



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:24 AM GMT

PDB ID : 3EI0
Title : Structure of the E221A mutant of the Gloebacter 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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

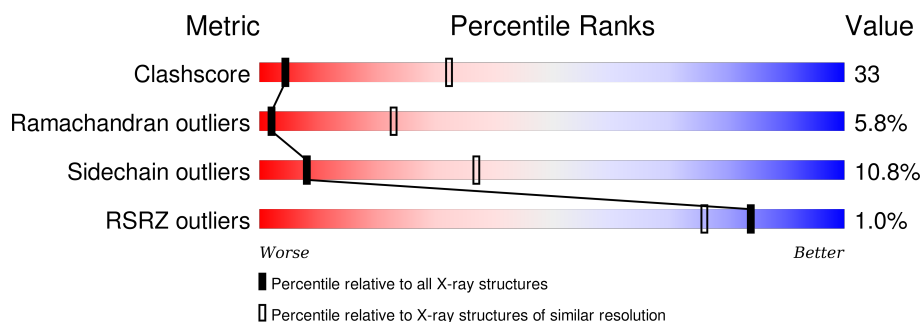
1 Overall quality at a glance

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	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (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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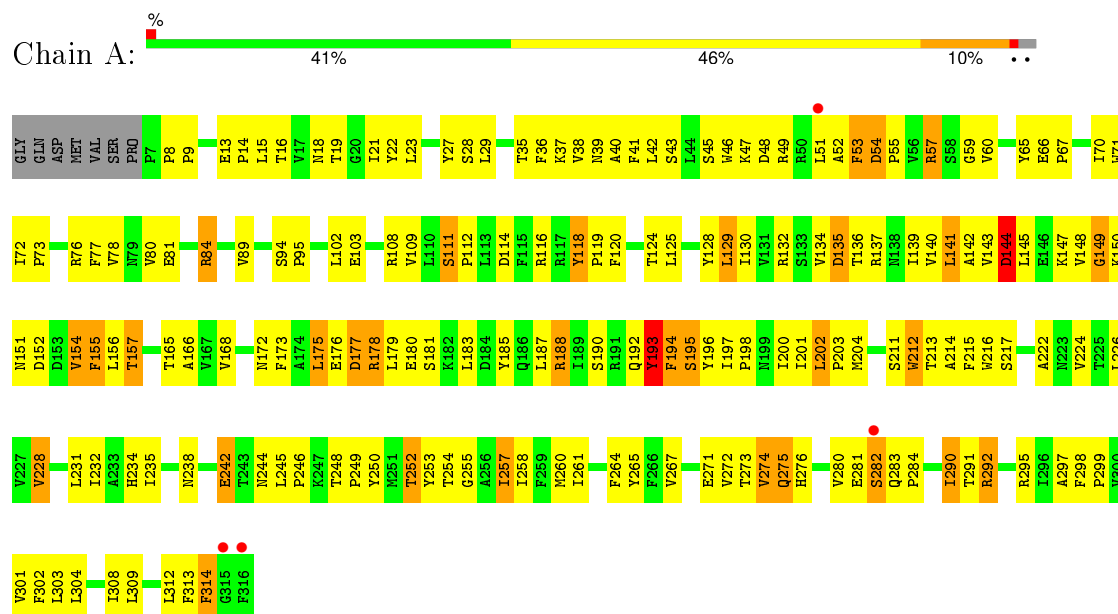
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Chain	Residue	Modelled	Actual	Comment	Reference
C	3	MET	-	EXPRESSION TAG	UNP Q7NDN8
C	4	VAL	-	EXPRESSION TAG	UNP Q7NDN8
C	5	SER	-	EXPRESSION TAG	UNP Q7NDN8
C	6	PRO	-	EXPRESSION TAG	UNP Q7NDN8
C	221	ALA	GLU	ENGINEERED	UNP Q7NDN8
D	0	GLY	-	EXPRESSION 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

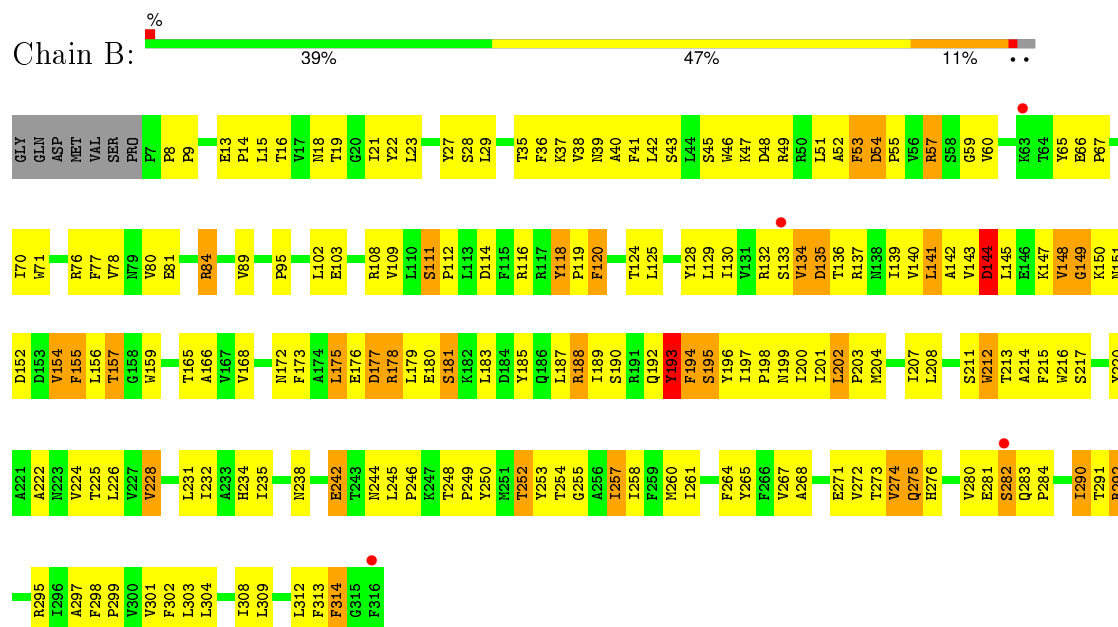
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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:

Sequence logo for Chain C. The y-axis represents information content in bits (0.00 to 0.15). The x-axis shows positions 1 to 100. A color scale at the top indicates conservation levels: 39% (green), 49% (yellow), and 9% (orange).

