



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:11 am GMT

PDB ID : 3EI0
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

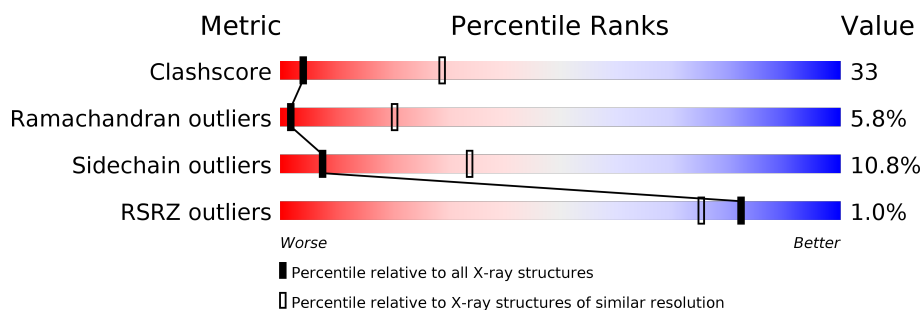
1 Overall quality at a glance

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	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)
RSRZ outliers	101464	1226 (3.60-3.40)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>%</div> <div> <div></div> <div>41%</div> <div>46%</div> <div>10%</div> <div>..</div> </div> </div>
1	B	317	<div> <div>%</div> <div> <div></div> <div>39%</div> <div>47%</div> <div>11%</div> <div>..</div> </div> </div>
1	C	317	<div> <div></div> <div> <div>39%</div> <div>49%</div> <div>9%</div> <div>..</div> </div> </div>
1	D	317	<div> <div>%</div> <div> <div></div> <div>40%</div> <div>47%</div> <div>9%</div> <div>..</div> </div> </div>
1	E	317	<div> <div>%</div> <div> <div></div> <div>41%</div> <div>47%</div> <div>10%</div> <div>..</div> </div> </div>

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	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	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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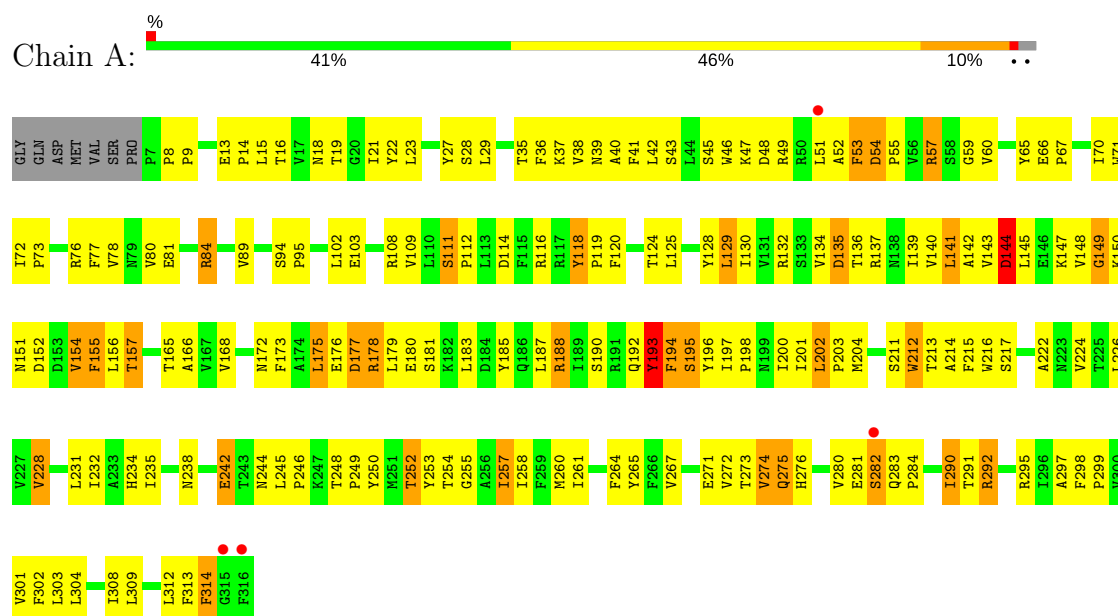
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Chain	Residue	Modelled	Actual	Comment	Reference
C	3	MET	-	EXPRESSION TAG	UNP Q7NDN8
C	4	VAL	-	EXPRESSION TAG	UNP Q7NDN8
C	5	SER	-	EXPRESSION TAG	UNP Q7NDN8
C	6	PRO	-	EXPRESSION TAG	UNP Q7NDN8
C	221	ALA	GLU	ENGINEERED	UNP Q7NDN8
D	0	GLY	-	EXPRESSION 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	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	UNP Q7NDN8

