



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:43 AM UTC

PDB ID : 3EI0 / pdb_00003ei0
Title : Structure of the E221A mutant of the *Gloeobacter violaceus* pentameric ligand gated ion channel (GLIC)
Authors : Hilf, R.J.C.; Dutzler, R.
Deposited on : 2008-09-15
Resolution : 3.50 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

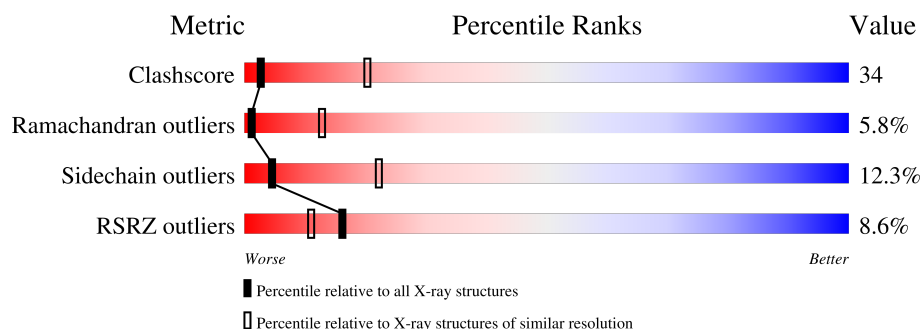
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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))
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	7% 40% 46% 10% ..
1	B	317	7% 38% 48% 10% ..
1	C	317	7% 37% 49% 11% ..
1	D	317	12% 39% 47% 10% ..
1	E	317	9% 38% 48% 10% ..

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 12585 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
			2517	1660	403	450	4			
1	B	310	Total	C	N	O	S	0	0	0
			2517	1660	403	450	4			
1	C	310	Total	C	N	O	S	0	0	0
			2517	1660	403	450	4			
1	D	310	Total	C	N	O	S	0	0	0
			2517	1660	403	450	4			
1	E	310	Total	C	N	O	S	0	0	0
			2517	1660	403	450	4			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q7NDN8
A	1	GLN	-	expression tag	UNP Q7NDN8
A	2	ASP	-	expression tag	UNP Q7NDN8
A	3	MET	-	expression tag	UNP Q7NDN8
A	4	VAL	-	expression tag	UNP Q7NDN8
A	5	SER	-	expression tag	UNP Q7NDN8
A	6	PRO	-	expression tag	UNP Q7NDN8
A	221	ALA	GLU	engineered mutation	UNP Q7NDN8
B	0	GLY	-	expression tag	UNP Q7NDN8
B	1	GLN	-	expression tag	UNP Q7NDN8
B	2	ASP	-	expression tag	UNP Q7NDN8
B	3	MET	-	expression tag	UNP Q7NDN8
B	4	VAL	-	expression tag	UNP Q7NDN8
B	5	SER	-	expression tag	UNP Q7NDN8
B	6	PRO	-	expression tag	UNP Q7NDN8
B	221	ALA	GLU	engineered mutation	UNP Q7NDN8
C	0	GLY	-	expression tag	UNP Q7NDN8
C	1	GLN	-	expression tag	UNP Q7NDN8
C	2	ASP	-	expression tag	UNP Q7NDN8

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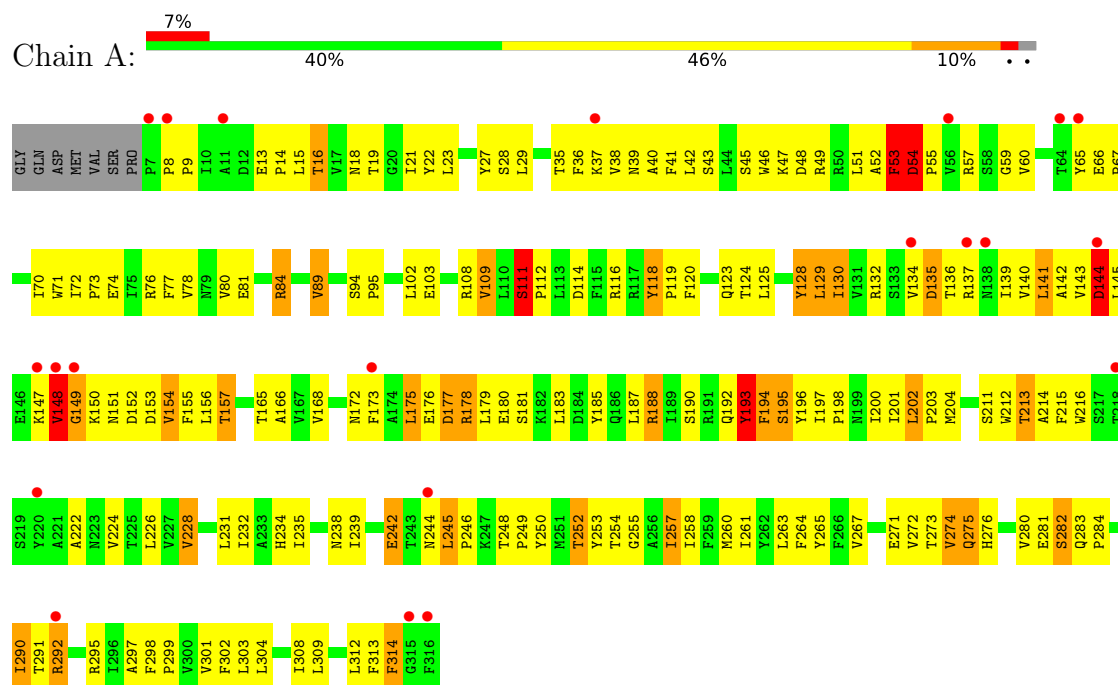
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Chain	Residue	Modelled	Actual	Comment	Reference
C	3	MET	-	expression tag	UNP Q7NDN8
C	4	VAL	-	expression tag	UNP Q7NDN8
C	5	SER	-	expression tag	UNP Q7NDN8
C	6	PRO	-	expression tag	UNP Q7NDN8
C	221	ALA	GLU	engineered mutation	UNP Q7NDN8
D	0	GLY	-	expression tag	UNP Q7NDN8
D	1	GLN	-	expression tag	UNP Q7NDN8
D	2	ASP	-	expression tag	UNP Q7NDN8
D	3	MET	-	expression tag	UNP Q7NDN8
D	4	VAL	-	expression tag	UNP Q7NDN8
D	5	SER	-	expression tag	UNP Q7NDN8
D	6	PRO	-	expression tag	UNP Q7NDN8
D	221	ALA	GLU	engineered mutation	UNP Q7NDN8
E	0	GLY	-	expression tag	UNP Q7NDN8
E	1	GLN	-	expression tag	UNP Q7NDN8
E	2	ASP	-	expression tag	UNP Q7NDN8
E	3	MET	-	expression tag	UNP Q7NDN8
E	4	VAL	-	expression tag	UNP Q7NDN8
E	5	SER	-	expression tag	UNP Q7NDN8
E	6	PRO	-	expression tag	UNP Q7NDN8
E	221	ALA	GLU	engineered mutation	UNP Q7NDN8

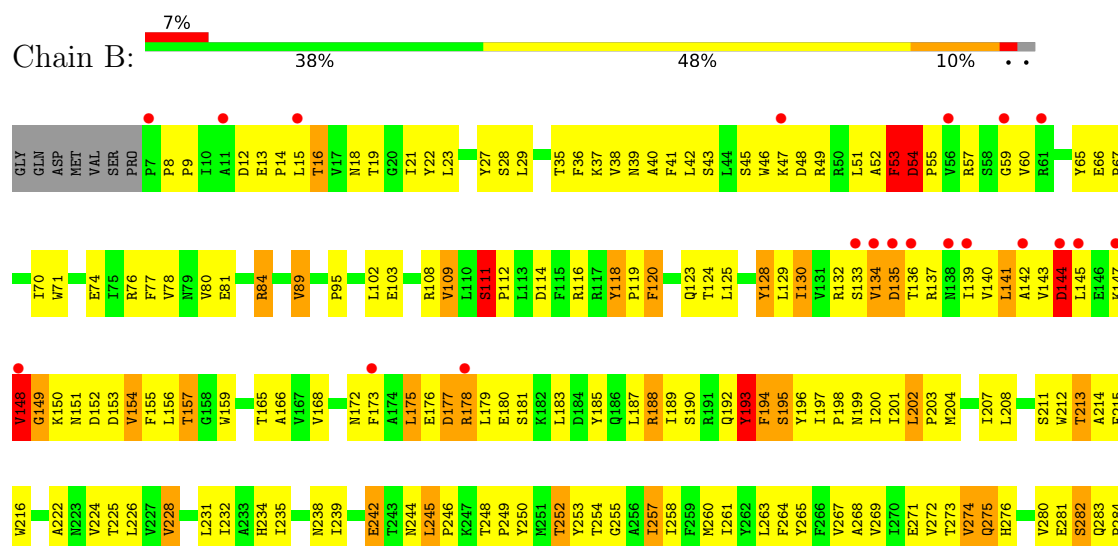
3 Residue-property plots

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

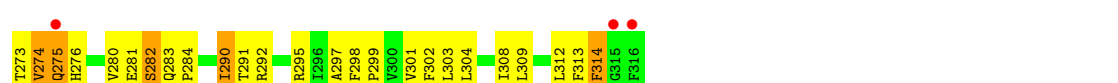
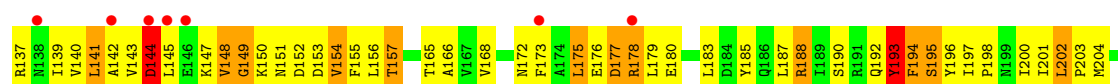


• Molecule 1: Glr4197 protein

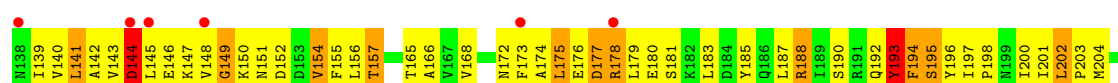
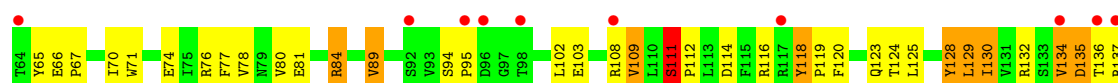
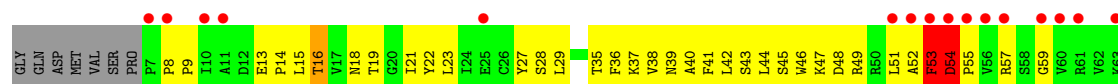




• Molecule 1: Glr4197 protein

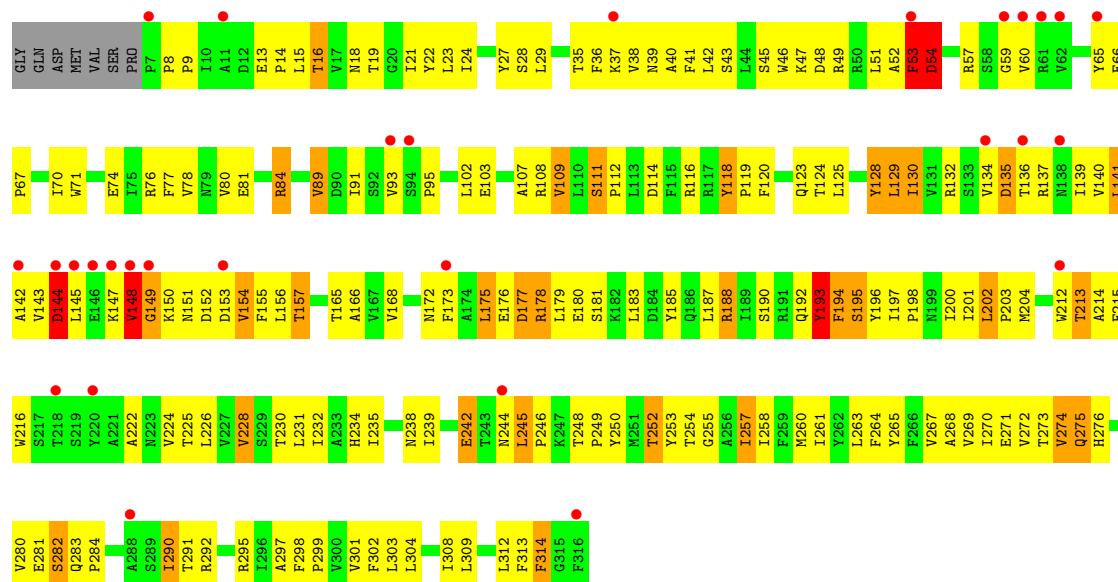


• Molecule 1: Glr4197 protein



• 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	179.64Å 133.76Å 161.65Å 90.00° 101.67° 90.00°	Depositor
Resolution (Å)	20.00 – 3.50 20.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-3.50) 98.6 (20.00-3.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 3.48Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.255 , 0.276 0.261 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	85.5	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 73.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12585	wwPDB-VP
Average B, all atoms (Å ²)	107.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.48	0/2585	0.91	9/3530 (0.3%)
1	B	0.48	0/2585	0.90	10/3530 (0.3%)
1	C	0.48	0/2585	0.91	10/3530 (0.3%)
1	D	0.50	0/2585	0.91	9/3530 (0.3%)
1	E	0.49	0/2585	0.91	10/3530 (0.3%)
All	All	0.49	0/12925	0.91	48/17650 (0.3%)