Position	Amino Acid	Information Content (bits)
1	I290	0.14
2	T291	0.14
3	R292	0.14
4	R295	0.14
5	I296	0.14
6	A297	0.14
7	F298	0.14
8	P299	0.14
9	V300	0.14
10	V301	0.14
11	F302	0.14
12	L303	0.14
13	L304	0.14
14	I308	0.14
15	L309	0.14
16	L312	0.14
17	F313	0.14
18	F314	0.14
19	G315	0.14
20	F316	0.14
21	S217	0.14
22	Y220	0.14
23	A221	0.14
24	A222	0.14
25	K223	0.14
26	V224	0.14
27	T225	0.14
28	L226	0.14
29	V227	0.14
30	V228	0.14
31	L231	0.14
32	L232	0.14
33	A233	0.14
34	H234	0.14
35	L235	0.14
36	M238	0.14
37	E242	0.14
38	T243	0.14
39	N244	0.14
40	L245	0.14
41	P246	0.14
42	T247	0.14
43	T248	0.14
44	P249	0.14
45	Y250	0.14
46	T251	0.14
47	T252	0.14
48	Y253	0.14
49	T254	0.14
50	G255	0.14
51	A256	0.14
52	T257	0.14
53	L258	0.14
54	F259	0.14
55	T260	0.14
56	L261	0.14
57	F264	0.14
58	Y265	0.14
59	F266	0.14
60	V267	0.14
61	A268	0.14
62	E271	0.14
63	V272	0.14
64	T273	0.14
65	V274	0.14
66	Q275	0.14
67	H276	0.14
68	V280	0.14
69	E281	0.14
70	S282	0.14
71	Q283	0.14
72	P284	0.14
73	E146	0.14
74	K147	0.14
75	V148	0.14
76	G149	0.14
77	K150	0.14
78	M151	0.14
79	D152	0.14
80	V154	0.14
81	F155	0.14
82	L156	0.14
83	T157	0.14
84	T165	0.14
85	A166	0.14
86	V167	0.14
87	V168	0.14
88	M172	0.14
89	F173	0.14
90	A174	0.14
91	L175	0.14
92	E176	0.14
93	D177	0.14
94	R178	0.14
95	L179	0.14
96	E180	0.14
97	L183	0.14
98	D184	0.14
99	I185	0.14
100	Q186	0.14
101	L187	0.14
102	R188	0.14
103	I189	0.14
104	S190	0.14
105	R191	0.14
106	Y193	0.14
107	F194	0.14
108	S195	0.14
109	I196	0.14
110	I197	0.14
111	P198	0.14
112	M199	0.14
113	L200	0.14
114	L201	0.14
115	L202	0.14
116	P203	0.14
117	M204	0.14
118	L207	0.14
119	L208	0.14
120	S211	0.14
121	T212	0.14
122	T213	0.14
123	A214	0.14
124	T215	0.14
125	F216	0.14
126	S217	0.14
127	Y220	0.14
128	A221	0.14
129	A222	0.14
130	K223	0.14
131	V224	0.14
132	T225	0.14
133	L226	

[illegible]

Chain E:

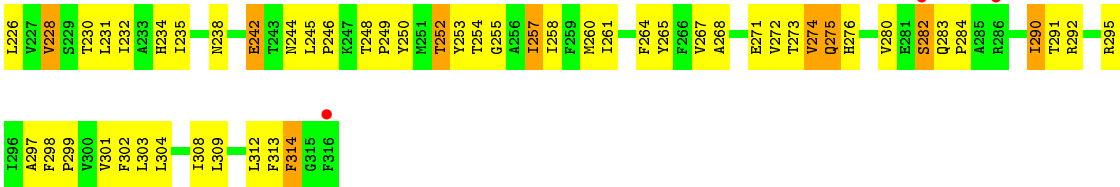
41% 47% 10%

GLY GLN ASP MET VAL SER PRO P7 P8 P9 E13 P14 L15 T16 V17 N18 T19 I21 Y22 L23 Y27 S28 L29 T35 F36 K37 V38 N39 A40 F41 L42 S43 L44 S45 W46 K47 D48 R49 R50 L51 A52 F53 D54 R57 S58 V60 Y65 E66 P67 I70 W71

0.00 0.05 0.10 0.15 0.20 0.25 0.30 0.35 0.40

R76 F77 V78 N79 Y80 E81 R84 V89 D90 T91 S92 S93 S94 P95 L102 E103 A107 R108 V109 L110 L113 D114 F115 R116 R117 Y118 P119 F120 Q123 T124 L125 Y128 L129 I130 V131 T132 S133 V134 D135 T136 R137 M138 T139 V140 L141 A142 V143 D144 L145 E146 V147 R148

G149 K150 K151 N151 D152 D153 V154 F155 L156 T157 T165 A166 V167 V168 N172 F173 A174 L175 E176 R177 R178 R179 L179 E180 S181 K182 K183 D184 Y185 Y186 L187 R188 L189 S190 S190 R191 Q192 Y193 F194 S195 Y196 L197 P198 P199 I200 I201 S133 L202 L202 P203 M204 S211 W212 T213 A214 F215 W216 A222 A223 V224 V225