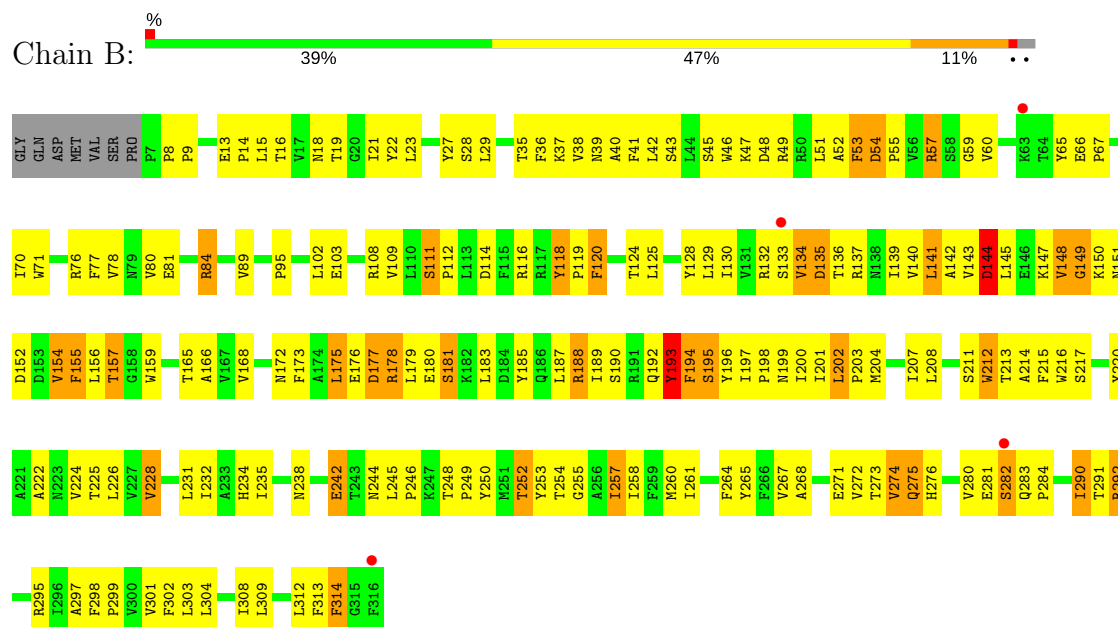
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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



Chain C: 39% 49% 9%

Amino Acid	Category	Percentage
GLY	Green	39%
GLN	Green	39%
VAL	Green	39%
SER	Green	39%
PRO	Green	39%
P8	Green	39%
P9	Green	39%
E13	Green	39%
P14	Green	39%
L15	Green	39%
T16	Green	39%
V17	Green	39%
N18	Green	39%
T19	Green	39%
G20	Green	39%
I21	Green	39%
Y22	Green	39%
L23	Green	39%
Y27	Green	39%
S28	Green	39%
L29	Green	39%
K32	Green	39%
T35	Green	39%
F36	Green	39%
K37	Green	39%
V38	Green	39%
N39	Green	39%
A40	Green	39%
F41	Green	39%
S43	Green	39%
L44	Green	39%
S45	Green	39%
N46	Green	39%
K47	Green	39%
D48	Green	39%
R49	Green	39%
R50	Green	39%
L51	Green	39%
A52	Green	39%
F53	Green	39%
D54	Green	39%
P55	Green	39%
V56	Green	39%
R57	Green	39%
K58	Green	39%
G59	Green	39%
V60	Green	39%
G65	Green	39%
E66	Green	39%
P67	Green	39%
I70	Orange	49%
W71	Orange	49%
R76	Orange	49%
F77	Orange	49%
Y78	Orange	49%
N79	Orange	49%
D80	Orange	49%
E81	Orange	49%
R84	Orange	49%
H89	Orange	49%
Q93	Orange	49%
P95	Orange	49%
V99	Orange	49%
L100	Orange	49%
S111	Orange	49%
P112	Orange	49%
L113	Orange	49%
D114	Orange	49%
F115	Orange	49%
R116	Orange	49%
R117	Orange	49%
Y118	Orange	49%
P119	Orange	49%
F120	Orange	49%
Q123	Orange	49%
T124	Orange	49%
L125	Orange	49%
Y128	Orange	49%
L129	Orange	49%
I130	Orange	49%
V131	Orange	49%
R132	Orange	49%
S133	Orange	49%
V134	Orange	49%
D135	Orange	49%
T136	Orange	49%
R137	Orange	49%
W138	Orange	49%
I139	Orange	49%
V140	Orange	49%
L141	Orange	49%
A142	Orange	49%
V143	Orange	49%
D144	Orange	49%
L145	Orange	49%
E146	Red	9%
K147	Red	9%
V148	Red	9%
G149	Red	9%
N150	Red	9%
D152	Red	9%
V154	Red	9%
F155	Red	9%
L156	Red	9%
T157	Red	9%
T165	Red	9%
A166	Red	9%
V167	Red	9%
V168	Red	9%
F172	Red	9%
F173	Red	9%
A174	Red	9%
L175	Red	9%
E176	Red	9%
D177	Red	9%
R178	Red	9%
L179	Red	9%
E180	Red	9%
L183	Red	9%
D184	Red	9%
V185	Red	9%
Q186	Red	9%
L187	Red	9%
R188	Red	9%
L189	Red	9%
S190	Red	9%
R191	Red	9%
Q192	Red	9%
F194	Red	9%
S195	Red	9%
V196	Red	9%
L197	Red	9%
P198	Red	9%
N199	Red	9%
L200	Red	9%
L201	Red	9%
L202	Red	9%
T203	Red	9%
M204	Red	9%
L207	Red	9%
L208	Red	9%
S211	Red	9%
W212	Red	9%
T213	Red	9%
A214	Red	9%
T215	Red	9%
F216	Red	9%
S217	Red	9%

[illegible]