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	SER	CA-C-N	8.54	129.06	119.92
1	A	111	SER	C-N-CA	8.54	129.06	119.92
1	C	245	LEU	CA-C-N	8.48	128.35	120.21
1	C	245	LEU	C-N-CA	8.48	128.35	120.21
1	E	245	LEU	CA-C-N	8.20	128.09	120.21
1	E	245	LEU	C-N-CA	8.20	128.09	120.21
1	E	111	SER	CA-C-N	7.18	128.81	119.84
1	E	111	SER	C-N-CA	7.18	128.81	119.84
1	D	245	LEU	CA-C-N	7.09	128.05	120.11
1	D	245	LEU	C-N-CA	7.09	128.05	120.11
1	B	245	LEU	CA-C-N	6.94	127.88	120.11
1	B	245	LEU	C-N-CA	6.94	127.88	120.11
1	A	245	LEU	CA-C-N	6.93	127.87	120.11
1	A	245	LEU	C-N-CA	6.93	127.87	120.11
1	D	111	SER	CA-C-N	6.87	128.43	119.84
1	D	111	SER	C-N-CA	6.87	128.43	119.84
1	C	111	SER	CA-C-N	6.84	128.39	119.84
1	C	111	SER	C-N-CA	6.84	128.39	119.84
1	B	111	SER	CA-C-N	6.49	127.95	119.84
1	B	111	SER	C-N-CA	6.49	127.95	119.84
1	E	213	THR	N-CA-C	-6.47	105.49	113.19
1	E	54	ASP	CA-C-N	6.38	127.81	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	54	ASP	C-N-CA	6.38	127.81	119.84
1	C	54	ASP	CA-C-N	6.31	127.73	119.84
1	C	54	ASP	C-N-CA	6.31	127.73	119.84
1	A	213	THR	N-CA-C	-6.28	105.72	113.19
1	B	54	ASP	CA-C-N	6.21	127.60	119.84
1	B	54	ASP	C-N-CA	6.21	127.60	119.84
1	D	54	ASP	CA-C-N	6.19	127.58	119.84
1	D	54	ASP	C-N-CA	6.19	127.58	119.84
1	A	54	ASP	CA-C-N	6.19	127.58	119.84
1	A	54	ASP	C-N-CA	6.19	127.58	119.84
1	C	128	TYR	N-CA-C	6.15	121.18	113.43
1	A	128	TYR	N-CA-C	6.08	121.09	113.43
1	E	53	PHE	N-CA-C	5.95	119.05	109.83
1	E	128	TYR	N-CA-C	5.94	120.92	113.43
1	D	53	PHE	N-CA-C	5.89	118.97	109.83
1	B	128	TYR	N-CA-C	5.88	120.84	113.43
1	D	128	TYR	N-CA-C	5.87	120.82	113.43
1	C	213	THR	N-CA-C	-5.85	106.23	113.19
1	B	213	THR	N-CA-C	-5.77	106.22	113.20
1	B	53	PHE	N-CA-C	5.72	118.70	109.83
1	D	213	THR	N-CA-C	-5.69	106.41	113.19
1	A	53	PHE	N-CA-C	5.58	118.48	109.83
1	C	53	PHE	N-CA-C	5.53	118.40	109.83
1	C	12	ASP	N-CA-C	-5.21	107.59	114.31
1	B	12	ASP	N-CA-C	-5.15	107.66	114.31
1	E	24	ILE	N-CA-C	-5.11	107.76	111.90

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	2517	0	2536	175	0
1	B	2517	0	2536	175	0
1	C	2517	0	2536	173	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2517	0	2536	172	0
1	E	2517	0	2536	178	0
All	All	12585	0	12680	850	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 34.