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 0.251 , (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 , 69.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 47328 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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:E:42:LEU:HB3	1:E:103:GLU:HG2	1.60	0.83
1:D:119:PRO:HG3	1:D:254:THR:HB	1.59	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:E:177:ASP:O	1:E:178:ARG:HB2	1.82	0.77
1:A:54:ASP:HB2	1:A:57:ARG:HG3	1.65	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:E:119:PRO:CG	1:E:254:THR:HB	2.15	0.77
1:B:177:ASP:O	1:B:178:ARG:HB2	1.84	0.77
1:D:54:ASP:HB2	1:D:57:ARG:HG3	1.66	0.76
1:A:42:LEU:HB3	1:A:103:GLU:HG2	1.65	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:84:ARG:HG3	1:B:84:ARG:HH11	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: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:D:13:GLU:HB3	1:D:14:PRO:CD	2.20	0.70
1:A:141:LEU:HD23	1:A:142:ALA:H	1.56	0.70
1:B:13:GLU:HB3	1:B:14:PRO:CD	2.21	0.70
1:A:257:ILE:O	1:A:261:ILE:HG12	1.92	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:D:257:ILE:O	1:D:261:ILE:HG12	1.94	0.67
1:A:297:ALA:O	1:A:301:VAL:HG23	1.94	0.67
1:C:84:ARG:HG2	1:C:84:ARG:HH11	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: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:C:81:GLU:HG3	1:C:108:ARG:HG3	1.78	0.65
1:A:140:VAL:HG23	1:A:183:LEU:HG	1.79	0.65
1:D:249:PRO:HD2	1:D:250:TYR:CD1	2.31	0.65
1:D:81:GLU:HG3	1:D:108:ARG:HG3	1.79	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:D:42:LEU:HB3	1:D:103:GLU:CG	2.29	0.62
1:B:81:GLU:HG3	1:B:108:ARG:HG3	1.80	0.62
1:D:214:ALA:HB2	1:D:226:LEU:HD23	1.82	0.62
1:B:298:PHE:HB2	1:B:299:PRO:HD3	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:D:274:VAL:C	1:D:276:HIS:H	2.02	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:D:175:LEU:HD22	1:D:176:GLU:HG3	1.83	0.61
1:B:314:PHE:H	1:B:314:PHE:HD1	1.48	0.61
1:C:21:ILE:O	1:C:149:GLY:HA3	2.01	0.61
1:A:84:ARG:NH1	1:A:84:ARG:HG3	2.15	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: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:51:LEU:HD11	1:E:70:ILE:HD12	1.83	0.61
1:A:214:ALA:HB2	1:A:226:LEU:HD23	1.83	0.61
1:E:274:VAL:C	1:E:276:HIS:H	2.03	0.61
1:B:140:VAL:HG23	1:B:183:LEU:HG	1.83	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:C:76:ARG:NH2	1:C:130:ILE:HD12	2.16	0.60
1:A:213:THR:OG1	1:A:226:LEU:HD21	2.01	0.60
1:C:214:ALA:HB2	1:C:226:LEU:HD23	1.82	0.60
1:C:155:PHE:CE1	1:D:112:PRO:HB3	2.36	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: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:151:ASN:O	1:A:154:VAL:HG22	2.01	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:E:53:PHE:O	1:E:53:PHE:CD1	2.56	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:B:304:LEU:O	1:B:308:ILE:HG12	2.02	0.59
1:E:21:ILE:O	1:E:149:GLY:HA3	2.02	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:314:PHE:N	1:E:314:PHE:CD1	2.71	0.59
1:C:298:PHE:HB2	1:C:299:PRO:HD3	1.83	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:E:304:LEU:O	1:E:308:ILE:HG12	2.02	0.59
1:D:27:TYR:CE1	1:D:37:LYS:HB3	2.38	0.59
1:C:314:PHE:CD1	1:C:314:PHE:N	2.71	0.59
1:E:140:VAL:HG23	1:E:183:LEU:HG	1.85	0.59
1:D:76:ARG:NH2	1:D:130:ILE:HD12	2.18	0.59
1:A:155:PHE:CE1	1:B:112:PRO:HB3	2.38	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:D:238:ASN:HA	1:D:258:ILE:HD11	1.85	0.58
1:C:177:ASP:O	1:C:178:ARG:CB	2.51	0.58
1:A:304:LEU:O	1:A:308:ILE:HG12	2.03	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:84:ARG:HG3	1:B:84:ARG:NH1	2.17	0.58
1:C:304:LEU:O	1:C:308:ILE:HG12	2.04	0.58
1:B:193:TYR:H	1:B:193:TYR:HD1	1.52	0.58
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:314:PHE:CD1	1:A:314:PHE:N	2.71	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:CD1	1:B:314:PHE:N	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:D:51:LEU:HD11	1:D:70:ILE:HD12	1.86	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: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:D:84:ARG:HD3	1:D:84:ARG:H	1.70	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:E:124:THR:HB	1:E:188:ARG:NE	2.20	0.56
1:C:238:ASN:HA	1:C:258:ILE:HD11	1.86	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:D:177:ASP:O	1:D:178:ARG:CB	2.52	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: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:D:53:PHE:O	1:D:53:PHE:CD1	2.59	0.56
1:B:51:LEU:HD11	1:B:70:ILE:HD12	1.88	0.56
1:E:147:LYS:C	1:E:149:GLY:H	2.09	0.56
1:B:84:ARG:H	1:B:84:ARG:HD3	1.71	0.56
1:A:255:GLY:HA2	1:A:258:ILE:HG22	1.88	0.56
1:A:114:ASP:OD2	1:A:116:ARG:HB2	2.06	0.56
1:E:140:VAL:CG2	1:E:183:LEU:HG	2.35	0.55
1:C:18:ASN:HB3	1:C:143:VAL:HG23	1.88	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:E:84:ARG:HG3	1:E:84:ARG:NH1	2.18	0.55
1:A:27:TYR:CE1	1:A:37:LYS:HB3	2.42	0.55
