



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:39 PM UTC

PDB ID : 3UDC / pdb_00003udc
Title : Crystal structure of a membrane protein
Authors : Li, W.; Ge, J.; Yang, M.
Deposited on : 2011-10-28
Resolution : 3.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

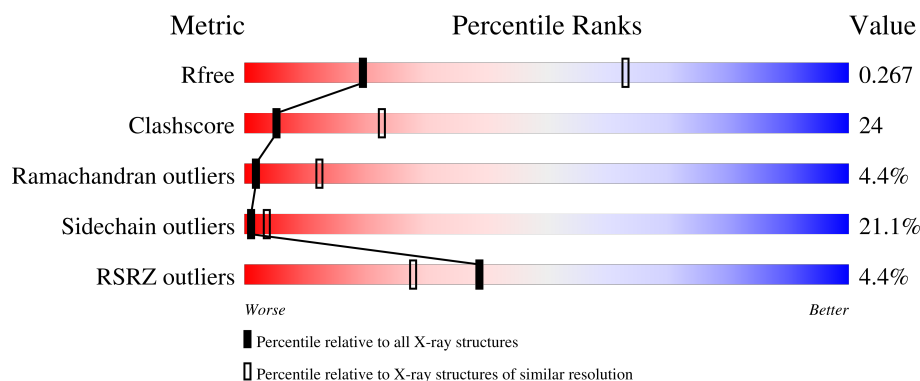
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	285	4% 43% 38% 12% 6%
1	B	285	0% 46% 36% 11% 6%
1	C	285	4% 44% 38% 10% 6%
1	D	285	7% 46% 36% 10% 6%
1	E	285	4% 44% 37% 12% 6%

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Mol	Chain	Length	Quality of chain
1	F	285	4%45%36%12%• 6%
1	G	285	5%44%37%11%• 6%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 14903 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.

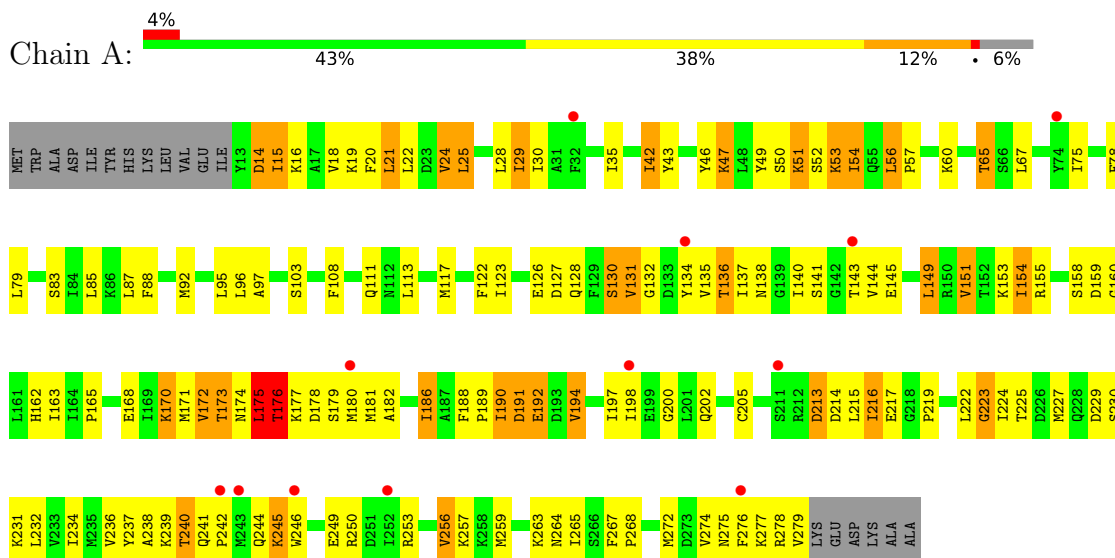
- Molecule 1 is a protein called Small-conductance mechanosensitive channel, C-terminal peptide from Small-conductance mechanosensitive channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2129	1391	343	384	11			
1	B	267	Total	C	N	O	S	0	0	0
			2129	1391	343	384	11			
1	C	267	Total	C	N	O	S	0	0	0
			2129	1391	343	384	11			
1	D	267	Total	C	N	O	S	0	0	0
			2129	1391	343	384	11			
1	E	267	Total	C	N	O	S	0	0	0
			2129	1391	343	384	11			
1	F	267	Total	C	N	O	S	0	0	0
			2129	1391	343	384	11			
1	G	267	Total	C	N	O	S	0	0	0
			2129	1391	343	384	11			