All (850) 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:D:22:TYR:HA	1:D:149:GLY:HA2	1.43	0.99
1:C:22:TYR:HA	1:C:149:GLY:HA2	1.45	0.98
1:B:22:TYR:HA	1:B:149:GLY:HA2	1.45	0.96
1:A:147:LYS:HE2	1:A:165:THR:HA	1.48	0.96
1:E:22:TYR:HA	1:E:149:GLY:HA2	1.44	0.96
1:C:147:LYS:HE2	1:C:165:THR:HA	1.48	0.95
1:A:22:TYR:HA	1:A:149:GLY:HA2	1.47	0.95
1:C:13:GLU:HB3	1:C:14:PRO:HD2	1.50	0.94
1:B:147:LYS:HE2	1:B:165:THR:HA	1.48	0.93
1:D:13:GLU:HB3	1:D:14:PRO:HD2	1.51	0.92
1:E:147:LYS:HE2	1:E:165:THR:HA	1.48	0.92
1:A:13:GLU:HB3	1:A:14:PRO:HD2	1.50	0.92
1:B:13:GLU:HB3	1:B:14:PRO:HD2	1.52	0.91
1:E:13:GLU:HB3	1:E:14:PRO:HD2	1.52	0.91
1:A:84:ARG:HH11	1:A:84:ARG:CG	1.84	0.90
1:D:147:LYS:HE2	1:D:165:THR:HA	1.52	0.88
1:B:84:ARG:CG	1:B:84:ARG:HH11	1.86	0.88
1:B:119:PRO:HG3	1:B:254:THR:HB	1.55	0.87
1:A:119:PRO:HG3	1:A:254:THR:HB	1.57	0.87
1:D:84:ARG:HH11	1:D:84:ARG:CG	1.88	0.87
1:E:84:ARG:CG	1:E:84:ARG:HH11	1.88	0.86
1:A:197:ILE:HB	1:A:198:PRO:HD3	1.57	0.86
1:C:84:ARG:HH11	1:C:84:ARG:CG	1.87	0.86
1:B:197:ILE:HB	1:B:198:PRO:HD3	1.58	0.85
1:C:119:PRO:HG3	1:C:254:THR:HB	1.56	0.85
1:B:22:TYR:HA	1:B:149:GLY:CA	2.07	0.84
1:E:22:TYR:HA	1:E:149:GLY:CA	2.07	0.84
1:D:22:TYR:HA	1:D:149:GLY:CA	2.07	0.84
1:E:119:PRO:HG3	1:E:254:THR:HB	1.57	0.83
1:D:197:ILE:HB	1:D:198:PRO:HD3	1.58	0.83
1:D:119:PRO:HG3	1:D:254:THR:HB	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:LEU:HB3	1:E:103:GLU:HG2	1.60	0.83
1:C:197:ILE:HB	1:C:198:PRO:HD3	1.60	0.82
1:E:197:ILE:HB	1:E:198:PRO:HD3	1.59	0.82
1:C:22:TYR:HA	1:C:149:GLY:CA	2.09	0.82
1:A:22:TYR:HA	1:A:149:GLY:CA	2.11	0.81
1:A:177:ASP:O	1:A:178:ARG:HB2	1.80	0.81
1:D:275:GLN:O	1:D:275:GLN:HG2	1.82	0.80
1:D:42:LEU:HB3	1:D:103:GLU:HG2	1.63	0.79
1:B:42:LEU:HB3	1:B:103:GLU:HG2	1.65	0.78
1:B:54:ASP:HB2	1:B:57:ARG:HG3	1.65	0.78
1:E:54:ASP:HB2	1:E:57:ARG:HG3	1.65	0.78
1:B:119:PRO:CG	1:B:254:THR:HB	2.13	0.78
1:E:275:GLN:O	1:E:275:GLN:HG2	1.84	0.78
1:C:177:ASP:O	1:C:178:ARG:HB2	1.82	0.78
1:A:54:ASP:HB2	1:A:57:ARG:HG3	1.65	0.77
1:E:177:ASP:O	1:E:178:ARG:HB2	1.82	0.77
1:B:275:GLN:HG2	1:B:275:GLN:O	1.83	0.77
1:A:119:PRO:CG	1:A:254:THR:HB	2.15	0.77
1:B:177:ASP:O	1:B:178:ARG:HB2	1.84	0.77
1:E:119:PRO:CG	1:E:254:THR:HB	2.15	0.77
1:A:42:LEU:HB3	1:A:103:GLU:HG2	1.65	0.76
1:D:54:ASP:HB2	1:D:57:ARG:HG3	1.66	0.76
1:C:42:LEU:HB3	1:C:103:GLU:HG2	1.68	0.76
1:A:275:GLN:O	1:A:275:GLN:HG2	1.84	0.76
1:C:54:ASP:HB2	1:C:57:ARG:HG3	1.65	0.76
1:C:275:GLN:O	1:C:275:GLN:HG2	1.85	0.76
1:D:177:ASP:O	1:D:178:ARG:HB2	1.84	0.76
1:E:141:LEU:HD23	1:E:142:ALA:H	1.51	0.75
1:C:119:PRO:CG	1:C:254:THR:HB	2.16	0.75
1:E:283:GLN:N	1:E:284:PRO:HD3	2.02	0.75
1:A:84:ARG:HH11	1:A:84:ARG:HG3	1.51	0.74
1:D:119:PRO:CG	1:D:254:THR:HB	2.17	0.74
1:B:141:LEU:HD23	1:B:142:ALA:H	1.53	0.74
1:D:141:LEU:HD23	1:D:142:ALA:H	1.52	0.74
1:C:141:LEU:HD23	1:C:142:ALA:H	1.53	0.73
1:C:283:GLN:N	1:C:284:PRO:HD3	2.03	0.73
1:A:283:GLN:N	1:A:284:PRO:HD3	2.02	0.73
1:B:84:ARG:HH11	1:B:84:ARG:HG3	1.52	0.72
1:B:283:GLN:N	1:B:284:PRO:HD3	2.03	0.72
1:C:13:GLU:HB3	1:C:14:PRO:CD	2.19	0.72
1:C:84:ARG:HH11	1:C:84:ARG:HG3	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:84:ARG:HH11	1:E:84:ARG:HG3	1.53	0.72
1:A:13:GLU:HB3	1:A:14:PRO:CD	2.19	0.72
1:D:283:GLN:N	1:D:284:PRO:HD3	2.03	0.71
1:B:257:ILE:O	1:B:261:ILE:HG12	1.91	0.70
1:A:141:LEU:HD23	1:A:142:ALA:H	1.56	0.70
1:D:13:GLU:HB3	1:D:14:PRO:CD	2.20	0.70
1:A:257:ILE:O	1:A:261:ILE:HG12	1.92	0.70
1:B:13:GLU:HB3	1:B:14:PRO:CD	2.21	0.70
1:D:84:ARG:HH11	1:D:84:ARG:HG3	1.56	0.69
1:C:257:ILE:O	1:C:261:ILE:HG12	1.92	0.69
1:A:249:PRO:HD2	1:A:250:TYR:CD1	2.27	0.69
1:E:257:ILE:O	1:E:261:ILE:HG12	1.92	0.69
1:B:274:VAL:C	1:B:276:HIS:H	2.01	0.69
1:E:13:GLU:HB3	1:E:14:PRO:CD	2.21	0.69
1:E:249:PRO:HD2	1:E:250:TYR:CD1	2.28	0.68
1:A:274:VAL:C	1:A:276:HIS:H	2.02	0.68
1:C:249:PRO:HD2	1:C:250:TYR:CD1	2.29	0.68
1:B:249:PRO:HD2	1:B:250:TYR:CD1	2.30	0.67
1:A:84:ARG:HH11	1:A:84:ARG:HG2	1.58	0.67
1:D:274:VAL:C	1:D:276:HIS:H	2.02	0.67
1:A:297:ALA:O	1:A:301:VAL:HG23	1.94	0.67
1:D:257:ILE:O	1:D:261:ILE:HG12	1.94	0.67
1:C:84:ARG:HH11	1:C:84:ARG:HG2	1.60	0.67
1:B:84:ARG:HH11	1:B:84:ARG:HG2	1.61	0.66
1:B:297:ALA:O	1:B:301:VAL:HG23	1.95	0.66
1:D:84:ARG:HH11	1:D:84:ARG:HG2	1.60	0.66
1:E:81:GLU:HG3	1:E:108:ARG:HG3	1.78	0.66
1:E:274:VAL:C	1:E:276:HIS:H	2.03	0.65
1:A:140:VAL:HG23	1:A:183:LEU:HG	1.79	0.65
1:C:81:GLU:HG3	1:C:108:ARG:HG3	1.78	0.65
1:D:81:GLU:HG3	1:D:108:ARG:HG3	1.79	0.65
1:D:249:PRO:HD2	1:D:250:TYR:CD1	2.31	0.65
1:E:260:MET:HE3	1:E:309:LEU:HD22	1.77	0.65
1:C:274:VAL:C	1:C:276:HIS:H	2.03	0.65
1:E:297:ALA:O	1:E:301:VAL:HG23	1.97	0.64
1:D:297:ALA:O	1:D:301:VAL:HG23	1.97	0.64
1:E:84:ARG:HH11	1:E:84:ARG:HG2	1.62	0.64
1:C:151:ASN:O	1:C:154:VAL:HG22	1.97	0.64
1:C:297:ALA:O	1:C:301:VAL:HG23	1.98	0.64
1:A:175:LEU:HD22	1:A:176:GLU:HG3	1.80	0.64
1:C:260:MET:HE3	1:C:309:LEU:HD22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:VAL:CG2	1:A:183:LEU:HG	2.29	0.63
1:B:260:MET:HE3	1:B:309:LEU:HD22	1.80	0.63
1:A:81:GLU:HG3	1:A:108:ARG:HG3	1.81	0.63
1:C:175:LEU:HD22	1:C:176:GLU:HG3	1.81	0.63
1:E:42:LEU:HB3	1:E:103:GLU:CG	2.29	0.62
1:B:151:ASN:O	1:B:154:VAL:HG22	1.98	0.62
1:B:214:ALA:HB2	1:B:226:LEU:HD23	1.82	0.62
1:D:260:MET:HE3	1:D:309:LEU:HD22	1.81	0.62
1:B:81:GLU:HG3	1:B:108:ARG:HG3	1.80	0.62
1:D:42:LEU:HB3	1:D:103:GLU:CG	2.29	0.62
1:B:298:PHE:HB2	1:B:299:PRO:HD3	1.82	0.62
1:D:214:ALA:HB2	1:D:226:LEU:HD23	1.82	0.62
1:D:21:ILE:O	1:D:149:GLY:HA3	2.00	0.62
1:E:214:ALA:HB2	1:E:226:LEU:HD23	1.82	0.62
1:E:151:ASN:O	1:E:154:VAL:HG22	2.00	0.61
1:A:147:LYS:C	1:A:149:GLY:H	2.07	0.61
1:E:298:PHE:HB2	1:E:299:PRO:HD3	1.81	0.61
1:D:298:PHE:HB2	1:D:299:PRO:HD3	1.83	0.61
1:B:314:PHE:HD1	1:B:314:PHE:H	1.48	0.61
1:D:175:LEU:HD22	1:D:176:GLU:HG3	1.83	0.61
1:A:84:ARG:HG3	1:A:84:ARG:NH1	2.15	0.61
1:C:21:ILE:O	1:C:149:GLY:HA3	2.01	0.61
1:E:213:THR:OG1	1:E:226:LEU:HD21	2.01	0.61
1:C:314:PHE:HD1	1:C:314:PHE:H	1.49	0.61
1:A:214:ALA:HB2	1:A:226:LEU:HD23	1.83	0.61
1:B:53:PHE:O	1:B:53:PHE:CD1	2.53	0.61
1:C:53:PHE:O	1:C:53:PHE:CD1	2.54	0.61
1:E:51:LEU:HD11	1:E:70:ILE:HD12	1.83	0.61
1:B:140:VAL:HG23	1:B:183:LEU:HG	1.83	0.60
1:C:76:ARG:NH2	1:C:130:ILE:HD12	2.16	0.60
1:C:213:THR:OG1	1:C:226:LEU:HD21	2.00	0.60
1:E:76:ARG:NH2	1:E:130:ILE:HD12	2.16	0.60
1:E:314:PHE:HD1	1:E:314:PHE:H	1.49	0.60
1:A:213:THR:OG1	1:A:226:LEU:HD21	2.01	0.60
1:C:155:PHE:CE1	1:D:112:PRO:HB3	2.36	0.60
1:C:214:ALA:HB2	1:C:226:LEU:HD23	1.82	0.60
1:E:147:LYS:C	1:E:149:GLY:H	2.09	0.60
1:B:42:LEU:HB3	1:B:103:GLU:CG	2.32	0.60
1:B:175:LEU:HD22	1:B:176:GLU:HG3	1.83	0.60
1:A:238:ASN:O	1:A:242:GLU:HB2	2.02	0.60
1:C:42:LEU:HB3	1:C:103:GLU:CG	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:THR:HB	1:D:188:ARG:NE	2.16	0.60
1:A:151:ASN:O	1:A:154:VAL:HG22	2.01	0.60
1:A:298:PHE:HB2	1:A:299:PRO:HD3	1.82	0.60
1:C:140:VAL:CG2	1:C:183:LEU:HG	2.32	0.60
1:C:140:VAL:HG23	1:C:183:LEU:HG	1.82	0.60
1:A:112:PRO:HB3	1:E:155:PHE:CE1	2.37	0.60
1:D:151:ASN:O	1:D:154:VAL:HG22	2.02	0.60
1:A:42:LEU:HB3	1:A:103:GLU:CG	2.32	0.60
1:E:175:LEU:HD22	1:E:176:GLU:HG3	1.83	0.60
1:B:238:ASN:HA	1:B:258:ILE:HD11	1.84	0.60
1:C:51:LEU:HD11	1:C:70:ILE:HD12	1.83	0.60
1:B:53:PHE:C	1:B:53:PHE:HD1	2.10	0.60
1:D:140:VAL:HG23	1:D:183:LEU:HG	1.83	0.60
1:C:27:TYR:CE1	1:C:37:LYS:HB3	2.37	0.59
1:A:314:PHE:HD1	1:A:314:PHE:H	1.49	0.59
1:B:21:ILE:O	1:B:149:GLY:HA3	2.02	0.59
1:B:27:TYR:CE1	1:B:37:LYS:HB3	2.37	0.59
1:B:304:LEU:O	1:B:308:ILE:HG12	2.02	0.59
1:E:53:PHE:O	1:E:53:PHE:CD1	2.56	0.59
1:A:51:LEU:HD11	1:A:70:ILE:HD12	1.83	0.59
1:A:177:ASP:O	1:A:178:ARG:CB	2.50	0.59
1:E:21:ILE:O	1:E:149:GLY:HA3	2.02	0.59
1:C:298:PHE:HB2	1:C:299:PRO:HD3	1.83	0.59
1:E:314:PHE:CD1	1:E:314:PHE:N	2.71	0.59
1:C:147:LYS:C	1:C:149:GLY:H	2.09	0.59
1:D:238:ASN:O	1:D:242:GLU:HB2	2.03	0.59
1:A:21:ILE:O	1:A:149:GLY:HA3	2.01	0.59
1:E:238:ASN:O	1:E:242:GLU:HB2	2.02	0.59
1:A:84:ARG:CG	1:A:84:ARG:NH1	2.54	0.59
1:B:140:VAL:CG2	1:B:183:LEU:HG	2.32	0.59
1:D:27:TYR:CE1	1:D:37:LYS:HB3	2.38	0.59
1:E:304:LEU:O	1:E:308:ILE:HG12	2.02	0.59
1:A:155:PHE:CE1	1:B:112:PRO:HB3	2.38	0.59
1:C:53:PHE:CD1	1:C:53:PHE:C	2.81	0.59
1:C:53:PHE:C	1:C:53:PHE:HD1	2.11	0.59
1:C:314:PHE:CD1	1:C:314:PHE:N	2.71	0.59
1:D:76:ARG:NH2	1:D:130:ILE:HD12	2.18	0.59
1:E:140:VAL:HG23	1:E:183:LEU:HG	1.85	0.59
1:B:147:LYS:C	1:B:149:GLY:H	2.11	0.58
1:E:27:TYR:CE1	1:E:37:LYS:HB3	2.38	0.58
1:D:304:LEU:O	1:D:308:ILE:HG12	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:PHE:HD1	1:E:53:PHE:C	2.11	0.58
1:A:304:LEU:O	1:A:308:ILE:HG12	2.03	0.58
1:C:177:ASP:O	1:C:178:ARG:CB	2.51	0.58
1:D:238:ASN:HA	1:D:258:ILE:HD11	1.85	0.58
1:D:314:PHE:HD1	1:D:314:PHE:H	1.51	0.58
1:C:141:LEU:HD23	1:C:142:ALA:N	2.19	0.58
1:D:314:PHE:CD1	1:D:314:PHE:N	2.72	0.58
1:B:48:ASP:CG	1:B:51:LEU:HD23	2.29	0.58
1:B:84:ARG:HG3	1:B:84:ARG:NH1	2.17	0.58
1:B:193:TYR:HD1	1:B:193:TYR:H	1.52	0.58
1:C:304:LEU:O	1:C:308:ILE:HG12	2.04	0.58
1:D:147:LYS:C	1:D:149:GLY:H	2.12	0.58
1:A:314:PHE:CD1	1:A:314:PHE:N	2.71	0.57
1:B:53:PHE:CD1	1:B:53:PHE:C	2.81	0.57
1:B:238:ASN:O	1:B:242:GLU:HB2	2.03	0.57
1:C:238:ASN:O	1:C:242:GLU:HB2	2.02	0.57
1:D:213:THR:OG1	1:D:226:LEU:HD21	2.03	0.57
1:A:53:PHE:O	1:A:53:PHE:CD1	2.56	0.57
1:C:48:ASP:CG	1:C:51:LEU:HD23	2.29	0.57
1:C:124:THR:HB	1:C:188:ARG:NE	2.19	0.57
1:B:314:PHE:N	1:B:314:PHE:CD1	2.70	0.57
1:D:140:VAL:CG2	1:D:183:LEU:HG	2.35	0.57
1:A:273:THR:HG21	1:E:213:THR:HB	1.86	0.57
1:B:124:THR:HB	1:B:188:ARG:NE	2.19	0.57
1:B:177:ASP:O	1:B:178:ARG:CB	2.52	0.57
1:B:213:THR:OG1	1:B:226:LEU:HD21	2.04	0.57
1:A:53:PHE:HD1	1:A:53:PHE:C	2.12	0.57
1:A:124:THR:HB	1:A:188:ARG:NE	2.20	0.57
1:B:114:ASP:OD2	1:B:116:ARG:HB2	2.04	0.57
1:D:51:LEU:HD11	1:D:70:ILE:HD12	1.86	0.57
1:A:260:MET:HE3	1:A:309:LEU:HD22	1.85	0.57
1:D:155:PHE:CE1	1:E:112:PRO:HB3	2.39	0.57
1:B:70:ILE:HG22	1:B:71:TRP:O	2.04	0.57
1:A:238:ASN:HA	1:A:258:ILE:HD11	1.86	0.57
1:E:141:LEU:HD23	1:E:142:ALA:N	2.19	0.57
1:E:193:TYR:HD1	1:E:193:TYR:H	1.53	0.57
1:B:197:ILE:HA	1:B:201:ILE:HB	1.86	0.56
1:E:177:ASP:O	1:E:178:ARG:CB	2.51	0.56
1:C:70:ILE:HG22	1:C:71:TRP:O	2.05	0.56
1:C:114:ASP:OD2	1:C:116:ARG:HB2	2.05	0.56
1:D:84:ARG:H	1:D:84:ARG:HD3	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:PHE:CD1	1:E:53:PHE:C	2.82	0.56
1:E:124:THR:HB	1:E:188:ARG:NE	2.20	0.56
1:B:141:LEU:HD23	1:B:142:ALA:N	2.20	0.56
1:C:224:VAL:O	1:C:228:VAL:HB	2.05	0.56
1:C:238:ASN:HA	1:C:258:ILE:HD11	1.86	0.56
1:A:53:PHE:CD1	1:A:53:PHE:C	2.82	0.56
1:A:193:TYR:H	1:A:193:TYR:HD1	1.54	0.56
1:C:18:ASN:HB3	1:C:143:VAL:CG2	2.36	0.56
1:D:177:ASP:O	1:D:178:ARG:CB	2.52	0.56
1:A:70:ILE:HG22	1:A:71:TRP:O	2.05	0.56
1:B:260:MET:CE	1:B:309:LEU:HD22	2.36	0.56
1:B:274:VAL:C	1:B:276:HIS:N	2.64	0.56
1:D:53:PHE:CD1	1:D:53:PHE:C	2.84	0.56
1:B:51:LEU:HD11	1:B:70:ILE:HD12	1.88	0.56
1:D:53:PHE:CD1	1:D:53:PHE:O	2.59	0.56
1:D:53:PHE:C	1:D:53:PHE:HD1	2.14	0.56
1:A:114:ASP:OD2	1:A:116:ARG:HB2	2.06	0.56
1:A:255:GLY:HA2	1:A:258:ILE:HG22	1.88	0.56
1:B:84:ARG:H	1:B:84:ARG:HD3	1.71	0.56
1:D:48:ASP:CG	1:D:51:LEU:HD23	2.31	0.56
1:C:18:ASN:HB3	1:C:143:VAL:HG23	1.88	0.55
1:E:140:VAL:CG2	1:E:183:LEU:HG	2.35	0.55
1:B:28:SER:O	1:B:36:PHE:HA	2.06	0.55
1:A:147:LYS:C	1:A:149:GLY:N	2.64	0.55
1:E:238:ASN:HA	1:E:258:ILE:HD11	1.88	0.55
1:A:27:TYR:CE1	1:A:37:LYS:HB3	2.42	0.55
1:E:84:ARG:HG3	1:E:84:ARG:NH1	2.18	0.55
1:A:76:ARG:NH2	1:A:130:ILE:HD12	2.22	0.55
1:A:283:GLN:N	1:A:284:PRO:CD	2.70	0.55
1:D:70:ILE:HG22	1:D:71:TRP:O	2.06	0.55
1:A:18:ASN:HB3	1:A:143:VAL:CG2	2.37	0.55
1:A:28:SER:O	1:A:36:PHE:HA	2.07	0.55
1:B:216:TRP:CH2	1:B:295:ARG:HB2	2.41	0.55
1:E:48:ASP:CG	1:E:51:LEU:HD23	2.32	0.55
1:E:216:TRP:CH2	1:E:295:ARG:HB2	2.41	0.55
1:E:274:VAL:C	1:E:276:HIS:N	2.65	0.55
1:A:48:ASP:CG	1:A:51:LEU:HD23	2.32	0.54
1:B:255:GLY:HA2	1:B:258:ILE:HG22	1.89	0.54
1:C:84:ARG:H	1:C:84:ARG:HD3	1.72	0.54
1:D:54:ASP:HB2	1:D:57:ARG:CG	2.37	0.54
1:D:216:TRP:CH2	1:D:295:ARG:HB2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ASN:HB3	1:A:143:VAL:HG23	1.88	0.54
1:C:216:TRP:CH2	1:C:295:ARG:HB2	2.43	0.54
1:E:114:ASP:OD2	1:E:116:ARG:HB2	2.07	0.54
1:E:255:GLY:HA2	1:E:258:ILE:HG22	1.90	0.54
1:C:283:GLN:N	1:C:284:PRO:CD	2.71	0.54
1:E:84:ARG:H	1:E:84:ARG:HD3	1.72	0.54
1:E:283:GLN:N	1:E:284:PRO:CD	2.69	0.54
1:B:76:ARG:NH2	1:B:130:ILE:HD12	2.22	0.54