1:B:53:PHE:C	1:B:53:PHE:HD1	2.10	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: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:A:18:ASN:HB3	1:A:143:VAL:CG2	2.37	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: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
1:E:255:GLY:HA2	1:E:258:ILE:HG22	1.90	0.54
1:A:18:ASN:HB3	1:A:143:VAL:HG23	1.88	0.54
1:E:114:ASP:OD2	1:E:116:ARG:HB2	2.07	0.54
1:C:216:TRP:CH2	1:C:295:ARG:HB2	2.43	0.54
1:C:147:LYS:C	1:C:149:GLY:H	2.09	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: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: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:B:76:ARG:NH2	1:B:130:ILE:HD12	2.22	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:B:147:LYS:C	1:B:149:GLY:H	2.11	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:H	1:C:193:TYR:HD1	1.54	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:A:216:TRP:CH2	1:A:295:ARG:HB2	2.43	0.53
1:D:197:ILE:HA	1:D:201:ILE:HB	1.90	0.53
1:E:53:PHE:HD1	1:E:53:PHE:C	2.11	0.53
1:D:28:SER:O	1:D:36:PHE:HA	2.08	0.53
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:C:155:PHE:CE2	1:C:157:THR:HG23	2.44	0.53
1:B:48:ASP:CG	1:B:51:LEU:HD23	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:53:PHE:CD1	1:B:53:PHE:C	2.81	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:D:141:LEU:HD23	1:D:142:ALA:N	2.19	0.53
1:C:48:ASP:CG	1:C:51:LEU:HD23	2.29	0.53
1:E:47:LYS:HD2	1:E:49:ARG:NH2	2.24	0.53
1:D:255:GLY:HA2	1:D:258:ILE:HG22	1.91	0.53
1:B:66:GLU:HG3	1:B:67:PRO:HD2	1.90	0.53
1:E:147:LYS:O	1:E:149:GLY:N	2.43	0.52
1:A:197:ILE:HA	1:A:201:ILE:HB	1.90	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:E:53:PHE:C	1:E:53:PHE:CD1	2.82	0.52
1:D:260:MET:CE	1:D:309:LEU:HD22	2.39	0.52
1:E:54:ASP:HB2	1:E:57:ARG:CG	2.39	0.52
1:D:213:THR:HB	1:E:273:THR:HG21	1.90	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:147:LYS:O	1:B:149:GLY:N	2.43	0.52
1:B:18:ASN:HB3	1:B:143:VAL:HG23	1.92	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:D:84:ARG:NH1	1:D:84:ARG:CG	2.58	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:E:66:GLU:HG3	1:E:67:PRO:HD2	1.92	0.51
1:D:53:PHE:C	1:D:53:PHE:CD1	2.84	0.51
1:C:28:SER:O	1:C:36:PHE:HA	2.11	0.51
1:B:274:VAL:C	1:B:276:HIS:N	2.64	0.51
1:C:147:LYS:O	1:C:149:GLY:N	2.44	0.51
1:A:54:ASP:HB2	1:A:57:ARG:CG	2.39	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:D:238:ASN:HA	1:D:258:ILE:CD1	2.40	0.51
1:A:260:MET:CE	1:A:309:LEU:HD22	2.40	0.51
1:D:35:THR:HG21	1:D:108:ARG:HH21	1.76	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:147:LYS:O	1:D:149:GLY:N	2.44	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:E:84:ARG:CG	1:E:84:ARG:NH1	2.57	0.51
1:A:271:GLU:OE2	1:A:272:VAL:N	2.44	0.51
1:E:18:ASN:HB3	1:E:143:VAL:HG23	1.92	0.51
1:D:47:LYS:HD2	1:D:49:ARG:NH2	2.27	0.51
1:B:22:TYR:CA	1:B:149:GLY:HA2	2.31	0.50
1:A:35:THR:HG21	1:A:108:ARG:HH21	1.76	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:E:52:ALA:HA	1:E:95:PRO:O	2.11	0.50
1:C:65:TYR:CD2	1:C:70:ILE:HD11	2.47	0.50
1:D:274:VAL:C	1:D:276:HIS:N	2.64	0.50
1:A:155:PHE:CE2	1:A:157:THR:HG23	2.46	0.50
1:B:78:VAL:HG22	1:B:130:ILE:HG12	1.93	0.50
1:A:224:VAL:O	1:A:228:VAL:HB	2.12	0.50
1:B:155:PHE:CE2	1:B:157:THR:HG23	2.47	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:B:232:ILE:HA	1:B:235:ILE:HD12	1.93	0.50
1:A:47:LYS:HD2	1:A:49:ARG:NH2	2.26	0.50
1:E:147:LYS:C	1:E:149:GLY:N	2.66	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:A:48:ASP:CG	1:A:51:LEU:HD23	2.32	0.50
1:D:224:VAL:O	1:D:228:VAL:HB	2.11	0.50
1:B:199:ASN:HD22	1:C:242:GLU:HG3	1.77	0.50
1:A:151:ASN:ND2	1:A:152:ASP:H	2.10	0.50
1:C:15:LEU:HD11	1:C:46:TRP:HB2	1.94	0.49
1:C:238:ASN:HA	1:C:258:ILE:CD1	2.41	0.49
1:C:166:ALA:HB2	1:C:185:TYR:CD2	2.47	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:E:151:ASN:ND2	1:E:152:ASP:H	2.10	0.49
1:B:47:LYS:HD2	1:B:49:ARG:NH2	2.26	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:C:47:LYS:HD2	1:C:49:ARG:NH2	2.27	0.49
1:B:222:ALA:O	1:B:226:LEU:HB2	2.12	0.49
1:E:149:GLY:O	1:E:150:LYS:HB2	2.13	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
1:D:144:ASP:HA	1:D:147:LYS:HB3	1.95	0.49
1:C:252:THR:HG23	1:C:255:GLY:HA3	1.93	0.49
1:B:53:PHE:HD1	1:B:53:PHE:O	1.96	0.49
1:C:54:ASP:HB2	1:C:57:ARG:CG	2.39	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: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:E:76:ARG:HH22	1:E:130:ILE:HD12	1.77	0.48
1:C:231:LEU:HD13	1:C:265:TYR:HB3	1.95	0.48
1:E:144:ASP:HA	1:E:147:LYS:HB3	1.95	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:A:15:LEU:HD11	1:A:46:TRP:HB2	1.94	0.48
1:C:147:LYS:C	1:C:149:GLY:N	2.66	0.48
1:B:147:LYS:C	1:B:149:GLY:N	2.66	0.48
1:C:245:LEU:HD12	1:C:246:PRO:HD2	1.94	0.48
1:D:53:PHE:CE1	1:D:95:PRO:HA	2.48	0.48
1:B:215:PHE:HZ	1:B:298:PHE:CE1	2.32	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: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:C:253:TYR:HB2	1:C:313:PHE:CD2	2.48	0.48