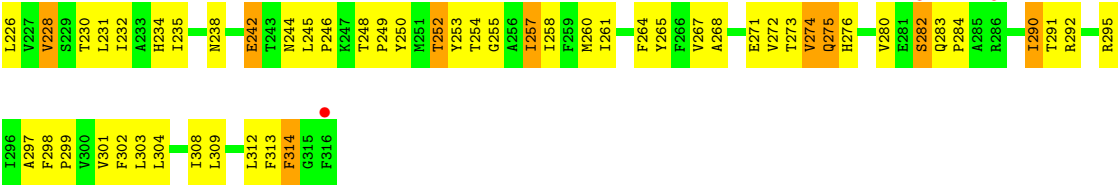
Chain E:

41% 47% 10%

GLY GLN ASP MET VAL SER PRO P7 P8 P9 E13 P14 L15 T16 V17 N18 T19 G20 Y21 Y22 Y23 Y27 Y28 L29 T35 F36 K37 V38 N39 A40 F41 F42 L43 S43 L44 S45 W46 K47 D48 R49 R50 L51 L52 A53 F53 D54 R57 S58 G59 V60 Y65 E66 P67 I70 W71

R76 F77 V78 N79 D79 V80 E81 R84 V89 D90 T91 S92 V93 S94 P95 L102 E103 A107 R108 V109 L110 S111 P112 L113 D114 F115 R116 R117 Y118 P119 F120 Q123 T124 L125 Y128 L129 T130 V131 R132 I133 S134 P135 D136 T137 M138 T139 V140 L141 A142 V143 D144 L145 E146 T147 H148

G149 K150 N151 D152 D153 V154 F155 L156 T157 T165 A166 V167 V168 N172 F173 A174 L175 E176 D177 R178 L179 E180 S181 K182 L183 D184 Y185 Q186 L187 R188 L189 S190 S191 R191 Q192 Y193 F194 S195 Y196 V197 I197 P198 P199 I200 I201 L202 P203 P204 M204 S211 W212 T213 T214 A214 F215 W216 A222 A223 V224 P225



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 39.58 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-3.50) 99.1 (39.58-3.50)	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 0.245 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	85.5	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 69.6	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	0.84	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	0.38	0/2585	0.54	0/3530
1	B	0.38	0/2585	0.54	0/3530
1	C	0.38	0/2585	0.54	0/3530
1	D	0.40	0/2585	0.55	0/3530
1	E	0.39	0/2585	0.54	0/3530
All	All	0.39	0/12925	0.54	0/17650

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2517	0	2536	168	0
1	B	2517	0	2536	172	0
1	C	2517	0	2536	170	0
1	D	2517	0	2536	170	0
1	E	2517	0	2536	170	0
All	All	12585	0	12680	825	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 33.