1:D:193:TYR:HD1	1:D:193:TYR:H	1.54	0.54
1:C:197:ILE:HA	1:C:201:ILE:HB	1.89	0.54
1:D:114:ASP:OD2	1:D:116:ARG:HB2	2.07	0.54
1:E:18:ASN:HB3	1:E:143:VAL:CG2	2.38	0.54
1:A:52:ALA:HA	1:A:95:PRO:O	2.08	0.54
1:A:84:ARG:H	1:A:84:ARG:HD3	1.72	0.54
1:B:283:GLN:N	1:B:284:PRO:CD	2.70	0.54
1:A:147:LYS:O	1:A:149:GLY:N	2.41	0.54
1:E:260:MET:CE	1:E:309:LEU:HD22	2.37	0.54
1:C:78:VAL:HG22	1:C:130:ILE:HG12	1.90	0.53
1:D:18:ASN:HB3	1:D:143:VAL:HG23	1.90	0.53
1:A:141:LEU:HD23	1:A:142:ALA:N	2.22	0.53
1:C:193:TYR:HD1	1:C:193:TYR:H	1.54	0.53
1:A:216:TRP:CH2	1:A:295:ARG:HB2	2.43	0.53
1:C:84:ARG:HG3	1:C:84:ARG:NH1	2.19	0.53
1:D:18:ASN:HB3	1:D:143:VAL:CG2	2.38	0.53
1:E:147:LYS:C	1:E:149:GLY:N	2.66	0.53
1:C:260:MET:CE	1:C:309:LEU:HD22	2.38	0.53
1:D:28:SER:O	1:D:36:PHE:HA	2.08	0.53
1:D:197:ILE:HA	1:D:201:ILE:HB	1.90	0.53
1:B:18:ASN:HB3	1:B:143:VAL:CG2	2.39	0.53
1:B:224:VAL:O	1:B:228:VAL:HB	2.08	0.53
1:C:155:PHE:CE2	1:C:157:THR:HG23	2.44	0.53
1:C:274:VAL:C	1:C:276:HIS:N	2.64	0.53
1:E:197:ILE:HA	1:E:201:ILE:HB	1.90	0.53
1:A:78:VAL:HG22	1:A:130:ILE:HG12	1.89	0.53
1:B:155:PHE:CE1	1:C:112:PRO:HB3	2.43	0.53
1:C:147:LYS:C	1:C:149:GLY:N	2.66	0.53
1:D:141:LEU:HD23	1:D:142:ALA:N	2.19	0.53
1:E:47:LYS:HD2	1:E:49:ARG:NH2	2.24	0.53
1:B:66:GLU:HG3	1:B:67:PRO:HD2	1.90	0.53
1:D:255:GLY:HA2	1:D:258:ILE:HG22	1.91	0.53
1:A:197:ILE:HA	1:A:201:ILE:HB	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:70:ILE:HG22	1:E:71:TRP:O	2.09	0.52
1:E:147:LYS:O	1:E:149:GLY:N	2.43	0.52
1:A:274:VAL:C	1:A:276:HIS:N	2.64	0.52
1:B:52:ALA:HA	1:B:95:PRO:O	2.09	0.52
1:D:260:MET:CE	1:D:309:LEU:HD22	2.39	0.52
1:C:135:ASP:OD2	1:C:135:ASP:C	2.53	0.52
1:B:147:LYS:C	1:B:149:GLY:N	2.66	0.52
1:D:213:THR:HB	1:E:273:THR:HG21	1.90	0.52
1:E:54:ASP:HB2	1:E:57:ARG:CG	2.39	0.52
1:E:65:TYR:CG	1:E:70:ILE:HD11	2.45	0.52
1:E:224:VAL:O	1:E:228:VAL:HB	2.10	0.52
1:B:238:ASN:HA	1:B:258:ILE:CD1	2.40	0.52
1:B:18:ASN:HB3	1:B:143:VAL:HG23	1.92	0.52
1:B:147:LYS:O	1:B:149:GLY:N	2.43	0.52
1:E:282:SER:C	1:E:284:PRO:HD3	2.35	0.52
1:D:52:ALA:HA	1:D:95:PRO:O	2.10	0.52
1:D:155:PHE:CE2	1:D:157:THR:HG23	2.45	0.51
1:E:193:TYR:O	1:E:195:SER:N	2.43	0.51
1:D:274:VAL:C	1:D:276:HIS:N	2.64	0.51
1:C:255:GLY:HA2	1:C:258:ILE:HG22	1.93	0.51
1:D:78:VAL:HG22	1:D:130:ILE:HG12	1.92	0.51
1:D:84:ARG:CG	1:D:84:ARG:NH1	2.58	0.51
1:E:66:GLU:HG3	1:E:67:PRO:HD2	1.92	0.51
1:C:28:SER:O	1:C:36:PHE:HA	2.11	0.51
1:A:54:ASP:HB2	1:A:57:ARG:CG	2.39	0.51
1:C:147:LYS:O	1:C:149:GLY:N	2.44	0.51
1:D:65:TYR:CG	1:D:70:ILE:HD11	2.45	0.51
1:C:52:ALA:HA	1:C:95:PRO:O	2.10	0.51
1:A:260:MET:CE	1:A:309:LEU:HD22	2.40	0.51
1:B:282:SER:C	1:B:284:PRO:HD3	2.36	0.51
1:D:35:THR:HG21	1:D:108:ARG:HH21	1.76	0.51
1:D:238:ASN:HA	1:D:258:ILE:CD1	2.40	0.51
1:B:65:TYR:CG	1:B:70:ILE:HD11	2.46	0.51
1:C:282:SER:C	1:C:284:PRO:HD3	2.36	0.51
1:D:147:LYS:O	1:D:149:GLY:N	2.44	0.51
1:A:271:GLU:OE2	1:A:272:VAL:N	2.44	0.51
1:D:47:LYS:HD2	1:D:49:ARG:NH2	2.27	0.51
1:E:18:ASN:HB3	1:E:143:VAL:HG23	1.92	0.51
1:E:84:ARG:CG	1:E:84:ARG:NH1	2.57	0.51
1:A:35:THR:HG21	1:A:108:ARG:HH21	1.76	0.50
1:B:22:TYR:CA	1:B:149:GLY:HA2	2.31	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:PHE:O	1:D:54:ASP:C	2.54	0.50
1:E:155:PHE:CE2	1:E:157:THR:HG23	2.47	0.50
1:E:232:ILE:HA	1:E:235:ILE:HD12	1.94	0.50
1:C:65:TYR:CG	1:C:70:ILE:HD11	2.47	0.50
1:C:65:TYR:CD2	1:C:70:ILE:HD11	2.47	0.50
1:E:52:ALA:HA	1:E:95:PRO:O	2.11	0.50
1:A:155:PHE:CE2	1:A:157:THR:HG23	2.46	0.50
1:A:224:VAL:O	1:A:228:VAL:HB	2.12	0.50
1:B:78:VAL:HG22	1:B:130:ILE:HG12	1.93	0.50
1:A:282:SER:C	1:A:284:PRO:HD3	2.37	0.50
1:B:155:PHE:CE2	1:B:157:THR:HG23	2.47	0.50
1:D:135:ASP:OD2	1:D:135:ASP:C	2.54	0.50
1:A:47:LYS:HD2	1:A:49:ARG:NH2	2.26	0.50
1:B:232:ILE:HA	1:B:235:ILE:HD12	1.93	0.50
1:D:84:ARG:HG3	1:D:84:ARG:NH1	2.20	0.50
1:D:147:LYS:C	1:D:149:GLY:N	2.67	0.50
1:E:275:GLN:HG3	1:E:291:THR:OG1	2.12	0.50
1:A:275:GLN:HG3	1:A:291:THR:OG1	2.11	0.50
1:C:248:THR:HB	1:C:250:TYR:CE1	2.47	0.50
1:D:224:VAL:O	1:D:228:VAL:HB	2.11	0.50
1:D:282:SER:C	1:D:284:PRO:HD3	2.36	0.50
1:A:151:ASN:ND2	1:A:152:ASP:H	2.10	0.50
1:B:199:ASN:HD22	1:C:242:GLU:HG3	1.77	0.50
1:A:53:PHE:O	1:A:54:ASP:C	2.55	0.49
1:C:15:LEU:HD11	1:C:46:TRP:HB2	1.94	0.49
1:B:53:PHE:O	1:B:54:ASP:C	2.55	0.49
1:C:166:ALA:HB2	1:C:185:TYR:CD2	2.47	0.49
1:C:238:ASN:HA	1:C:258:ILE:CD1	2.41	0.49
1:C:271:GLU:OE2	1:C:272:VAL:N	2.45	0.49
1:E:135:ASP:OD2	1:E:135:ASP:C	2.55	0.49
1:A:238:ASN:HA	1:A:258:ILE:CD1	2.41	0.49
1:B:47:LYS:HD2	1:B:49:ARG:NH2	2.26	0.49
1:B:135:ASP:OD2	1:B:135:ASP:C	2.55	0.49
1:E:151:ASN:ND2	1:E:152:ASP:H	2.10	0.49
1:C:47:LYS:HD2	1:C:49:ARG:NH2	2.27	0.49
1:D:252:THR:HG23	1:D:255:GLY:HA3	1.93	0.49
1:B:222:ALA:O	1:B:226:LEU:HB2	2.12	0.49
1:E:53:PHE:O	1:E:54:ASP:C	2.54	0.49
1:A:135:ASP:C	1:A:135:ASP:OD2	2.55	0.49
1:B:119:PRO:HG3	1:B:254:THR:CB	2.36	0.49
1:E:78:VAL:HG22	1:E:130:ILE:HG12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:PHE:O	1:B:53:PHE:HD1	1.96	0.49
1:C:54:ASP:HB2	1:C:57:ARG:CG	2.39	0.49
1:C:252:THR:HG23	1:C:255:GLY:HA3	1.93	0.49
1:D:144:ASP:HA	1:D:147:LYS:HB3	1.95	0.49
1:E:149:GLY:O	1:E:150:LYS:HB2	2.13	0.49
1:E:212:TRP:HB2	1:E:215:PHE:CE1	2.48	0.49
1:C:179:LEU:C	1:C:179:LEU:HD12	2.38	0.49
1:D:271:GLU:OE2	1:D:272:VAL:N	2.46	0.49
1:E:271:GLU:OE2	1:E:272:VAL:N	2.45	0.49
1:A:53:PHE:CE1	1:A:95:PRO:HA	2.47	0.48
1:A:248:THR:HB	1:A:250:TYR:CE1	2.48	0.48
1:B:213:THR:HB	1:C:273:THR:HG21	1.95	0.48
1:C:231:LEU:HD13	1:C:265:TYR:HB3	1.95	0.48
1:E:76:ARG:HH22	1:E:130:ILE:HD12	1.77	0.48
1:A:15:LEU:HD11	1:A:46:TRP:HB2	1.94	0.48
1:B:53:PHE:CE1	1:B:95:PRO:HA	2.48	0.48
1:D:66:GLU:HG3	1:D:67:PRO:HD2	1.94	0.48
1:E:144:ASP:HA	1:E:147:LYS:HB3	1.95	0.48
1:C:245:LEU:HD12	1:C:246:PRO:HD2	1.94	0.48
1:A:65:TYR:CG	1:A:70:ILE:HD11	2.48	0.48
1:A:166:ALA:HB2	1:A:185:TYR:CD2	2.49	0.48
1:B:215:PHE:HZ	1:B:298:PHE:CE1	2.32	0.48
1:D:53:PHE:CE1	1:D:95:PRO:HA	2.48	0.48
1:A:119:PRO:HG3	1:A:254:THR:CB	2.38	0.48
1:D:275:GLN:HG3	1:D:291:THR:OG1	2.13	0.48
1:A:144:ASP:HA	1:A:147:LYS:HB3	1.96	0.48
1:C:275:GLN:HG3	1:C:291:THR:OG1	2.13	0.48
1:D:193:TYR:O	1:D:195:SER:N	2.47	0.48
1:B:15:LEU:HD11	1:B:46:TRP:HB2	1.94	0.48
1:C:253:TYR:HB2	1:C:313:PHE:CD2	2.48	0.48
1:B:35:THR:HG21	1:B:108:ARG:HH21	1.78	0.48
1:B:252:THR:HG23	1:B:255:GLY:HA3	1.95	0.48
1:B:275:GLN:HG3	1:B:291:THR:OG1	2.13	0.48
1:C:66:GLU:HG3	1:C:67:PRO:HD2	1.94	0.48
1:E:15:LEU:HD11	1:E:46:TRP:HB2	1.95	0.48
1:E:65:TYR:CD2	1:E:70:ILE:HD11	2.48	0.48
1:A:66:GLU:HG3	1:A:67:PRO:HD2	1.95	0.48
1:B:84:ARG:CG	1:B:84:ARG:NH1	2.56	0.48
1:B:248:THR:HB	1:B:250:TYR:CE1	2.49	0.48
1:C:192:GLN:NE2	1:D:249:PRO:HG3	2.29	0.48
1:D:179:LEU:HD12	1:D:179:LEU:C	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:GLN:N	1:D:284:PRO:CD	2.71	0.48
1:B:271:GLU:OE2	1:B:272:VAL:N	2.47	0.48
1:C:118:TYR:O	1:C:119:PRO:C	2.55	0.48
1:D:15:LEU:HD11	1:D:46:TRP:HB2	1.96	0.48
1:D:248:THR:HB	1:D:250:TYR:CE1	2.49	0.48
1:D:253:TYR:HB2	1:D:313:PHE:CD2	2.49	0.48
1:A:222:ALA:O	1:A:226:LEU:HB2	2.14	0.47
1:A:253:TYR:HB2	1:A:313:PHE:CD2	2.49	0.47
1:C:36:PHE:CE1	1:C:109:VAL:HB	2.48	0.47
1:D:89:VAL:HG11	1:D:102:LEU:HD23	1.96	0.47
1:E:215:PHE:HZ	1:E:298:PHE:CE1	2.32	0.47
1:A:23:LEU:HA	1:A:40:ALA:HB2	1.96	0.47
1:A:252:THR:HG23	1:A:255:GLY:HA3	1.96	0.47
1:B:65:TYR:CD2	1:B:70:ILE:HD11	2.49	0.47
1:B:151:ASN:ND2	1:B:152:ASP:H	2.12	0.47
1:C:257:ILE:HG22	1:C:309:LEU:HD23	1.96	0.47
1:E:89:VAL:HG11	1:E:102:LEU:HD23	1.96	0.47
1:E:238:ASN:HA	1:E:258:ILE:CD1	2.43	0.47
1:A:193:TYR:O	1:A:195:SER:N	2.48	0.47
1:B:149:GLY:O	1:B:150:LYS:HB2	2.14	0.47
1:D:151:ASN:ND2	1:D:152:ASP:H	2.12	0.47
1:D:166:ALA:HB2	1:D:185:TYR:CD2	2.49	0.47
1:E:257:ILE:HG22	1:E:309:LEU:HD23	1.96	0.47
1:A:179:LEU:C	1:A:179:LEU:HD12	2.39	0.47
1:C:232:ILE:HA	1:C:235:ILE:HD12	1.96	0.47
1:D:8:PRO:HA	1:D:71:TRP:CD1	2.49	0.47
1:D:222:ALA:O	1:D:226:LEU:HB2	2.14	0.47
1:D:231:LEU:HD13	1:D:265:TYR:HB3	1.96	0.47
1:E:245:LEU:HD12	1:E:246:PRO:HD2	1.97	0.47
1:B:144:ASP:HA	1:B:147:LYS:HB3	1.95	0.47
1:B:197:ILE:HB	1:B:198:PRO:CD	2.38	0.47
1:C:53:PHE:O	1:C:54:ASP:C	2.56	0.47
1:C:84:ARG:CG	1:C:84:ARG:NH1	2.57	0.47
1:E:8:PRO:HA	1:E:71:TRP:CD1	2.50	0.47
1:E:248:THR:HB	1:E:250:TYR:CE1	2.49	0.47
1:A:35:THR:O	1:A:36:PHE:HB3	2.15	0.47
1:A:212:TRP:HB2	1:A:215:PHE:CE1	2.49	0.47
1:A:253:TYR:HA	1:A:313:PHE:CE2	2.50	0.47
1:B:54:ASP:HB2	1:B:57:ARG:CG	2.38	0.47
1:C:23:LEU:HA	1:C:40:ALA:HB2	1.95	0.47
1:C:144:ASP:HA	1:C:147:LYS:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:GLY:O	1:C:150:LYS:HB2	2.15	0.47
1:D:15:LEU:HD12	1:D:16:THR:N	2.29	0.47
1:D:253:TYR:HA	1:D:313:PHE:CE2	2.49	0.47
1:E:53:PHE:CE1	1:E:95:PRO:HA	2.50	0.47
1:E:252:THR:HG23	1:E:255:GLY:HA3	1.96	0.47
1:A:36:PHE:CE1	1:A:109:VAL:HB	2.49	0.47
1:C:151:ASN:ND2	1:C:152:ASP:H	2.13	0.47
1:C:222:ALA:O	1:C:226:LEU:HB2	2.14	0.47
1:D:149:GLY:O	1:D:150:LYS:HB2	2.13	0.47
1:D:212:TRP:HB2	1:D:215:PHE:CE1	2.50	0.47
1:D:231:LEU:HD13	1:D:265:TYR:CB	2.45	0.47
1:E:179:LEU:C	1:E:179:LEU:HD12	2.39	0.47
1:E:253:TYR:HA	1:E:313:PHE:CE2	2.49	0.47
1:A:245:LEU:HD12	1:A:246:PRO:HD2	1.96	0.47
1:B:143:VAL:O	1:B:145:LEU:N	2.48	0.47
1:D:132:ARG:HA	1:D:180:GLU:HG2	1.97	0.47
1:E:222:ALA:O	1:E:226:LEU:HB2	2.14	0.47
1:B:8:PRO:HA	1:B:71:TRP:CD1	2.50	0.47
1:B:225:THR:HG21	1:C:224:VAL:HG23	1.96	0.47
1:B:253:TYR:HB2	1:B:313:PHE:CD2	2.50	0.47
1:C:267:VAL:HG23	1:C:298:PHE:CZ	2.50	0.47
1:B:15:LEU:HD12	1:B:16:THR:N	2.29	0.46
1:B:132:ARG:HA	1:B:180:GLU:HG2	1.96	0.46
1:C:197:ILE:HB	1:C:198:PRO:CD	2.40	0.46
1:D:257:ILE:HG22	1:D:309:LEU:HD23	1.97	0.46
1:E:28:SER:O	1:E:36:PHE:HA	2.14	0.46
1:B:253:TYR:HA	1:B:313:PHE:CE2	2.50	0.46
1:C:231:LEU:HD13	1:C:265:TYR:CB	2.45	0.46
1:C:253:TYR:HA	1:C:313:PHE:CE2	2.50	0.46
1:E:15:LEU:HD12	1:E:16:THR:N	2.30	0.46
1:E:35:THR:HG21	1:E:108:ARG:HH21	1.80	0.46
1:E:231:LEU:HD13	1:E:265:TYR:HB3	1.96	0.46
1:A:65:TYR:CD2	1:A:70:ILE:HD11	2.49	0.46
1:D:65:TYR:CD2	1:D:70:ILE:HD11	2.50	0.46
1:A:281:GLU:O	1:A:282:SER:C	2.58	0.46
1:D:245:LEU:HD12	1:D:246:PRO:HD2	1.97	0.46
1:A:249:PRO:HG3	1:E:192:GLN:NE2	2.31	0.46
1:B:118:TYR:O	1:B:119:PRO:C	2.58	0.46
1:D:36:PHE:CE1	1:D:109:VAL:HB	2.51	0.46
1:A:89:VAL:HG11	1:A:102:LEU:HD23	1.96	0.46
1:A:309:LEU:O	1:A:312:LEU:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:VAL:HG11	1:C:102:LEU:HD23	1.97	0.46
1:C:281:GLU:O	1:C:282:SER:C	2.59	0.46
1:E:166:ALA:HB2	1:E:185:TYR:CD2	2.49	0.46
1:D:35:THR:O	1:D:36:PHE:HB3	2.16	0.46
1:D:118:TYR:O	1:D:119:PRO:C	2.55	0.46
1:E:253:TYR:HB2	1:E:313:PHE:CD2	2.50	0.46
1:B:212:TRP:HB2	1:B:215:PHE:CE1	2.50	0.46
1:B:245:LEU:HD12	1:B:246:PRO:HD2	1.97	0.46
1:D:281:GLU:O	1:D:282:SER:C	2.58	0.46
1:E:231:LEU:HD13	1:E:265:TYR:CB	2.45	0.46
1:B:276:HIS:O	1:B:280:VAL:HG22	2.16	0.46
1:E:36:PHE:CE1	1:E:109:VAL:HB	2.51	0.46
1:A:215:PHE:HZ	1:A:298:PHE:CE1	2.34	0.46
1:A:276:HIS:O	1:A:280:VAL:HG22	2.16	0.46
1:D:9:PRO:HD3	1:D:71:TRP:CE3	2.51	0.46
1:E:123:GLN:C	1:E:188:ARG:HH21	2.24	0.46
1:E:196:TYR:N	1:E:196:TYR:HD1	2.14	0.46
1:A:231:LEU:HD13	1:A:265:TYR:CB	2.46	0.45
1:C:41:PHE:HE2	1:D:175:LEU:HD13	1.80	0.45
1:A:53:PHE:O	1:A:53:PHE:HD1	2.00	0.45
1:A:149:GLY:O	1:A:150:LYS:HB2	2.16	0.45
1:B:193:TYR:O	1:B:195:SER:N	2.49	0.45
1:C:193:TYR:O	1:C:195:SER:N	2.49	0.45
1:C:212:TRP:HB2	1:C:215:PHE:CE1	2.52	0.45
1:C:309:LEU:O	1:C:312:LEU:HB3	2.16	0.45
1:D:23:LEU:HA	1:D:40:ALA:HB2	1.98	0.45
1:D:119:PRO:HG3	1:D:254:THR:CB	2.41	0.45
1:D:136:THR:HG22	1:D:137:ARG:N	2.31	0.45
1:E:298:PHE:CB	1:E:299:PRO:HD3	2.45	0.45
1:A:231:LEU:HD13	1:A:265:TYR:HB3	1.97	0.45
1:B:36:PHE:CE1	1:B:109:VAL:HB	2.51	0.45
1:A:136:THR:HG22	1:A:137:ARG:N	2.31	0.45
1:B:231:LEU:HD13	1:B:265:TYR:HB3	1.98	0.45
1:E:197:ILE:HB	1:E:198:PRO:CD	2.40	0.45
1:E:276:HIS:O	1:E:280:VAL:HG22	2.17	0.45
1:A:9:PRO:HD3	1:A:71:TRP:CE3	2.51	0.45
1:C:53:PHE:CE1	1:C:95:PRO:HA	2.51	0.45
1:E:118:TYR:O	1:E:119:PRO:C	2.58	0.45
1:B:23:LEU:HA	1:B:40:ALA:HB2	1.99	0.45
1:B:298:PHE:CB	1:B:299:PRO:HD3	2.46	0.45
1:C:132:ARG:HA	1:C:180:GLU:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:TYR:N	1:C:196:TYR:CD1	2.85	0.45
1:D:309:LEU:O	1:D:312:LEU:HB3	2.16	0.45
1:A:22:TYR:HB3	1:A:41:PHE:HB2	1.98	0.45
1:C:123:GLN:C	1:C:188:ARG:HH21	2.25	0.45
1:D:38:VAL:HG22	1:D:39:ASN:N	2.31	0.45
1:E:9:PRO:HD3	1:E:71:TRP:CE3	2.52	0.45
1:B:179:LEU:HD12	1:B:179:LEU:C	2.41	0.45