1:B:15:LEU:HD11	1:B:46:TRP:HB2	1.94	0.48
1:B:252:THR:HG23	1:B:255:GLY:HA3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:GLN:HG3	1:B:291:THR:OG1	2.13	0.48
1:B:35:THR:HG21	1:B:108:ARG:HH21	1.78	0.48
1:E:65:TYR:CD2	1:E:70:ILE:HD11	2.48	0.48
1:E:15:LEU:HD11	1:E:46:TRP:HB2	1.95	0.48
1:C:66:GLU:HG3	1:C:67:PRO:HD2	1.94	0.48
1:B:84:ARG:NH1	1:B:84:ARG:CG	2.56	0.48
1:D:283:GLN:N	1:D:284:PRO:CD	2.71	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:A:66:GLU:HG3	1:A:67:PRO:HD2	1.95	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: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:C:36:PHE:CE1	1:C:109:VAL:HB	2.48	0.47
1:E:215:PHE:HZ	1:E:298:PHE:CE1	2.32	0.47
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:D:89:VAL:HG11	1:D:102:LEU:HD23	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:A:23:LEU:HA	1:A:40:ALA:HB2	1.96	0.47
1:E:238:ASN:HA	1:E:258:ILE:CD1	2.43	0.47
1:C:257:ILE:HG22	1:C:309:LEU:HD23	1.96	0.47
1:B:151:ASN:ND2	1:B:152:ASP:H	2.12	0.47
1:E:89:VAL:HG11	1:E:102:LEU:HD23	1.96	0.47
1:B:149:GLY:O	1:B:150:LYS:HB2	2.14	0.47
1:E:257:ILE:HG22	1:E:309:LEU:HD23	1.96	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:A:193:TYR:O	1:A:195:SER:N	2.48	0.47
1:C:135:ASP:C	1:C:135:ASP:OD2	2.53	0.47
1:D:222:ALA:O	1:D:226:LEU:HB2	2.14	0.47
1:D:8:PRO:HA	1:D:71:TRP:CD1	2.49	0.47
1:C:232:ILE:HA	1:C:235:ILE:HD12	1.96	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:C:84:ARG:NH1	1:C:84:ARG:CG	2.57	0.47
1:B:197:ILE:HB	1:B:198:PRO:CD	2.38	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:D:147:LYS:C	1:D:149:GLY:N	2.67	0.47
1:C:144:ASP:HA	1:C:147:LYS:HB3	1.97	0.47
1:C:149:GLY:O	1:C:150:LYS:HB2	2.15	0.47
1:E:252:THR:HG23	1:E:255:GLY:HA3	1.96	0.47
1:B:54:ASP:HB2	1:B:57:ARG:CG	2.38	0.47
1:E:53:PHE:CE1	1:E:95:PRO:HA	2.50	0.47
1:E:282:SER:C	1:E:284:PRO:HD3	2.35	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:D:253:TYR:HA	1:D:313:PHE:CE2	2.49	0.47
1:D:15:LEU:HD12	1:D:16:THR:N	2.29	0.47
1:C:23:LEU:HA	1:C:40:ALA:HB2	1.95	0.47
1:C:151:ASN:ND2	1:C:152:ASP:H	2.13	0.47
1:A:36:PHE:CE1	1:A:109:VAL:HB	2.49	0.47
1:D:212:TRP:HB2	1:D:215:PHE:CE1	2.50	0.47
1:C:222:ALA:O	1:C:226:LEU:HB2	2.14	0.47
1:E:253:TYR:HA	1:E:313:PHE:CE2	2.49	0.47
1:D:231:LEU:HD13	1:D:265:TYR:CB	2.45	0.47
1:E:222:ALA:O	1:E:226:LEU:HB2	2.14	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:A:245:LEU:HD12	1:A:246:PRO:HD2	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: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: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: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:E:35:THR:HG21	1:E:108:ARG:HH21	1.80	0.46
1:B:253:TYR:HA	1:B:313:PHE:CE2	2.50	0.46
1:C:253:TYR:HA	1:C:313:PHE:CE2	2.50	0.46
1:C:231:LEU:HD13	1:C:265:TYR:CB	2.45	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:A:249:PRO:HG3	1:E:192:GLN:NE2	2.31	0.46
1:D:36:PHE:CE1	1:D:109:VAL:HB	2.51	0.46
1:C:282:SER:C	1:C:284:PRO:HD3	2.36	0.46
1:A:309:LEU:O	1:A:312:LEU:HB3	2.15	0.46
1:E:166:ALA:HB2	1:E:185:TYR:CD2	2.49	0.46
1:A:89:VAL:HG11	1:A:102:LEU:HD23	1.96	0.46
1:C:89:VAL:HG11	1:C:102:LEU:HD23	1.97	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:E:231:LEU:HD13	1:E:265:TYR:CB	2.45	0.46
1:B:245:LEU:HD12	1:B:246:PRO:HD2	1.97	0.46
1:D:53:PHE:O	1:D:54:ASP:C	2.54	0.46
1:A:260:MET:HE3	1:A:309:LEU:HD22	1.98	0.46
1:E:36:PHE:CE1	1:E:109:VAL:HB	2.51	0.46
1:B:276:HIS:O	1:B:280:VAL:HG22	2.16	0.46
1:A:276:HIS:O	1:A:280:VAL:HG22	2.16	0.46
1:A:215:PHE:HZ	1:A:298:PHE:CE1	2.34	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:C:41:PHE:HE2	1:D:175:LEU:HD13	1.80	0.45
1:A:231:LEU:HD13	1:A:265:TYR:CB	2.46	0.45
1:A:149:GLY:O	1:A:150:LYS:HB2	2.16	0.45
1:D:119:PRO:HG3	1:D:254:THR:CB	2.41	0.45
1:A:53:PHE:HD1	1:A:53:PHE:O	2.00	0.45
1:C:309:LEU:O	1:C:312:LEU:HB3	2.16	0.45
1:E:298:PHE:CB	1:E:299:PRO:HD3	2.45	0.45
1:C:212:TRP:HB2	1:C:215:PHE:CE1	2.52	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: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:A:282:SER:C	1:A:284:PRO:HD3	2.37	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:LEU:HD13	1:B:265:TYR:HB3	1.98	0.45
1:A:136:THR:HG22	1:A:137:ARG:N	2.31	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:A:9:PRO:HD3	1:A:71:TRP:CE3	2.51	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: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:B:23:LEU:HA	1:B:40:ALA:HB2	1.99	0.45
1:C:196:TYR:N	1:C:196:TYR:CD1	2.85	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:53:PHE:O	1:B:54:ASP:C	2.55	0.45
1:E:143:VAL:O	1:E:145:LEU:N	2.50	0.45
1:C:245:LEU:HA	1:C:246:PRO:HD2	1.77	0.45
1:B:196:TYR:HD1	1:B:196:TYR:N	2.14	0.45
1:B:234:HIS:CE1	1:B:258:ILE:O	2.70	0.45
1:A:234:HIS:CE1	1:A:258:ILE:O	2.70	0.45
1:C:76:ARG:HH22	1:C:130:ILE:HD12	1.81	0.45