All (825) 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:HH11	1:B:84:ARG:CG	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:CG	1:D:84:ARG:HH11	1.88	0.87
1:E:84:ARG:HH11	1:E:84:ARG:CG	1.88	0.86
1:A:197:ILE:HB	1:A:198:PRO:HD3	1.57	0.86
1:C:84:ARG:CG	1:C:84:ARG:HH11	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG2	1:A:275:GLN:O	1.84	0.76
1:C:54:ASP:HB2	1:C:57:ARG:HG3	1.65	0.76
1:C:275:GLN:HG2	1:C:275:GLN:O	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:283:GLN:N	1:B:284:PRO:HD3	2.03	0.72
1:B:84:ARG:HH11	1:B:84:ARG:HG3	1.52	0.72
1:C:13:GLU:HB3	1:C:14:PRO:CD	2.19	0.72
1:C:84:ARG:HG3	1:C:84:ARG:HH11	1.54	0.72
1:E:84:ARG:HG3	1:E:84:ARG:HH11	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:HG3	1:D:84:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:257:ILE:O	1:E:261:ILE:HG12	1.92	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: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:HG2	1:A:84:ARG:HH11	1.58	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:HG2	1:C:84:ARG:HH11	1.60	0.67
1:B:297:ALA:O	1:B:301:VAL:HG23	1.95	0.66
1:B:84:ARG:HH11	1:B:84:ARG:HG2	1.61	0.66
1:D:84:ARG:HG2	1:D:84:ARG:HH11	1.60	0.66
1:E:81:GLU:HG3	1:E:108:ARG:HG3	1.78	0.66
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: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:B:274:VAL:C	1:B:276:HIS:H	2.01	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:A:140:VAL:CG2	1:A:183:LEU:HG	2.29	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:A:274:VAL:C	1:A:276:HIS:H	2.02	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: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:D:274:VAL:C	1:D:276:HIS:H	2.02	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:PHE:H	1:B:314:PHE:HD1	1.48	0.61
1:D:175:LEU:HD22	1:D:176:GLU:HG3	1.83	0.61
1:A:84:ARG:NH1	1:A:84:ARG:HG3	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:H	1:C:314:PHE:HD1	1.49	0.61
1:A:214:ALA:HB2	1:A:226:LEU:HD23	1.83	0.61
1:B:53:PHE:CD1	1:B:53:PHE:O	2.53	0.61
1:C:53:PHE:CD1	1:C:53:PHE:O	2.54	0.61
1:E:274:VAL:C	1:E:276:HIS:H	2.03	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:314:PHE:HD1	1:E:314:PHE:H	1.49	0.60
1:E:76:ARG:NH2	1:E:130:ILE:HD12	2.16	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:B:175:LEU:HD22	1:B:176:GLU:HG3	1.83	0.60
1:B:42:LEU:HB3	1:B:103:GLU:CG	2.32	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
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:D:151:ASN:O	1:D:154:VAL:HG22	2.02	0.60
1:A:112:PRO:HB3	1:E:155:PHE:CE1	2.37	0.60
1:A:42:LEU:HB3	1:A:103:GLU:CG	2.32	0.60
1:C:274:VAL:C	1:C:276:HIS:H	2.03	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: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:304:LEU:O	1:B:308:ILE:HG12	2.02	0.59
1:B:27:TYR:CE1	1:B:37:LYS:HB3	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:PHE:O	1:E:53:PHE:CD1	2.56	0.59
1:A:177:ASP:O	1:A:178:ARG:CB	2.50	0.59
1:A:51:LEU:HD11	1:A:70:ILE:HD12	1.83	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:N	1:E:314:PHE:CD1	2.71	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:NH1	1:A:84:ARG:CG	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: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: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
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:H	1:D:314:PHE:HD1	1.51	0.58
1:C:141:LEU:HD23	1:C:142:ALA:N	2.19	0.58
1:D:314:PHE:N	1:D:314:PHE:CD1	2.72	0.58
1:B:193:TYR:H	1:B:193:TYR:HD1	1.52	0.58
1:B:84:ARG:NH1	1:B:84:ARG:HG3	2.17	0.58
1:C:304:LEU:O	1:C:308:ILE:HG12	2.04	0.58
1:A:314:PHE:CD1	1:A:314:PHE:N	2.71	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:CD1	1:A:53:PHE:O	2.56	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:147:LYS:C	1:A:149:GLY:H	2.07	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:114:ASP:OD2	1:C:116:ARG:HB2	2.05	0.56
1:C:70:ILE:HG22	1:C:71:TRP:O	2.05	0.56
1:D:84:ARG:HD3	1:D:84:ARG:H	1.70	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: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:51:LEU:HD11	1:B:70:ILE:HD12	1.88	0.56
1:D:53:PHE:O	1:D:53:PHE:CD1	2.59	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:E:147:LYS:C	1:E:149:GLY:H	2.09	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: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:B:53:PHE:C	1:B:53:PHE:HD1	2.10	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:216:TRP:CH2	1:E:295:ARG:HB2	2.41	0.55
1:B:255:GLY:HA2	1:B:258:ILE:HG22	1.89	0.54
1:C:84:ARG:HD3	1:C:84:ARG:H	1.72	0.54
1:D:216:TRP:CH2	1:D:295:ARG:HB2	2.42	0.54
1:D:54:ASP:HB2	1:D:57:ARG:CG	2.37	0.54
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:147:LYS:C	1:C:149:GLY:H	2.09	0.54
1:C:283:GLN:N	1:C:284:PRO:CD	2.71	0.54
1:C:260:MET:CE	1:C:309:LEU:HD22	2.38	0.54
1:E:283:GLN:N	1:E:284:PRO:CD	2.69	0.54
1:E:84:ARG:H	1:E:84:ARG:HD3	1.72	0.54
1:B:76:ARG:NH2	1:B:130:ILE:HD12	2.22	0.54
1:C:53:PHE:CD1	1:C:53:PHE:C	2.81	0.54
1:C:53:PHE:HD1	1:C:53:PHE:C	2.11	0.54
1:D:193:TYR:H	1:D:193:TYR:HD1	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:B:147:LYS:C	1:B:149:GLY:H	2.11	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:H	1:C:193:TYR:HD1	1.54	0.53
1:A:216:TRP:CH2	1:A:295:ARG:HB2	2.43	0.53
1:C:84:ARG:NH1	1:C:84:ARG:HG3	2.19	0.53
1:D:18:ASN:HB3	1:D:143:VAL:CG2	2.38	0.53
1:D:197:ILE:HA	1:D:201:ILE:HB	1.90	0.53
1:D:28:SER:O	1:D:36:PHE:HA	2.08	0.53
1:E:53:PHE:HD1	1:E:53:PHE:C	2.11	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:B:48:ASP:CG	1:B:51:LEU:HD23	2.29	0.53
1:C:155:PHE:CE2	1:C:157:THR:HG23	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:LYS:C	1:D:149:GLY:H	2.12	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:B:53:PHE:CD1	1:B:53:PHE:C	2.81	0.53
1:C:48:ASP:CG	1:C:51:LEU:HD23	2.29	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
1:E:147:LYS:O	1:E:149:GLY:N	2.43	0.52
1:E:70:ILE:HG22	1:E:71:TRP:O	2.09	0.52
1:A:53:PHE:HD1	1:A:53:PHE:C	2.12	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:E:53:PHE:C	1:E:53:PHE:CD1	2.82	0.52
1:E:224:VAL:O	1:E:228:VAL:HB	2.10	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: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: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:A:53:PHE:CD1	1:A:53:PHE:C	2.82	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:NH1	1:D:84:ARG:CG	2.58	0.51
1:E:66:GLU:HG3	1:E:67:PRO:HD2	1.92	0.51
1:B:274:VAL:C	1:B:276:HIS:N	2.64	0.51