1:B:196:TYR:N	1:B:196:TYR:HD1	2.14	0.45
1:C:245:LEU:HA	1:C:246:PRO:HD2	1.77	0.45
1:E:143:VAL:O	1:E:145:LEU:N	2.50	0.45
1:A:139:ILE:HG12	1:A:172:ASN:HD21	1.81	0.45
1:A:196:TYR:HD1	1:A:196:TYR:N	2.15	0.45
1:A:234:HIS:CE1	1:A:258:ILE:O	2.70	0.45
1:A:267:VAL:HG23	1:A:298:PHE:CZ	2.52	0.45
1:B:89:VAL:HG11	1:B:102:LEU:HD23	1.98	0.45
1:B:196:TYR:N	1:B:196:TYR:CD1	2.84	0.45
1:B:234:HIS:CE1	1:B:258:ILE:O	2.70	0.45
1:C:15:LEU:HD12	1:C:16:THR:N	2.32	0.45
1:C:76:ARG:HH22	1:C:130:ILE:HD12	1.81	0.45
1:C:143:VAL:O	1:C:145:LEU:N	2.50	0.45
1:E:132:ARG:HA	1:E:180:GLU:HG2	1.98	0.45
1:A:8:PRO:HA	1:A:71:TRP:CD1	2.52	0.45
1:B:136:THR:HG22	1:B:137:ARG:N	2.32	0.45
1:C:9:PRO:HD3	1:C:71:TRP:CE3	2.52	0.45
1:C:77:PHE:HB3	1:C:80:VAL:HG23	1.99	0.45
1:C:78:VAL:HB	1:C:128:TYR:HB2	1.99	0.45
1:C:139:ILE:HG12	1:C:172:ASN:HD21	1.82	0.45
1:C:215:PHE:HZ	1:C:298:PHE:CE1	2.35	0.45
1:D:264:PHE:CE2	1:D:302:PHE:HB2	2.52	0.45
1:A:232:ILE:HA	1:A:235:ILE:HD12	1.98	0.44
1:A:271:GLU:O	1:A:274:VAL:N	2.50	0.44
1:B:254:THR:O	1:B:258:ILE:HB	2.17	0.44
1:D:196:TYR:N	1:D:196:TYR:CD1	2.85	0.44
1:E:254:THR:O	1:E:258:ILE:HB	2.17	0.44
1:E:281:GLU:O	1:E:282:SER:C	2.60	0.44
1:A:143:VAL:O	1:A:145:LEU:N	2.50	0.44
1:B:38:VAL:HG22	1:B:39:ASN:N	2.33	0.44
1:C:22:TYR:HB3	1:C:41:PHE:HB2	1.99	0.44
1:D:22:TYR:HA	1:D:149:GLY:HA3	1.97	0.44
1:D:253:TYR:CD1	1:D:314:PHE:HE1	2.35	0.44
1:D:276:HIS:O	1:D:280:VAL:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:253:TYR:CD1	1:E:314:PHE:HE1	2.36	0.44
1:B:22:TYR:HB3	1:B:41:PHE:HB2	1.99	0.44
1:B:257:ILE:HG22	1:B:309:LEU:HD23	1.99	0.44
1:B:281:GLU:O	1:B:282:SER:C	2.59	0.44
1:C:29:LEU:HB2	1:C:156:LEU:HD11	2.00	0.44
1:C:196:TYR:N	1:C:196:TYR:HD1	2.15	0.44
1:C:253:TYR:CD1	1:C:314:PHE:HE1	2.35	0.44
1:A:192:GLN:NE2	1:B:249:PRO:HG3	2.32	0.44
1:B:130:ILE:HA	1:B:181:SER:O	2.18	0.44
1:C:35:THR:HG21	1:C:108:ARG:HH21	1.82	0.44
1:C:136:THR:HG22	1:C:137:ARG:N	2.33	0.44
1:D:54:ASP:HA	1:D:55:PRO:HD2	1.65	0.44
1:D:123:GLN:C	1:D:188:ARG:HH21	2.26	0.44
1:D:215:PHE:HZ	1:D:298:PHE:CE1	2.34	0.44
1:E:139:ILE:HG12	1:E:172:ASN:HD21	1.81	0.44
1:A:118:TYR:O	1:A:119:PRO:C	2.59	0.44
1:B:253:TYR:CD1	1:B:314:PHE:HE1	2.36	0.44
1:E:136:THR:HG22	1:E:137:ARG:N	2.33	0.44
1:E:234:HIS:CE1	1:E:258:ILE:O	2.71	0.44
1:A:15:LEU:HD12	1:A:16:THR:N	2.33	0.44
1:B:77:PHE:HB3	1:B:80:VAL:HG23	2.00	0.44
1:B:166:ALA:HB2	1:B:185:TYR:CD2	2.52	0.44
1:C:77:PHE:HB3	1:C:80:VAL:CG2	2.48	0.44
1:D:35:THR:CG2	1:D:108:ARG:HH21	2.31	0.44
1:D:76:ARG:HH22	1:D:130:ILE:HD12	1.81	0.44
1:D:196:TYR:N	1:D:196:TYR:HD1	2.15	0.44
1:E:196:TYR:N	1:E:196:TYR:CD1	2.85	0.44
1:A:257:ILE:HG22	1:A:309:LEU:HD23	2.00	0.44
1:B:22:TYR:HA	1:B:149:GLY:HA3	1.96	0.44
1:B:231:LEU:HD13	1:B:265:TYR:CB	2.47	0.44
1:B:267:VAL:HG23	1:B:298:PHE:CZ	2.53	0.44
1:B:309:LEU:O	1:B:312:LEU:HB3	2.17	0.44
1:D:22:TYR:HB3	1:D:41:PHE:HB2	2.00	0.44
1:D:139:ILE:HG12	1:D:172:ASN:HD21	1.82	0.44
1:D:245:LEU:HA	1:D:246:PRO:HD2	1.78	0.44
1:E:78:VAL:HB	1:E:128:TYR:HB2	1.99	0.44
1:A:54:ASP:HA	1:A:55:PRO:HD2	1.77	0.44
1:A:77:PHE:HB3	1:A:80:VAL:CG2	2.48	0.44
1:A:111:SER:HA	1:A:112:PRO:HD2	1.75	0.44
1:A:196:TYR:N	1:A:196:TYR:CD1	2.85	0.44
1:C:128:TYR:O	1:C:129:LEU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:LEU:HD22	1:C:185:TYR:CE1	2.53	0.44
1:D:125:LEU:HB2	1:D:187:LEU:HB3	2.00	0.44
1:D:298:PHE:CB	1:D:299:PRO:HD3	2.47	0.44
1:B:139:ILE:HG12	1:B:172:ASN:HD21	1.83	0.43
1:D:202:LEU:HB2	1:D:203:PRO:HD3	2.00	0.43
1:A:128:TYR:O	1:A:129:LEU:HB2	2.17	0.43
1:A:213:THR:HB	1:B:273:THR:HG21	1.99	0.43
1:B:77:PHE:HB3	1:B:80:VAL:CG2	2.47	0.43
1:B:78:VAL:HB	1:B:128:TYR:HB2	1.99	0.43
1:C:54:ASP:HA	1:C:55:PRO:HD2	1.77	0.43
1:E:53:PHE:O	1:E:53:PHE:HD1	1.98	0.43
1:A:253:TYR:CD1	1:A:314:PHE:HE1	2.36	0.43
1:C:8:PRO:HA	1:C:71:TRP:CD1	2.53	0.43
1:D:143:VAL:O	1:D:145:LEU:N	2.51	0.43
1:A:125:LEU:HB2	1:A:187:LEU:HB3	2.00	0.43
1:E:35:THR:O	1:E:36:PHE:HB3	2.18	0.43
1:E:89:VAL:CG1	1:E:102:LEU:HD23	2.47	0.43
1:D:130:ILE:HA	1:D:181:SER:O	2.18	0.43
1:D:264:PHE:O	1:D:268:ALA:HB2	2.19	0.43
1:E:255:GLY:HA2	1:E:258:ILE:CG2	2.48	0.43
1:A:123:GLN:C	1:A:188:ARG:HH21	2.26	0.43
1:A:254:THR:O	1:A:258:ILE:HB	2.18	0.43
1:B:125:LEU:HB2	1:B:187:LEU:HB3	2.01	0.43
1:B:264:PHE:CE2	1:B:302:PHE:HB2	2.53	0.43
1:C:81:GLU:HG3	1:C:108:ARG:CG	2.47	0.43
1:C:276:HIS:O	1:C:280:VAL:HG22	2.18	0.43
1:A:202:LEU:HB2	1:A:203:PRO:HD3	2.01	0.43
1:B:9:PRO:HD3	1:B:71:TRP:CE3	2.53	0.43
1:C:19:THR:HA	1:C:43:SER:O	2.19	0.43
1:C:48:ASP:OD2	1:C:51:LEU:HD23	2.19	0.43
1:D:192:GLN:NE2	1:E:249:PRO:HG3	2.33	0.43
1:D:234:HIS:CE1	1:D:258:ILE:O	2.71	0.43
1:D:267:VAL:HG23	1:D:298:PHE:CZ	2.54	0.43
1:E:77:PHE:HB3	1:E:80:VAL:HG23	2.01	0.43
1:A:19:THR:HA	1:A:43:SER:O	2.18	0.43
1:A:35:THR:CG2	1:A:108:ARG:HH21	2.31	0.43
1:B:255:GLY:O	1:B:258:ILE:HG22	2.18	0.43
1:E:202:LEU:HB2	1:E:203:PRO:HD3	2.01	0.43
1:B:81:GLU:HG3	1:B:108:ARG:CG	2.48	0.43
1:C:125:LEU:HB2	1:C:187:LEU:HB3	2.01	0.43
1:E:125:LEU:HB2	1:E:187:LEU:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:200:ILE:O	1:E:204:MET:HB3	2.18	0.43
1:A:224:VAL:HG23	1:E:225:THR:HG21	2.00	0.43
1:B:264:PHE:O	1:B:268:ALA:HB2	2.19	0.43
1:C:202:LEU:HB2	1:C:203:PRO:HD3	2.01	0.43
1:C:298:PHE:CB	1:C:299:PRO:HD3	2.48	0.43
1:D:146:GLU:HG3	1:E:176:GLU:CD	2.44	0.43
1:E:77:PHE:HB3	1:E:80:VAL:CG2	2.48	0.43
1:A:193:TYR:CD1	1:A:193:TYR:N	2.86	0.42
1:C:22:TYR:CA	1:C:149:GLY:HA2	2.33	0.42
1:C:254:THR:O	1:C:258:ILE:HB	2.19	0.42
1:E:81:GLU:HG3	1:E:108:ARG:CG	2.47	0.42
1:A:78:VAL:HB	1:A:128:TYR:HB2	2.01	0.42
1:A:77:PHE:HB3	1:A:80:VAL:HG23	2.00	0.42
1:B:111:SER:HA	1:B:112:PRO:HD2	1.77	0.42
1:B:290:ILE:HG22	1:B:291:THR:N	2.35	0.42
1:A:255:GLY:O	1:A:258:ILE:HG22	2.20	0.42
1:B:54:ASP:HA	1:B:55:PRO:HD2	1.76	0.42
1:B:123:GLN:C	1:B:188:ARG:HH21	2.28	0.42
1:A:212:TRP:C	1:A:214:ALA:H	2.27	0.42
1:B:35:THR:O	1:B:36:PHE:HB3	2.19	0.42
1:B:193:TYR:CG	1:B:194:PHE:N	2.87	0.42
1:B:255:GLY:HA2	1:B:258:ILE:CG2	2.49	0.42
1:C:264:PHE:CE2	1:C:302:PHE:HB2	2.54	0.42
1:D:19:THR:HA	1:D:43:SER:O	2.20	0.42
1:D:271:GLU:O	1:D:274:VAL:N	2.51	0.42
1:E:151:ASN:C	1:E:153:ASP:H	2.27	0.42
1:A:38:VAL:HG22	1:A:39:ASN:N	2.34	0.42
1:A:41:PHE:HE2	1:B:175:LEU:HD13	1.85	0.42
1:C:35:THR:O	1:C:36:PHE:HB3	2.18	0.42
1:C:94:SER:OG	1:C:95:PRO:HD2	2.19	0.42
1:A:298:PHE:CB	1:A:299:PRO:HD3	2.47	0.42
1:B:13:GLU:CB	1:B:14:PRO:CD	2.92	0.42
1:B:29:LEU:HB2	1:B:156:LEU:HD11	2.01	0.42
1:B:150:LYS:HB3	1:B:150:LYS:HE2	1.89	0.42
1:B:194:PHE:C	1:B:196:TYR:N	2.77	0.42
1:C:264:PHE:O	1:C:268:ALA:HB2	2.19	0.42
1:D:197:ILE:HB	1:D:198:PRO:CD	2.39	0.42
1:E:27:TYR:CE1	1:E:37:LYS:CB	3.03	0.42
1:B:35:THR:CG2	1:B:108:ARG:HH21	2.32	0.42
1:B:89:VAL:CG1	1:B:102:LEU:HD23	2.50	0.42
1:D:77:PHE:HB3	1:D:80:VAL:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:193:TYR:CG	1:E:194:PHE:N	2.88	0.42
1:E:216:TRP:CH2	1:E:295:ARG:CB	3.03	0.42
1:E:255:GLY:O	1:E:258:ILE:HG22	2.20	0.42
1:A:22:TYR:HA	1:A:149:GLY:HA3	2.00	0.42
1:A:234:HIS:HE1	1:A:258:ILE:O	2.02	0.42
1:A:255:GLY:HA2	1:A:258:ILE:CG2	2.48	0.42
1:B:133:SER:HB3	1:B:136:THR:O	2.19	0.42
1:B:148:VAL:O	1:B:149:GLY:C	2.63	0.42
1:C:234:HIS:CE1	1:C:258:ILE:O	2.72	0.42
1:C:271:GLU:O	1:C:274:VAL:N	2.50	0.42
1:C:290:ILE:HG22	1:C:291:THR:N	2.34	0.42
1:D:193:TYR:CD1	1:D:193:TYR:N	2.86	0.42
1:E:19:THR:HA	1:E:43:SER:O	2.20	0.42
1:E:23:LEU:HA	1:E:40:ALA:HB2	2.00	0.42
1:E:38:VAL:HG22	1:E:39:ASN:N	2.34	0.42
1:E:194:PHE:C	1:E:196:TYR:N	2.77	0.42
1:D:128:TYR:O	1:D:129:LEU:HB2	2.19	0.42
1:E:130:ILE:HA	1:E:181:SER:O	2.20	0.42
1:E:264:PHE:CE2	1:E:302:PHE:HB2	2.54	0.42
1:E:309:LEU:O	1:E:312:LEU:HB3	2.19	0.42
1:A:29:LEU:HB2	1:A:156:LEU:HD11	2.02	0.41
1:A:89:VAL:CG1	1:A:102:LEU:HD23	2.49	0.41
1:A:94:SER:OG	1:A:95:PRO:HD2	2.20	0.41
1:B:216:TRP:CH2	1:B:295:ARG:CB	3.03	0.41
1:B:292:ARG:HD2	1:B:295:ARG:HD2	2.02	0.41
1:C:93:VAL:HG22	1:C:99:VAL:HG13	2.02	0.41
1:C:104:ARG:HD2	1:D:76:ARG:NH1	2.35	0.41
1:D:174:ALA:HA	1:D:179:LEU:HA	2.02	0.41
1:A:194:PHE:C	1:A:196:TYR:N	2.77	0.41
1:A:290:ILE:HG22	1:A:291:THR:N	2.35	0.41
1:B:192:GLN:NE2	1:C:249:PRO:HG3	2.35	0.41
1:C:155:PHE:CZ	1:C:157:THR:HG23	2.55	0.41
1:C:207:ILE:HG13	1:C:208:LEU:N	2.35	0.41
1:D:232:ILE:HA	1:D:235:ILE:HD12	2.02	0.41
1:E:29:LEU:HB2	1:E:156:LEU:HD11	2.02	0.41
1:E:148:VAL:O	1:E:149:GLY:C	2.62	0.41
1:A:81:GLU:HG3	1:A:108:ARG:CG	2.50	0.41
1:A:249:PRO:HD2	1:A:250:TYR:HD1	1.81	0.41
1:B:76:ARG:HH22	1:B:130:ILE:HD12	1.85	0.41
1:C:193:TYR:CG	1:C:194:PHE:N	2.88	0.41
1:C:194:PHE:C	1:C:196:TYR:N	2.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:TRP:CH2	1:D:295:ARG:CB	3.03	0.41
1:D:225:THR:HG21	1:E:224:VAL:HG23	2.02	0.41
1:A:264:PHE:CE2	1:A:302:PHE:HB2	2.54	0.41
1:B:234:HIS:HE1	1:B:258:ILE:O	2.03	0.41
1:C:193:TYR:CD1	1:C:193:TYR:N	2.86	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:HB3	2.21	0.41
1:E:267:VAL:HG23	1:E:298:PHE:CZ	2.55	0.41
1:E:269:VAL:O	1:E:270:ILE:C	2.64	0.41
1:A:132:ARG:HA	1:A:180:GLU:HG2	2.02	0.41
1:C:89:VAL:CG1	1:C:102:LEU:HD23	2.50	0.41
1:C:151:ASN:C	1:C:153:ASP:H	2.27	0.41
1:D:124:THR:HB	1:D:188:ARG:HE	1.83	0.41
1:E:271:GLU:O	1:E:274:VAL:N	2.53	0.41
1:A:193:TYR:CG	1:A:194:PHE:N	2.87	0.41
1:C:38:VAL:HG22	1:C:39:ASN:N	2.36	0.41
1:C:134:VAL:HG12	1:C:135:ASP:H	1.85	0.41
1:D:194:PHE:C	1:D:196:TYR:N	2.77	0.41
1:D:255:GLY:HA2	1:D:258:ILE:CG2	2.50	0.41
1:E:22:TYR:HA	1:E:149:GLY:HA3	1.96	0.41
1:E:22:TYR:HB3	1:E:41:PHE:HB2	2.02	0.41
1:E:51:LEU:HB3	1:E:93:VAL:HG11	2.03	0.41
1:D:78:VAL:HB	1:D:128:TYR:HB2	2.01	0.41
1:D:94:SER:OG	1:D:95:PRO:HD2	2.21	0.41
1:D:129:LEU:HD22	1:D:185:TYR:CE1	2.56	0.41
1:D:254:THR:O	1:D:258:ILE:HB	2.21	0.41
1:A:151:ASN:C	1:A:153:ASP:H	2.28	0.41
1:B:151:ASN:C	1:B:153:ASP:H	2.28	0.41
1:C:32:LYS:HD3	1:C:243:THR:O	2.21	0.41
1:C:269:VAL:O	1:C:270:ILE:C	2.63	0.41
1:A:130:ILE:HA	1:A:181:SER:O	2.21	0.41
1:A:155:PHE:HB3	1:A:156:LEU:H	1.71	0.41
1:A:255:GLY:C	1:A:258:ILE:HG22	2.46	0.41
1:A:261:ILE:O	1:A:265:TYR:HD1	2.04	0.41
1:A:292:ARG:HD2	1:A:295:ARG:HD2	2.03	0.41
1:B:202:LEU:HB2	1:B:203:PRO:HD3	2.02	0.41
1:D:134:VAL:HG12	1:D:135:ASP:H	1.85	0.41
1:D:150:LYS:HB3	1:D:150:LYS:HE2	1.90	0.41
1:E:84:ARG:CB	1:E:107:ALA:HB2	2.51	0.41
1:E:128:TYR:O	1:E:129:LEU:HB2	2.20	0.41
1:E:150:LYS:HB3	1:E:150:LYS:HE2	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:234:HIS:HE1	1:E:258:ILE:O	2.03	0.41
1:A:212:TRP:C	1:A:214:ALA:N	2.79	0.41
1:B:119:PRO:HB2	1:B:120:PHE:CE1	2.56	0.41
1:B:255:GLY:C	1:B:258:ILE:HG22	2.46	0.41
1:D:234:HIS:HE1	1:D:258:ILE:O	2.04	0.41
1:E:249:PRO:HD2	1:E:250:TYR:HD1	1.82	0.41
1:A:200:ILE:O	1:A:204:MET:HB3	2.21	0.40
1:B:200:ILE:O	1:B:204:MET:HB3	2.21	0.40
1:E:65:TYR:O	1:E:91:ILE:HD13	2.21	0.40
1:E:212:TRP:C	1:E:214:ALA:H	2.28	0.40
1:E:290:ILE:HG22	1:E:291:THR:N	2.35	0.40
1:A:76:ARG:HH22	1:A:130:ILE:HD12	1.86	0.40
1:A:118:TYR:HD2	1:A:254:THR:HG21	1.86	0.40
1:A:148:VAL:O	1:A:149:GLY:C	2.64	0.40
1:C:134:VAL:HG12	1:C:135:ASP:N	2.37	0.40
1:C:200:ILE:O	1:C:204:MET:HB3	2.20	0.40
1:C:216:TRP:CH2	1:C:295:ARG:CB	3.05	0.40
1:D:111:SER:HA	1:D:112:PRO:HD2	1.76	0.40
1:E:129:LEU:HD22	1:E:185:TYR:CE1	2.57	0.40
1:E:140:VAL:HG22	1:E:181:SER:HB3	2.03	0.40
1:E:216:TRP:HA	1:E:295:ARG:HH21	1.86	0.40
1:B:19:THR:HA	1:B:43:SER:O	2.20	0.40
1:B:207:ILE:HG13	1:B:208:LEU:N	2.37	0.40
1:C:212:TRP:C	1:C:214:ALA:H	2.29	0.40
1:C:213:THR:HB	1:D:273:THR:HG21	2.04	0.40
1:D:123:GLN:HA	1:D:123:GLN:NE2	2.37	0.40
1:D:128:TYR:O	1:D:183:LEU:O	2.40	0.40
1:E:183:LEU:HD23	1:E:183:LEU:HA	1.84	0.40
1:E:264:PHE:O	1:E:268:ALA:HB2	2.22	0.40
1:A:72:ILE:HA	1:A:73:PRO:HD3	1.99	0.40
1:A:216:TRP:CH2	1:A:295:ARG:CB	3.04	0.40
1:B:134:VAL:HG12	1:B:135:ASP:H	1.86	0.40
1:E:119:PRO:HG3	1:E:254:THR:CB	2.39	0.40
1:E:255:GLY:C	1:E:258:ILE:HG22	2.46	0.40
1:B:159:TRP:CE3	1:B:189:ILE:HD12	2.57	0.40
1:C:32:LYS:HD3	1:C:245:LEU:H	1.86	0.40
1:D:18:ASN:O	1:D:44:LEU:HA	2.21	0.40
1:D:155:PHE:CZ	1:D:157:THR:HG23	2.57	0.40
1:D:193:TYR:CG	1:D:194:PHE:N	2.88	0.40
1:E:230:THR:OG1	1:E:265:TYR:HE2	2.04	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%)	246 (80%)	44 (14%)	18 (6%)	1	13
1	B	308/317 (97%)	250 (81%)	40 (13%)	18 (6%)	1	13
1	C	308/317 (97%)	247 (80%)	43 (14%)	18 (6%)	1	13
1	D	308/317 (97%)	249 (81%)	42 (14%)	17 (6%)	1	13
1	E	308/317 (97%)	247 (80%)	43 (14%)	18 (6%)	1	13
All	All	1540/1585 (97%)	1239 (80%)	212 (14%)	89 (6%)	1	13