1:A:267:VAL:HG23	1:A:298:PHE:CZ	2.52	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:B:196:TYR:N	1:B:196:TYR:CD1	2.84	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: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:B:89:VAL:HG11	1:B:102:LEU:HD23	1.98	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:A:8:PRO:HA	1:A:71:TRP:CD1	2.52	0.45
1:C:215:PHE:HZ	1:C:298:PHE:CE1	2.35	0.45
1:C:139:ILE:HG12	1:C:172:ASN:HD21	1.82	0.45
1:D:264:PHE:CE2	1:D:302:PHE:HB2	2.52	0.45
1:B:136:THR:HG22	1:B:137:ARG:N	2.32	0.45
1:B:135:ASP:OD2	1:B:135:ASP:C	2.55	0.45
1:C:77:PHE:HB3	1:C:80:VAL:HG23	1.99	0.45
1:B:254:THR:O	1:B:258:ILE:HB	2.17	0.44
1:E:254:THR:O	1:E:258:ILE:HB	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:PHE:O	1:E:54:ASP:C	2.54	0.44
1:A:271:GLU:O	1:A:274:VAL:N	2.50	0.44
1:D:196:TYR:N	1:D:196:TYR:CD1	2.85	0.44
1:A:232:ILE:HA	1:A:235:ILE:HD12	1.98	0.44
1:D:22:TYR:HA	1:D:149:GLY:HA3	1.97	0.44
1:C:22:TYR:HB3	1:C:41:PHE:HB2	1.99	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:D:253:TYR:CD1	1:D:314:PHE:HE1	2.35	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:A:135:ASP:OD2	1:A:135:ASP:C	2.55	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:C:253:TYR:CD1	1:C:314:PHE:HE1	2.35	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:D:54:ASP:HA	1:D:55:PRO:HD2	1.65	0.44
1:A:192:GLN:NE2	1:B:249:PRO:HG3	2.32	0.44
1:C:35:THR:HG21	1:C:108:ARG:HH21	1.82	0.44
1:D:215:PHE:HZ	1:D:298:PHE:CE1	2.34	0.44
1:B:130:ILE:HA	1:B:181:SER:O	2.18	0.44
1:C:136:THR:HG22	1:C:137:ARG:N	2.33	0.44
1:E:139:ILE:HG12	1:E:172:ASN:HD21	1.81	0.44
1:E:234:HIS:CE1	1:E:258:ILE:O	2.71	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: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:A:15:LEU:HD12	1:A:16:THR:N	2.33	0.44
1:E:196:TYR:CD1	1:E:196:TYR:N	2.85	0.44
1:C:77:PHE:HB3	1:C:80:VAL:CG2	2.48	0.44
1:D:196:TYR:N	1:D:196:TYR:HD1	2.15	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:D:22:TYR:HB3	1:D:41:PHE:HB2	2.00	0.44
1:B:22:TYR:HA	1:B:149:GLY:HA3	1.96	0.44
1:B:309:LEU:O	1:B:312:LEU:HB3	2.17	0.44
1:A:257:ILE:HG22	1:A:309:LEU:HD23	2.00	0.44
1:B:267:VAL:HG23	1:B:298:PHE:CZ	2.53	0.44
1:E:78:VAL:HB	1:E:128:TYR:HB2	1.99	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:B:231:LEU:HD13	1:B:265:TYR:CB	2.47	0.44
1:D:139:ILE:HG12	1:D:172:ASN:HD21	1.82	0.44
1:A:54:ASP:HA	1:A:55:PRO:HD2	1.77	0.44
1:C:128:TYR:O	1:C:129:LEU:HB2	2.17	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:77:PHE:HB3	1:A:80:VAL:CG2	2.48	0.44
1:D:298:PHE:CB	1:D:299:PRO:HD3	2.47	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:C:179:LEU:C	1:C:179:LEU:HD12	2.38	0.44
1:D:202:LEU:HB2	1:D:203:PRO:HD3	2.00	0.43
1:B:139:ILE:HG12	1:B:172:ASN:HD21	1.83	0.43
1:E:53:PHE:HD1	1:E:53:PHE:O	1.98	0.43
1:C:54:ASP:HA	1:C:55:PRO:HD2	1.77	0.43
1:A:213:THR:HB	1:B:273:THR:HG21	1.99	0.43
1:A:128:TYR:O	1:A:129:LEU:HB2	2.17	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:8:PRO:HA	1:C:71:TRP:CD1	2.53	0.43
1:A:253:TYR:CD1	1:A:314:PHE:HE1	2.36	0.43
1:D:143:VAL:O	1:D:145:LEU:N	2.51	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:A:125:LEU:HB2	1:A:187:LEU:HB3	2.00	0.43
1:E:255:GLY:HA2	1:E:258:ILE:CG2	2.48	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:A:254:THR:O	1:A:258:ILE:HB	2.18	0.43
1:C:118:TYR:O	1:C:119:PRO:C	2.55	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:B:125:LEU:HB2	1:B:187:LEU:HB3	2.01	0.43
1:D:179:LEU:C	1:D:179:LEU:HD12	2.39	0.43
1:B:264:PHE:CE2	1:B:302:PHE:HB2	2.53	0.43
1:D:234:HIS:CE1	1:D:258:ILE:O	2.71	0.43
1:D:192:GLN:NE2	1:E:249:PRO:HG3	2.33	0.43
1:D:267:VAL:HG23	1:D:298:PHE:CZ	2.54	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:B:9:PRO:HD3	1:B:71:TRP:CE3	2.53	0.43
1:E:77:PHE:HB3	1:E:80:VAL:HG23	2.01	0.43
1:C:19:THR:HA	1:C:43:SER:O	2.19	0.43
1:A:202:LEU:HB2	1:A:203:PRO:HD3	2.01	0.43
1:B:255:GLY:O	1:B:258:ILE:HG22	2.18	0.43
1:A:35:THR:CG2	1:A:108:ARG:HH21	2.31	0.43
1:E:202:LEU:HB2	1:E:203:PRO:HD3	2.01	0.43
1:A:19:THR:HA	1:A:43:SER:O	2.18	0.43
1:B:81:GLU:HG3	1:B:108:ARG:CG	2.48	0.43
1:E:200:ILE:O	1:E:204:MET:HB3	2.18	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: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:B:264:PHE:O	1:B:268:ALA:HB2	2.19	0.43
1:E:77:PHE:HB3	1:E:80:VAL:CG2	2.48	0.43
1:C:202:LEU:HB2	1:C:203:PRO:HD3	2.01	0.43
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: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:193:TYR:N	1:A:193:TYR:CD1	2.86	0.42
1:C:217:SER:HG	1:D:220:TYR:HE2	1.66	0.42
1:A:78:VAL:HB	1:A:128:TYR:HB2	2.01	0.42
1:A:179:LEU:HD12	1:A:179:LEU:C	2.39	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:B:111:SER:HA	1:B:112:PRO:HD2	1.77	0.42
1:A:77:PHE:HB3	1:A:80:VAL:HG23	2.00	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: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:D:271:GLU:O	1:D:274:VAL:N	2.51	0.42
1:B:193:TYR:CG	1:B:194:PHE:N	2.87	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:A:41:PHE:HE2	1:B:175:LEU:HD13	1.85	0.42