1:C:28:SER:O	1:C:36:PHE:HA	2.11	0.51
1:D:53:PHE:C	1:D:53:PHE:CD1	2.84	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:53:PHE:C	1:D:53:PHE:HD1	2.14	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:D:48:ASP:CG	1:D:51:LEU:HD23	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:MET:CE	1:A:309:LEU:HD22	2.40	0.51
1:A:274:VAL:C	1:A:276:HIS:N	2.64	0.51
1:C:274:VAL:C	1:C:276:HIS:N	2.64	0.51
1:D:238:ASN:HA	1:D:258:ILE:CD1	2.40	0.51
1:D:35:THR:HG21	1:D:108:ARG:HH21	1.76	0.51
1:A:147:LYS:C	1:A:149:GLY:N	2.64	0.51
1:B:65:TYR:CG	1:B:70:ILE:HD11	2.46	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
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:D:274:VAL:C	1:D:276:HIS:N	2.64	0.50
1:B:155:PHE:CE2	1:B:157:THR:HG23	2.47	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:NH1	1:D:84:ARG:HG3	2.20	0.50
1:E:275:GLN:HG3	1:E:291:THR:OG1	2.12	0.50
1:E:48:ASP:CG	1:E:51:LEU:HD23	2.32	0.50
1:A:275:GLN:HG3	1:A:291:THR:OG1	2.11	0.50
1:A:48:ASP:CG	1:A:51:LEU:HD23	2.32	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:E:147:LYS:C	1:E:149:GLY:N	2.66	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:C:15:LEU:HD11	1:C:46:TRP:HB2	1.94	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:A:238:ASN:HA	1:A:258:ILE:CD1	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:LYS:HD2	1:B:49:ARG:NH2	2.26	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:E:274:VAL:C	1:E:276:HIS:N	2.65	0.49
1:B:222:ALA:O	1:B:226:LEU:HB2	2.12	0.49
1:B:119:PRO:HG3	1:B:254:THR:CB	2.36	0.49
1:E:149:GLY:O	1:E:150:LYS:HB2	2.13	0.49
1:E:78:VAL:HG22	1:E:130:ILE:HG12	1.93	0.49
1:B:53:PHE:HD1	1:B:53:PHE:O	1.96	0.49
1:C:252:THR:HG23	1:C:255:GLY:HA3	1.93	0.49
1:C:54:ASP:HB2	1:C:57:ARG:CG	2.39	0.49
1:D:144:ASP:HA	1:D:147:LYS:HB3	1.95	0.49
1:D:149:GLY:O	1:D:150:LYS:HB2	2.13	0.49
1:E:212:TRP:HB2	1:E:215:PHE:CE1	2.48	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:248:THR:HB	1:A:250:TYR:CE1	2.48	0.48
1:A:53:PHE:CE1	1:A:95:PRO:HA	2.47	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:B:147:LYS:C	1:B:149:GLY:N	2.66	0.48
1:C:147:LYS:C	1:C:149:GLY:N	2.66	0.48
1:C:245:LEU:HD12	1:C:246:PRO:HD2	1.94	0.48
1:A:166:ALA:HB2	1:A:185:TYR:CD2	2.49	0.48
1:A:65:TYR:CG	1:A:70:ILE:HD11	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:248:THR:HB	1:B:250:TYR:CE1	2.49	0.48
1:B:84:ARG:NH1	1:B:84:ARG:CG	2.56	0.48
1:C:192:GLN:NE2	1:D:249:PRO:HG3	2.29	0.48
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: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:252:THR:HG23	1:A:255:GLY:HA3	1.96	0.47
1:A:23:LEU:HA	1:A:40:ALA:HB2	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:238:ASN:HA	1:E:258:ILE:CD1	2.43	0.47
1:E:89:VAL:HG11	1:E:102:LEU:HD23	1.96	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:C:135:ASP:C	1:C:135:ASP:OD2	2.53	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:C:232:ILE:HA	1:C:235:ILE:HD12	1.96	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:D:8:PRO:HA	1:D:71:TRP:CD1	2.49	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:84:ARG:NH1	1:C:84:ARG:CG	2.57	0.47
1:E:248:THR:HB	1:E:250:TYR:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:PRO:HA	1:E:71:TRP:CD1	2.50	0.47
1:A:253:TYR:HA	1:A:313:PHE:CE2	2.50	0.47
1:A:35:THR:O	1:A:36:PHE:HB3	2.15	0.47
1:B:54:ASP:HB2	1:B:57:ARG:CG	2.38	0.47
1:C:144:ASP:HA	1:C:147:LYS:HB3	1.97	0.47
1:D:147:LYS:C	1:D:149:GLY:N	2.67	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:252:THR:HG23	1:E:255:GLY:HA3	1.96	0.47
1:E:282:SER:C	1:E:284:PRO:HD3	2.35	0.47
1:A:212:TRP:HB2	1:A:215:PHE:CE1	2.49	0.47
1:C:149:GLY:O	1:C:150:LYS:HB2	2.15	0.47
1:C:23:LEU:HA	1:C:40:ALA:HB2	1.95	0.47
1:E:53:PHE:CE1	1:E:95:PRO:HA	2.50	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: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: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:253:TYR:HB2	1:B:313:PHE:CD2	2.50	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: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:35:THR:HG21	1:E:108:ARG:HH21	1.80	0.46
1:E:15:LEU:HD12	1:E:16:THR:N	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:LEU:HD12	1:D:246:PRO:HD2	1.97	0.46
1:B:282:SER:C	1:B:284:PRO:HD3	2.36	0.46
1:D:36:PHE:CE1	1:D:109:VAL:HB	2.51	0.46
1:A:249:PRO:HG3	1:E:192:GLN:NE2	2.31	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
1:C:282:SER:C	1:C:284:PRO:HD3	2.36	0.46
1:C:89:VAL:HG11	1:C:102:LEU:HD23	1.97	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: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:E:231:LEU:HD13	1:E:265:TYR:CB	2.45	0.46
1:A:260:MET:HE3	1:A:309:LEU:HD22	1.98	0.46
1:B:276:HIS:O	1:B:280:VAL:HG22	2.16	0.46
1:D:53:PHE:O	1:D:54:ASP:C	2.54	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: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:149:GLY:O	1:A:150:LYS:HB2	2.16	0.45
1:A:53:PHE:HD1	1:A:53:PHE:O	2.00	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: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:D:23:LEU:HA	1:D:40:ALA:HB2	1.98	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:A:282:SER:C	1:A:284:PRO:HD3	2.37	0.45
1:B:36:PHE:CE1	1:B:109:VAL:HB	2.51	0.45
1:D:135:ASP:OD2	1:D:135:ASP:C	2.54	0.45
1:D:38:VAL:HG22	1:D:39:ASN:N	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:282:SER:C	1:D:284:PRO:HD3	2.36	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
1:C:196:TYR:N	1:C:196:TYR:CD1	2.85	0.45
1:D:260:MET:HE2	1:D:309:LEU:HD22	1.99	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:A:53:PHE:O	1:A:54:ASP:C	2.55	0.45
1:E:9:PRO:HD3	1:E:71:TRP:CE3	2.52	0.45
1:B:196:TYR:HD1	1:B:196:TYR:N	2.14	0.45
1:B:53:PHE:O	1:B:54:ASP:C	2.55	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:143:VAL:O	1:C:145:LEU:N	2.50	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:E:135:ASP:OD2	1:E:135:ASP:C	2.55	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:135:ASP:OD2	1:B:135:ASP:C	2.55	0.45
1:B:136:THR:HG22	1:B:137:ARG:N	2.32	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: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:9:PRO:HD3	1:C:71:TRP:CE3	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:53:PHE:O	1:E:54:ASP:C	2.54	0.44
1:A:135:ASP:OD2	1:A:135:ASP:C	2.55	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
1:E:253:TYR:CD1	1:E:314:PHE:HE1	2.36	0.44
1:B:257:ILE:HG22	1:B:309:LEU:HD23	1.99	0.44
1:B:22:TYR:HB3	1:B:41:PHE:HB2	1.99	0.44
1:C:196:TYR:HD1	1:C:196:TYR:N	2.15	0.44