All (89) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	149	GLY
1	A	178	ARG
1	A	193	TYR
1	B	149	GLY
1	B	178	ARG
1	B	193	TYR
1	C	149	GLY
1	C	178	ARG
1	C	193	TYR
1	D	149	GLY
1	D	178	ARG
1	D	193	TYR
1	E	149	GLY
1	E	178	ARG
1	E	193	TYR
1	A	59	GLY
1	A	144	ASP
1	A	148	VAL
1	A	173	PHE
1	A	194	PHE
1	A	242	GLU

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Mol	Chain	Res	Type
1	A	275	GLN
1	B	59	GLY
1	B	144	ASP
1	B	173	PHE
1	B	194	PHE
1	B	242	GLU
1	B	275	GLN
1	B	282	SER
1	C	59	GLY
1	C	144	ASP
1	C	148	VAL
1	C	173	PHE
1	C	194	PHE
1	C	242	GLU
1	C	275	GLN
1	D	59	GLY
1	D	144	ASP
1	D	148	VAL
1	D	173	PHE
1	D	194	PHE
1	D	242	GLU
1	D	275	GLN
1	E	59	GLY
1	E	144	ASP
1	E	148	VAL
1	E	173	PHE
1	E	194	PHE
1	E	242	GLU
1	E	275	GLN
1	A	134	VAL
1	A	282	SER
1	B	134	VAL
1	B	148	VAL
1	C	134	VAL
1	C	282	SER
1	D	134	VAL
1	D	282	SER
1	E	134	VAL
1	E	282	SER
1	A	129	LEU
1	A	177	ASP
1	A	195	SER