1:E:118:TYR:O	1:E:119:PRO:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:SER:OG	1:C:95:PRO:HD2	2.19	0.42
1:C:35:THR:O	1:C:36:PHE:HB3	2.18	0.42
1:A:38:VAL:HG22	1:A:39:ASN:N	2.34	0.42
1:B:150:LYS:HB3	1:B:150:LYS:HE2	1.89	0.42
1:B:13:GLU:CB	1:B:14:PRO:CD	2.92	0.42
1:D:197:ILE:HB	1:D:198:PRO:CD	2.39	0.42
1:A:298:PHE:CB	1:A:299:PRO:HD3	2.47	0.42
1:E:27:TYR:CE1	1:E:37:LYS:CB	3.03	0.42
1:C:264:PHE:O	1:C:268:ALA:HB2	2.19	0.42
1:B:29:LEU:HB2	1:B:156:LEU:HD11	2.01	0.42
1:E:255:GLY:O	1:E:258:ILE:HG22	2.20	0.42
1:B:35:THR:CG2	1:B:108:ARG:HH21	2.32	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: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
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:C:234:HIS:CE1	1:C:258:ILE:O	2.72	0.42
1:C:290:ILE:HG22	1:C:291:THR:N	2.34	0.42
1:D:281:GLU:O	1:D:282:SER:C	2.58	0.42
1:C:271:GLU:O	1:C:274:VAL:N	2.50	0.42
1:D:193:TYR:N	1:D:193:TYR:CD1	2.86	0.42
1:B:133:SER:HB3	1:B:136:THR:O	2.19	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:309:LEU:O	1:E:312:LEU:HB3	2.19	0.42
1:E:130:ILE:HA	1:E:181:SER:O	2.20	0.42
1:D:128:TYR:O	1:D:129:LEU:HB2	2.19	0.42
1:E:264:PHE:CE2	1:E:302:PHE:HB2	2.54	0.42
1:A:94:SER:OG	1:A:95:PRO:HD2	2.20	0.41
1:C:104:ARG:HD2	1:D:76:ARG:NH1	2.35	0.41
1:A:29:LEU:HB2	1:A:156:LEU:HD11	2.02	0.41
1:B:292:ARG:HD2	1:B:295:ARG:HD2	2.02	0.41
1:B:216:TRP:CH2	1:B:295:ARG:CB	3.03	0.41
1:A:89:VAL:CG1	1:A:102:LEU:HD23	2.49	0.41
1:D:174:ALA:HA	1:D:179:LEU:HA	2.02	0.41
1:C:93:VAL:HG22	1:C:99:VAL:HG13	2.02	0.41
1:A:290:ILE:HG22	1:A:291:THR:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:GLU:O	1:A:282:SER:C	2.58	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: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:C:207:ILE:HG13	1:C:208:LEU:N	2.35	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:D:216:TRP:CH2	1:D:295:ARG:CB	3.03	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:225:THR:HG21	1:E:224:VAL:HG23	2.02	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:281:GLU:O	1:C:282:SER:C	2.59	0.41
1:E:267:VAL:HG23	1:E:298:PHE:CZ	2.55	0.41
1:C:193:TYR:CD1	1:C:193:TYR:N	2.86	0.41
1:D:200:ILE:O	1:D:204:MET:HB3	2.21	0.41
1:A:264:PHE:CE2	1:A:302:PHE:HB2	2.54	0.41
1:D:29:LEU:HB2	1:D:156:LEU:HD11	2.02	0.41
1:E:271:GLU:O	1:E:274:VAL:N	2.53	0.41
1:D:124:THR:HB	1:D:188:ARG:HE	1.83	0.41
1:C:89:VAL:CG1	1:C:102:LEU:HD23	2.50	0.41
1:A:132:ARG:HA	1:A:180:GLU:HG2	2.02	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:D:255:GLY:HA2	1:D:258:ILE:CG2	2.50	0.41
1:E:51:LEU:HB3	1:E:93:VAL:HG11	2.03	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:254:THR:O	1:D:258:ILE:HB	2.21	0.41
1:D:94:SER:OG	1:D:95:PRO:HD2	2.21	0.41
1:D:78:VAL:HB	1:D:128:TYR:HB2	2.01	0.41
1:D:129:LEU:HD22	1:D:185:TYR:CE1	2.56	0.41
1:E:123:GLN:C	1:E:188:ARG:HH21	2.24	0.41
1:C:32:LYS:HD3	1:C:243:THR:O	2.21	0.41
1:D:150:LYS:HE2	1:D:150:LYS:HB3	1.90	0.41
1:E:150:LYS:HE2	1:E:150:LYS:HB3	1.90	0.41
1:E:84:ARG:CB	1:E:107:ALA:HB2	2.51	0.41
1:E:234:HIS:HE1	1:E:258:ILE:O	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:ILE:O	1:A:265:TYR:HD1	2.04	0.41
1:E:128:TYR:O	1:E:129:LEU:HB2	2.20	0.41
1:A:155:PHE:HB3	1:A:156:LEU:H	1.71	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:D:134:VAL:HG12	1:D:135:ASP:H	1.85	0.41
1:B:202:LEU:HB2	1:B:203:PRO:HD3	2.02	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: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:217:SER:HG	1:B:220:TYR:HE2	1.64	0.40
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:B:217:SER:HG	1:C:220:TYR:HE2	1.66	0.40
1:A:118:TYR:HD2	1:A:254:THR:HG21	1.86	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:D:111:SER:HA	1:D:112:PRO:HD2	1.76	0.40
1:A:76:ARG:HH22	1:A:130:ILE:HD12	1.86	0.40
1:E:216:TRP:HA	1:E:295:ARG:HH21	1.86	0.40
1:C:216:TRP:CH2	1:C:295:ARG:CB	3.05	0.40
1:C:134:VAL:HG12	1:C:135:ASP:N	2.37	0.40
1:B:179:LEU:HD12	1:B:179:LEU:C	2.41	0.40
1:C:200:ILE:O	1:C:204:MET:HB3	2.20	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:D:128:TYR:O	1:D:183:LEU:O	2.40	0.40
1:E:264:PHE:O	1:E:268:ALA:HB2	2.22	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:B:207:ILE:HG13	1:B:208:LEU:N	2.37	0.40
1:E:119:PRO:HG3	1:E:254:THR:CB	2.39	0.40
1:C:123:GLN:C	1:C:188:ARG:HH21	2.25	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:A:72:ILE:HA	1:A:73:PRO:HD3	1.99	0.40
1:B:281:GLU:O	1:B:282:SER:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:ASN:O	1:D:44:LEU:HA	2.21	0.40
1:C:32:LYS:HD3	1:C:245:LEU:H	1.86	0.40
1:E:230:THR:OG1	1:E:265:TYR:HE2	2.04	0.40
1:B:159:TRP:CE3	1:B:189:ILE:HD12	2.57	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	23
1	B	308/317 (97%)	250 (81%)	40 (13%)	18 (6%)	2	23
1	C	308/317 (97%)	247 (80%)	43 (14%)	18 (6%)	2	23
1	D	308/317 (97%)	249 (81%)	42 (14%)	17 (6%)	2	24
1	E	308/317 (97%)	247 (80%)	43 (14%)	18 (6%)	2	23
All	All	1540/1585 (97%)	1239 (80%)	212 (14%)	89 (6%)	2	23