1:C:29:LEU:HB2	1:C:156:LEU:HD11	2.00	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:215:PHE:HZ	1:D:298:PHE:CE1	2.34	0.44
1:D:54:ASP:HA	1:D:55:PRO:HD2	1.65	0.44
1:E:139:ILE:HG12	1:E:172:ASN:HD21	1.81	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:166:ALA:HB2	1:B:185:TYR:CD2	2.52	0.44
1:B:77:PHE:HB3	1:B:80:VAL:HG23	2.00	0.44
1:C:77:PHE:HB3	1:C:80:VAL:CG2	2.48	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:D:35:THR:CG2	1:D:108:ARG:HH21	2.31	0.44
1:E:196:TYR:CD1	1:E:196:TYR:N	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:139:ILE:HG12	1:D:172:ASN:HD21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:LEU:HA	1:D:246:PRO:HD2	1.78	0.44
1:D:22:TYR:HB3	1:D:41:PHE:HB2	2.00	0.44
1:E:78:VAL:HB	1:E:128:TYR:HB2	1.99	0.44
1:A:111:SER:HA	1:A:112:PRO:HD2	1.75	0.44
1:A:196:TYR:CD1	1:A:196:TYR:N	2.85	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:C:128:TYR:O	1:C:129:LEU:HB2	2.17	0.44
1:C:179:LEU:C	1:C:179:LEU:HD12	2.38	0.44
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:78:VAL:HB	1:B:128:TYR:HB2	1.99	0.43
1:B:77:PHE:HB3	1:B:80:VAL:CG2	2.47	0.43
1:C:54:ASP:HA	1:C:55:PRO:HD2	1.77	0.43
1:E:53:PHE:HD1	1:E:53:PHE:O	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:B:260:MET:HE3	1:B:309:LEU:HD22	2.00	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:179:LEU:HD12	1:E:179:LEU:C	2.39	0.43
1:E:255:GLY:HA2	1:E:258:ILE:CG2	2.48	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:118:TYR:O	1:C:119:PRO:C	2.55	0.43
1:C:276:HIS:O	1:C:280:VAL:HG22	2.18	0.43
1:C:81:GLU:HG3	1:C:108:ARG:CG	2.47	0.43
1:D:179:LEU:C	1:D:179:LEU:HD12	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:35:THR:CG2	1:A:108:ARG:HH21	2.31	0.43
1:A:19:THR:HA	1:A:43:SER:O	2.18	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
1:E:200:ILE:O	1:E:204:MET:HB3	2.18	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:A:224:VAL:HG23	1:E:225:THR:HG21	2.00	0.43
1:E:77:PHE:HB3	1:E:80:VAL:CG2	2.48	0.43
1:A:193:TYR:N	1:A:193:TYR:CD1	2.86	0.42
1:C:22:TYR:CA	1:C:149:GLY:HA2	2.33	0.42
1:C:217:SER:HG	1:D:220:TYR:HE2	1.66	0.42
1:C:254:THR:O	1:C:258:ILE:HB	2.19	0.42
1:D:118:TYR:O	1:D:119:PRO:C	2.55	0.42
1:E:260:MET:HE3	1:E:309:LEU:HD22	2.01	0.42
1:E:81:GLU:HG3	1:E:108:ARG:CG	2.47	0.42
1:A:179:LEU:HD12	1:A:179:LEU:C	2.39	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:C:53:PHE:O	1:C:54:ASP:C	2.56	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: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:B:35:THR:O	1:B:36:PHE:HB3	2.19	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:118:TYR:O	1:E:119:PRO:C	2.58	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:150:LYS:HB3	1:B:150:LYS:HE2	1.89	0.42
1:B:29:LEU:HB2	1:B:156:LEU:HD11	2.01	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:89:VAL:CG1	1:B:102:LEU:HD23	2.50	0.42
1:B:35:THR:CG2	1:B:108:ARG:HH21	2.32	0.42
1:D:77:PHE:HB3	1:D:80:VAL:CG2	2.50	0.42
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:255:GLY:HA2	1:A:258:ILE:CG2	2.48	0.42
1:A:234:HIS:HE1	1:A:258:ILE:O	2.02	0.42
1:B:133:SER:HB3	1:B:136:THR:O	2.19	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:N	1:D:193:TYR:CD1	2.86	0.42
1:D:281:GLU:O	1:D:282:SER:C	2.58	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:19:THR:HA	1:E:43:SER:O	2.20	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:104:ARG:HD2	1:D:76:ARG:NH1	2.35	0.41
1:C:93:VAL:HG22	1:C:99:VAL:HG13	2.02	0.41
1:D:174:ALA:HA	1:D:179:LEU:HA	2.02	0.41
1:A:281:GLU:O	1:A:282:SER:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:ILE:HG22	1:A:291:THR:N	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:B:192:GLN:NE2	1:C:249:PRO:HG3	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:A:249:PRO:HD2	1:A:250:TYR:HD1	1.81	0.41
1:A:81:GLU:HG3	1:A:108:ARG:CG	2.50	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: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:118:TYR:O	1:B:119:PRO:C	2.58	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:C:281:GLU:O	1:C:282:SER:C	2.59	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: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: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:134:VAL:HG12	1:C:135:ASP:H	1.85	0.41
1:C:38:VAL:HG22	1:C:39:ASN:N	2.36	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: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: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:C:32:LYS:HD3	1:C:243:THR:O	2.21	0.41
1:E:123:GLN:C	1:E:188:ARG:HH21	2.24	0.41
1:A:130:ILE:HA	1:A:181:SER:O	2.21	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:150:LYS:HE2	1:D:150:LYS:HB3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE2	1:E:150:LYS:HB3	1.90	0.41
1:E:234:HIS:HE1	1:E:258:ILE:O	2.03	0.41
1:A:155:PHE:HB3	1:A:156:LEU:H	1.71	0.41
1:A:261:ILE:O	1:A:265:TYR:HD1	2.04	0.41
1:D:134:VAL:HG12	1:D:135:ASP:H	1.85	0.41
1:B:119:PRO:HB2	1:B:120:PHE:CE1	2.56	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:A:217:SER:HG	1:B:220:TYR:HE2	1.64	0.40
1:B:200:ILE:O	1:B:204:MET:HB3	2.21	0.40
1:B:217:SER:HG	1:C:220:TYR:HE2	1.66	0.40
1:E:290:ILE:HG22	1:E:291:THR:N	2.35	0.40
1:E:65:TYR:O	1:E:91:ILE:HD13	2.21	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:B:179:LEU:HD12	1:B:179:LEU:C	2.41	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:207:ILE:HG13	1:B:208:LEU:N	2.37	0.40
1:B:19:THR:HA	1:B:43:SER:O	2.20	0.40
1:D:123:GLN:NE2	1:D:123:GLN:HA	2.37	0.40
1:D:128:TYR:O	1:D:183:LEU:O	2.40	0.40
1:C:213:THR:HB	1:D:273:THR:HG21	2.04	0.40
1:E:183:LEU:HA	1:E:183:LEU:HD23	1.84	0.40
1:E:264:PHE:O	1:E:268:ALA:HB2	2.22	0.40
1:A:216:TRP:CH2	1:A:295:ARG:CB	3.04	0.40
1:A:72:ILE:HA	1:A:73:PRO:HD3	1.99	0.40
1:B:134:VAL:HG12	1:B:135:ASP:H	1.86	0.40
1:C:123:GLN:C	1:C:188:ARG:HH21	2.25	0.40
1:E:119:PRO:HG3	1:E:254:THR:CB	2.39	0.40
1:B:159:TRP:CE3	1:B:189:ILE:HD12	2.57	0.40
1:B:281:GLU:O	1:B:282:SER:C	2.59	0.40
1:C:32:LYS:HD3	1:C:245:LEU:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:18:ASN:O	1:D:44:LEU:HA	2.21	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 [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	308/317 (97%)	246 (80%)	44 (14%)	18 (6%)	2	20
1	B	308/317 (97%)	250 (81%)	40 (13%)	18 (6%)	2	20
1	C	308/317 (97%)	247 (80%)	43 (14%)	18 (6%)	2	20
1	D	308/317 (97%)	249 (81%)	42 (14%)	17 (6%)	2	22
1	E	308/317 (97%)	247 (80%)	43 (14%)	18 (6%)	2	20
All	All	1540/1585 (97%)	1239 (80%)	212 (14%)	89 (6%)	2	20