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Mol	Chain	Res	Type
1	B	129	LEU
1	B	177	ASP
1	B	195	SER
1	C	177	ASP
1	D	177	ASP
1	D	195	SER
1	E	129	LEU
1	E	177	ASP
1	C	129	LEU
1	C	195	SER
1	D	129	LEU
1	E	195	SER
1	A	54	ASP
1	B	54	ASP
1	C	54	ASP
1	C	118	TYR
1	D	54	ASP
1	E	54	ASP
1	D	118	TYR
1	A	118	TYR
1	B	118	TYR
1	E	118	TYR
1	A	60	VAL
1	C	60	VAL
1	B	60	VAL
1	E	60	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	277/283 (98%)	243 (88%)	34 (12%)	4	22
1	B	277/283 (98%)	242 (87%)	35 (13%)	4	21
1	C	277/283 (98%)	243 (88%)	34 (12%)	4	22
1	D	277/283 (98%)	243 (88%)	34 (12%)	4	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	277/283 (98%)	244 (88%)	33 (12%)	5	23
All	All	1385/1415 (98%)	1215 (88%)	170 (12%)	4	22

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	THR
1	A	45	SER
1	A	53	PHE
1	A	74	GLU
1	A	84	ARG
1	A	89	VAL
1	A	109	VAL
1	A	111	SER
1	A	120	PHE
1	A	130	ILE
1	A	135	ASP
1	A	141	LEU
1	A	144	ASP
1	A	148	VAL
1	A	154	VAL
1	A	157	THR
1	A	168	VAL
1	A	175	LEU
1	A	188	ARG
1	A	190	SER
1	A	193	TYR
1	A	202	LEU
1	A	211	SER
1	A	228	VAL
1	A	239	ILE
1	A	244	ASN
1	A	252	THR
1	A	257	ILE
1	A	263	LEU
1	A	274	VAL
1	A	290	ILE
1	A	292	ARG
1	A	303	LEU
1	A	314	PHE
1	B	16	THR
1	B	45	SER