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	38
1	B	277/283 (98%)	246 (89%)	31 (11%)	7	35
1	C	277/283 (98%)	248 (90%)	29 (10%)	8	38
1	D	277/283 (98%)	248 (90%)	29 (10%)	8	38
1	E	277/283 (98%)	246 (89%)	31 (11%)	7	35
All	All	1385/1415 (98%)	1236 (89%)	149 (11%)	8	37

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%)	-0.21	4 (1%) 79 70	76, 103, 142, 169	0
1	B	310/317 (97%)	-0.24	4 (1%) 79 70	76, 103, 142, 169	0
1	C	310/317 (97%)	-0.26	1 (0%) 94 91	76, 103, 142, 169	0
1	D	310/317 (97%)	-0.22	2 (0%) 90 85	76, 103, 142, 169	0
1	E	310/317 (97%)	-0.25	4 (1%) 79 70	76, 103, 142, 169	0
All	All	1550/1585 (97%)	-0.24	15 (0%) 84 76	76, 103, 143, 169	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	316	PHE	3.7
1	A	316	PHE	3.1
1	E	282	SER	2.9
1	D	282	SER	2.6
1	E	316	PHE	2.6
1	B	282	SER	2.6
1	D	55	PRO	2.5
1	A	315	GLY	2.5
1	B	316	PHE	2.5
1	A	282	SER	2.3
1	B	63	LYS	2.3
1	E	60	VAL	2.3
1	E	286	ARG	2.2
1	B	133	SER	2.2
1	A	51	LEU	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.