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	248 (90%)	29 (10%)	8	35
1	B	277/283 (98%)	246 (89%)	31 (11%)	7	32
1	C	277/283 (98%)	248 (90%)	29 (10%)	8	35
1	D	277/283 (98%)	248 (90%)	29 (10%)	8	35
1	E	277/283 (98%)	246 (89%)	31 (11%)	7	32
All	All	1385/1415 (98%)	1236 (89%)	149 (11%)	7	34

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	SER
1	A	53	PHE
1	A	57	ARG
1	A	84	ARG
1	A	111	SER
1	A	120	PHE
1	A	135	ASP
1	A	141	LEU
1	A	144	ASP
1	A	154	VAL
1	A	155	PHE
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	212	TRP
1	A	228	VAL
1	A	244	ASN
1	A	252	THR
1	A	257	ILE
1	A	274	VAL
1	A	290	ILE
1	A	292	ARG

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Mol	Chain	Res	Type
1	A	303	LEU
1	A	314	PHE
1	B	45	SER
1	B	53	PHE
1	B	57	ARG
1	B	84	ARG
1	B	111	SER
1	B	120	PHE
1	B	135	ASP
1	B	141	LEU
1	B	144	ASP
1	B	148	VAL
1	B	154	VAL
1	B	155	PHE
1	B	157	THR
1	B	168	VAL
1	B	175	LEU
1	B	181	SER
1	B	188	ARG
1	B	190	SER
1	B	193	TYR
1	B	202	LEU
1	B	211	SER
1	B	212	TRP
1	B	228	VAL
1	B	244	ASN
1	B	252	THR
1	B	257	ILE
1	B	274	VAL
1	B	290	ILE
1	B	292	ARG
1	B	303	LEU
1	B	314	PHE
1	C	45	SER
1	C	53	PHE
1	C	57	ARG
1	C	84	ARG
1	C	111	SER
1	C	120	PHE
1	C	135	ASP
1	C	141	LEU
1	C	144	ASP