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Mol	Chain	Res	Type
1	B	53	PHE
1	B	74	GLU
1	B	84	ARG
1	B	89	VAL
1	B	109	VAL
1	B	111	SER
1	B	120	PHE
1	B	130	ILE
1	B	135	ASP
1	B	141	LEU
1	B	144	ASP
1	B	148	VAL
1	B	154	VAL
1	B	157	THR
1	B	168	VAL
1	B	175	LEU
1	B	188	ARG
1	B	190	SER
1	B	193	TYR
1	B	202	LEU
1	B	211	SER
1	B	228	VAL
1	B	239	ILE
1	B	244	ASN
1	B	252	THR
1	B	257	ILE
1	B	263	LEU
1	B	269	VAL
1	B	274	VAL
1	B	290	ILE
1	B	292	ARG
1	B	303	LEU
1	B	314	PHE
1	C	16	THR
1	C	45	SER
1	C	53	PHE
1	C	74	GLU
1	C	84	ARG
1	C	89	VAL
1	C	109	VAL
1	C	111	SER
1	C	120	PHE

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Mol	Chain	Res	Type
1	C	130	ILE
1	C	135	ASP
1	C	141	LEU
1	C	144	ASP
1	C	148	VAL
1	C	154	VAL
1	C	157	THR
1	C	168	VAL
1	C	175	LEU
1	C	188	ARG
1	C	190	SER
1	C	193	TYR
1	C	202	LEU
1	C	211	SER
1	C	228	VAL
1	C	239	ILE
1	C	244	ASN
1	C	252	THR
1	C	257	ILE
1	C	263	LEU
1	C	274	VAL
1	C	290	ILE
1	C	292	ARG
1	C	303	LEU
1	C	314	PHE
1	D	16	THR
1	D	45	SER
1	D	53	PHE
1	D	74	GLU
1	D	84	ARG
1	D	89	VAL
1	D	109	VAL
1	D	111	SER
1	D	120	PHE
1	D	130	ILE
1	D	135	ASP
1	D	141	LEU
1	D	144	ASP
1	D	154	VAL
1	D	157	THR
1	D	168	VAL
1	D	175	LEU

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Mol	Chain	Res	Type
1	D	188	ARG
1	D	190	SER
1	D	193	TYR
1	D	202	LEU
1	D	211	SER
1	D	228	VAL
1	D	239	ILE
1	D	244	ASN
1	D	252	THR
1	D	257	ILE
1	D	263	LEU
1	D	269	VAL
1	D	274	VAL
1	D	290	ILE
1	D	292	ARG
1	D	303	LEU
1	D	314	PHE
1	E	16	THR
1	E	45	SER
1	E	53	PHE
1	E	74	GLU
1	E	84	ARG
1	E	89	VAL
1	E	109	VAL
1	E	111	SER
1	E	120	PHE
1	E	130	ILE
1	E	135	ASP
1	E	141	LEU
1	E	144	ASP
1	E	148	VAL
1	E	154	VAL
1	E	157	THR
1	E	168	VAL
1	E	175	LEU
1	E	188	ARG
1	E	190	SER
1	E	193	TYR
1	E	202	LEU
1	E	228	VAL
1	E	239	ILE
1	E	244	ASN

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Mol	Chain	Res	Type
1	E	252	THR
1	E	257	ILE
1	E	263	LEU
1	E	274	VAL
1	E	290	ILE
1	E	292	ARG
1	E	303	LEU
1	E	314	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	ASN
1	A	172	ASN
1	A	192	GLN
1	A	199	ASN
1	A	234	HIS
1	A	238	ASN
1	A	306	ASN
1	B	123	GLN
1	B	151	ASN
1	B	172	ASN
1	B	192	GLN
1	B	199	ASN
1	B	234	HIS
1	B	238	ASN
1	B	306	ASN
1	C	123	GLN
1	C	151	ASN
1	C	192	GLN
1	C	199	ASN
1	C	234	HIS
1	C	238	ASN
1	C	306	ASN
1	D	151	ASN
1	D	172	ASN
1	D	192	GLN
1	D	199	ASN
1	D	234	HIS
1	D	238	ASN
1	D	306	ASN
1	E	82	ASN

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Mol	Chain	Res	Type
1	E	151	ASN
1	E	172	ASN
1	E	192	GLN
1	E	199	ASN
1	E	234	HIS
1	E	238	ASN
1	E	306	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.65	21 (6%)	23	14	76, 103, 142, 169	0
1	B	310/317 (97%)	0.68	23 (7%)	20	13	76, 103, 142, 169	0
1	C	310/317 (97%)	0.63	23 (7%)	20	13	76, 103, 142, 169	0
1	D	310/317 (97%)	0.79	37 (11%)	9	6	76, 103, 142, 169	0
1	E	310/317 (97%)	0.68	29 (9%)	14	9	76, 103, 142, 169	0
All	All	1550/1585 (97%)	0.69	133 (8%)	16	11	76, 103, 143, 169	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	55	PRO	5.4
1	A	7	PRO	4.5
1	E	173	PHE	4.1
1	B	134	VAL	4.0
1	E	136	THR	4.0
1	B	144	ASP	3.9
1	B	11	ALA	3.9
1	E	218	THR	3.8
1	B	7	PRO	3.7
1	E	60	VAL	3.7
1	E	7	PRO	3.6
1	D	7	PRO	3.5
1	D	60	VAL	3.5
1	C	316	PHE	3.5
1	D	11	ALA	3.5
1	C	138	ASN	3.4
1	A	316	PHE	3.4
1	B	173	PHE	3.4
1	E	11	ALA	3.3
1	A	144	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	7	PRO	3.3
1	B	136	THR	3.3
1	D	56	VAL	3.2
1	A	138	ASN	3.2
1	D	59	GLY	3.2
1	C	142	ALA	3.1
1	C	11	ALA	3.1
1	D	54	ASP	3.1
1	E	316	PHE	3.1
1	D	144	ASP	3.1
1	D	148	VAL	3.1
1	D	95	PRO	3.1
1	A	11	ALA	3.0
1	E	144	ASP	3.0
1	D	173	PHE	3.0
1	C	173	PHE	2.9
1	D	8	PRO	2.9
1	B	61	ARG	2.9
1	A	220	TYR	2.9
1	E	146	GLU	2.9
1	A	173	PHE	2.9
1	C	315	GLY	2.8
1	B	148	VAL	2.8
1	C	53	PHE	2.8
1	D	218	THR	2.8
1	C	144	ASP	2.7
1	D	63	LYS	2.7
1	D	52	ALA	2.7
1	D	138	ASN	2.7
1	B	56	VAL	2.7
1	B	316	PHE	2.7
1	D	212	TRP	2.6
1	D	25	GLU	2.6
1	E	53	PHE	2.6
1	B	138	ASN	2.6
1	B	59	GLY	2.6
1	B	285	ALA	2.6
1	D	315	GLY	2.6
1	A	244	ASN	2.6
1	C	51	LEU	2.6
1	E	59	GLY	2.6
1	A	315	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	47	LYS	2.5
1	A	56	VAL	2.5
1	D	51	LEU	2.5
1	C	55	PRO	2.5
1	A	37	LYS	2.5
1	B	15	LEU	2.5
1	E	94	SER	2.5
1	D	96	ASP	2.5
1	D	137	ARG	2.5
1	C	63	LYS	2.4
1	B	135	ASP	2.4
1	D	136	THR	2.4
1	A	148	VAL	2.4
1	D	64	THR	2.4
1	C	275	GLN	2.4
1	D	134	VAL	2.4
1	A	149	GLY	2.4
1	B	315	GLY	2.4
1	D	53	PHE	2.4
1	E	148	VAL	2.4
1	C	220	TYR	2.4
1	E	147	LYS	2.3
1	E	145	LEU	2.3
1	E	153	ASP	2.3
1	C	65	TYR	2.3
1	A	134	VAL	2.3
1	C	64	THR	2.3
1	E	138	ASN	2.3
1	B	178	ARG	2.3
1	C	87	ASP	2.3
1	E	37	LYS	2.3
1	A	137	ARG	2.3
1	E	244	ASN	2.2
1	D	92	SER	2.2
1	C	178	ARG	2.2
1	D	61	ARG	2.2
1	B	142	ALA	2.2
1	D	243	THR	2.2
1	D	117	ARG	2.2
1	B	145	LEU	2.2
1	E	61	ARG	2.2
1	E	93	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	147	LYS	2.2
1	B	133	SER	2.1
1	E	212	TRP	2.1
1	E	149	GLY	2.1
1	E	288	ALA	2.1
1	C	56	VAL	2.1
1	C	60	VAL	2.1
1	D	10	ILE	2.1
1	A	218	THR	2.1
1	E	65	TYR	2.1
1	C	146	GLU	2.1
1	D	145	LEU	2.1
1	A	292	ARG	2.1
1	D	57	ARG	2.1
1	A	65	TYR	2.1
1	C	145	LEU	2.1
1	D	98	THR	2.1
1	B	139	ILE	2.1
1	C	82	ASN	2.1
1	D	316	PHE	2.1
1	E	134	VAL	2.1
1	D	178	ARG	2.0
1	E	62	VAL	2.0
1	A	8	PRO	2.0
1	D	108	ARG	2.0
1	B	147	LYS	2.0
1	E	220	TYR	2.0
1	A	64	THR	2.0
1	E	142	ALA	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.