	2.4
1	A	179	LEU	2.4
1	B	86	ALA	2.4
1	B	25	GLU	2.4
1	D	178	ARG	2.4
1	B	15	LEU	2.4
1	C	145	LEU	2.4
1	E	175	LEU	2.4
1	E	138	ASN	2.4
1	A	307	ILE	2.4
1	C	162	GLU	2.4
1	D	164	PHE	2.4
1	D	190	SER	2.4
1	A	160	ASP	2.4
1	C	220	TYR	2.4
1	D	204	MET	2.4
1	B	206	PHE	2.4
1	A	226	LEU	2.4
1	D	162	GLU	2.4
1	B	26	CYS	2.4
1	C	136	THR	2.4
1	C	288	ALA	2.4
1	B	247	LYS	2.4
1	C	263	LEU	2.4
1	E	285	ALA	2.3
1	D	67	PRO	2.3
1	B	207	ILE	2.3
1	C	76	ARG	2.3
1	D	185	TYR	2.3
1	D	110	LEU	2.3
1	E	275	GLN	2.3
1	D	200	ILE	2.3
1	E	166	ALA	2.3
1	D	154	VAL	2.3
1	D	14	PRO	2.3
1	D	95	PRO	2.3
1	D	308	ILE	2.3
1	C	106	SER	2.3
1	D	165	THR	2.3
1	E	165	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	118	TYR	2.3
1	E	266	PHE	2.3
1	A	96	ASP	2.3
1	C	192	GLN	2.3
1	D	236	ALA	2.3
1	A	124	THR	2.3
1	E	312	LEU	2.3
1	E	111	SER	2.3
1	E	280	VAL	2.3
1	A	15	LEU	2.2
1	E	220	TYR	2.2
1	B	138	ASN	2.2
1	C	63	LYS	2.2
1	C	276	HIS	2.2
1	D	63	LYS	2.2
1	D	147	LYS	2.2
1	E	292	ARG	2.2
1	E	217	SER	2.2
1	A	228	VAL	2.2
1	B	177	ASP	2.2
1	C	81	GLU	2.2
1	C	242	GLU	2.2
1	B	83	ALA	2.2
1	D	260	MET	2.2
1	E	55	PRO	2.2
1	E	83	ALA	2.2
1	E	149	GLY	2.2
1	B	137	ARG	2.2
1	B	94	SER	2.2
1	B	42	LEU	2.2
1	B	251	MET	2.2
1	D	25	GLU	2.2
1	D	130	ILE	2.1
1	A	205	LEU	2.1
1	B	147	LYS	2.1
1	A	146	GLU	2.1
1	B	281	GLU	2.1
1	A	95	PRO	2.1
1	C	57	ARG	2.1
1	E	112	PRO	2.1
1	E	137	ARG	2.1
1	E	301	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	150	LYS	2.1
1	A	57	ARG	2.1
1	A	61	ARG	2.1
1	A	229	SER	2.1
1	E	162	GLU	2.1
1	E	62	VAL	2.1
1	C	182	LYS	2.1
1	E	125	LEU	2.1
1	E	200	ILE	2.1
1	E	208	LEU	2.1
1	A	282	SER	2.1
1	D	15	LEU	2.1
1	D	44	LEU	2.1
1	D	96	ASP	2.1
1	D	183	LEU	2.1
1	E	85	ASP	2.1
1	B	55	PRO	2.1
1	D	168	VAL	2.1
1	D	138	ASN	2.1
1	B	156	LEU	2.1
1	C	261	ILE	2.1
1	C	292	ARG	2.1
1	C	296	ILE	2.1
1	E	226	LEU	2.1
1	A	128	TYR	2.1
1	C	64	THR	2.1
1	D	220	TYR	2.1
1	A	86	ALA	2.1
1	D	170	PRO	2.1
1	E	78	VAL	2.0
1	E	247	LYS	2.0
1	A	72	ILE	2.0
1	A	200	ILE	2.0
1	B	244	ASN	2.0
1	D	199	ASN	2.0
1	E	179	LEU	2.0
1	B	285	ALA	2.0
1	C	160	ASP	2.0
1	C	53	PHE	2.0
1	C	264	PHE	2.0
1	D	275	GLN	2.0
1	C	170	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	42	LEU	2.0
1	B	179	LEU	2.0
1	E	244	ASN	2.0
1	D	262	TYR	2.0
1	A	135	ASP	2.0
1	A	164	PHE	2.0
1	B	209	PHE	2.0
1	C	247	LYS	2.0
1	B	224	VAL	2.0
1	D	68	GLU	2.0
1	D	312	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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	ARS	C	1316	1/1	0.95	0.37	130,130,130,130	0

6.5 Other polymers [i](#)

There are no such residues in this entry.