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Mol	Chain	Res	Type
1	C	154	VAL
1	C	155	PHE
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	212	TRP
1	C	228	VAL
1	C	244	ASN
1	C	252	THR
1	C	257	ILE
1	C	274	VAL
1	C	290	ILE
1	C	292	ARG
1	C	303	LEU
1	C	314	PHE
1	D	45	SER
1	D	53	PHE
1	D	57	ARG
1	D	84	ARG
1	D	111	SER
1	D	120	PHE
1	D	135	ASP
1	D	141	LEU
1	D	144	ASP
1	D	154	VAL
1	D	155	PHE
1	D	157	THR
1	D	168	VAL
1	D	175	LEU
1	D	188	ARG
1	D	190	SER
1	D	193	TYR
1	D	202	LEU
1	D	211	SER
1	D	212	TRP
1	D	228	VAL
1	D	244	ASN

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Mol	Chain	Res	Type
1	D	252	THR
1	D	257	ILE
1	D	274	VAL
1	D	290	ILE
1	D	292	ARG
1	D	303	LEU
1	D	314	PHE
1	E	45	SER
1	E	53	PHE
1	E	57	ARG
1	E	84	ARG
1	E	111	SER
1	E	120	PHE
1	E	135	ASP
1	E	141	LEU
1	E	144	ASP
1	E	148	VAL
1	E	154	VAL
1	E	155	PHE
1	E	157	THR
1	E	168	VAL
1	E	175	LEU
1	E	181	SER
1	E	188	ARG
1	E	190	SER
1	E	193	TYR
1	E	202	LEU
1	E	211	SER
1	E	212	TRP
1	E	228	VAL
1	E	244	ASN
1	E	252	THR
1	E	257	ILE
1	E	274	VAL
1	E	290	ILE
1	E	292	ARG
1	E	303	LEU
1	E	314	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	GLN
1	A	151	ASN
1	A	192	GLN
1	A	234	HIS
1	A	238	ASN
1	B	123	GLN
1	B	151	ASN
1	B	192	GLN
1	B	199	ASN
1	B	234	HIS
1	C	39	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	D	39	ASN
1	D	123	GLN
1	D	151	ASN
1	D	192	GLN
1	D	199	ASN
1	D	234	HIS
1	E	151	ASN
1	E	192	GLN
1	E	234	HIS

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 carbohydrates 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.24	4 (1%) 77 69	76, 103, 142, 169	0
1	B	310/317 (97%)	-0.27	4 (1%) 77 69	76, 103, 142, 169	0
1	C	310/317 (97%)	-0.29	1 (0%) 93 90	76, 103, 142, 169	0
1	D	310/317 (97%)	-0.25	2 (0%) 89 84	76, 103, 142, 169	0
1	E	310/317 (97%)	-0.27	4 (1%) 77 69	76, 103, 142, 169	0
All	All	1550/1585 (97%)	-0.26	15 (0%) 82 75	76, 103, 143, 169	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	316	PHE	3.6
1	A	316	PHE	3.1
1	E	282	SER	2.8
1	E	316	PHE	2.6
1	A	315	GLY	2.6
1	D	55	PRO	2.5
1	D	282	SER	2.5
1	B	282	SER	2.5
1	B	316	PHE	2.5
1	B	63	LYS	2.3
1	E	286	ARG	2.3
1	E	60	VAL	2.3
1	A	282	SER	2.3
1	A	51	LEU	2.1
1	B	133	SER	2.1

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 carbohydrates 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.