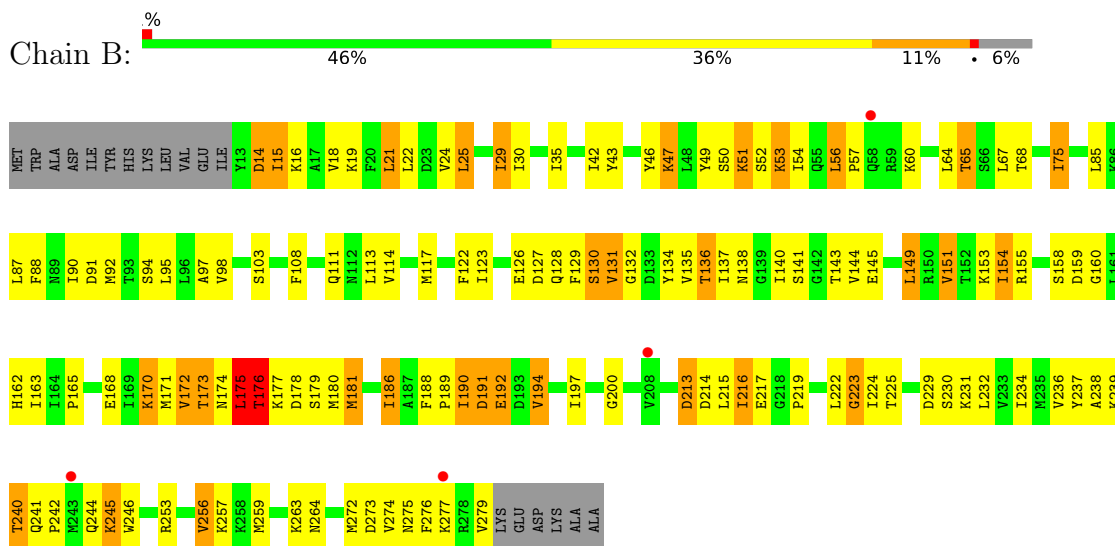
3 Residue-property plots

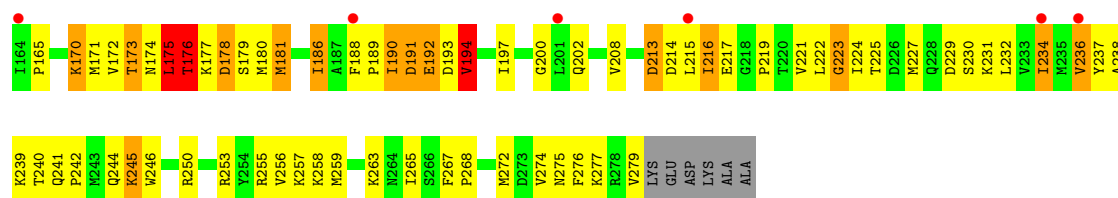
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Small-conductance mechanosensitive channel, C-terminal peptide from Small-conductance mechanosensitive channel

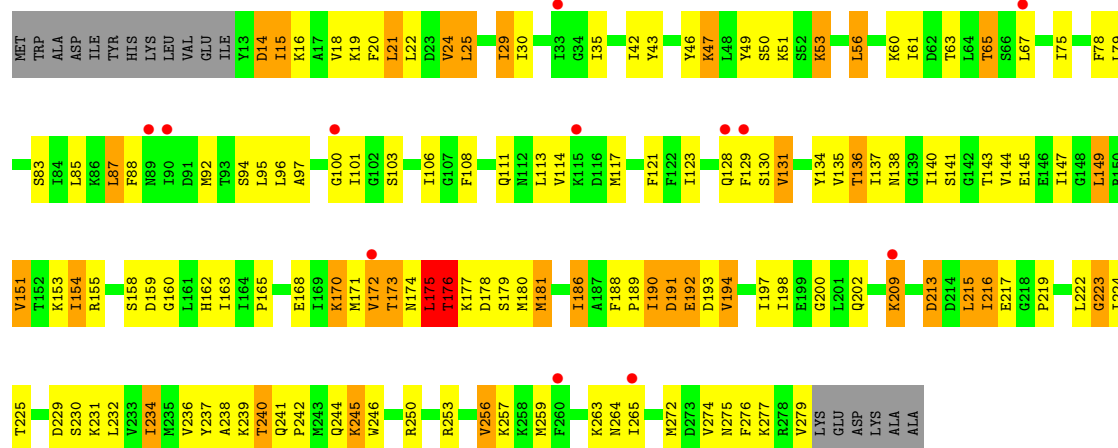
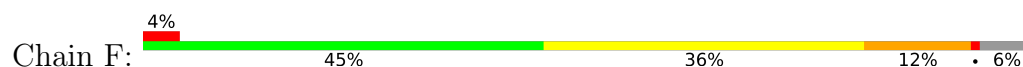


- Molecule 1: Small-conductance mechanosensitive channel, C-terminal peptide from Small-conductance mechanosensitive channel

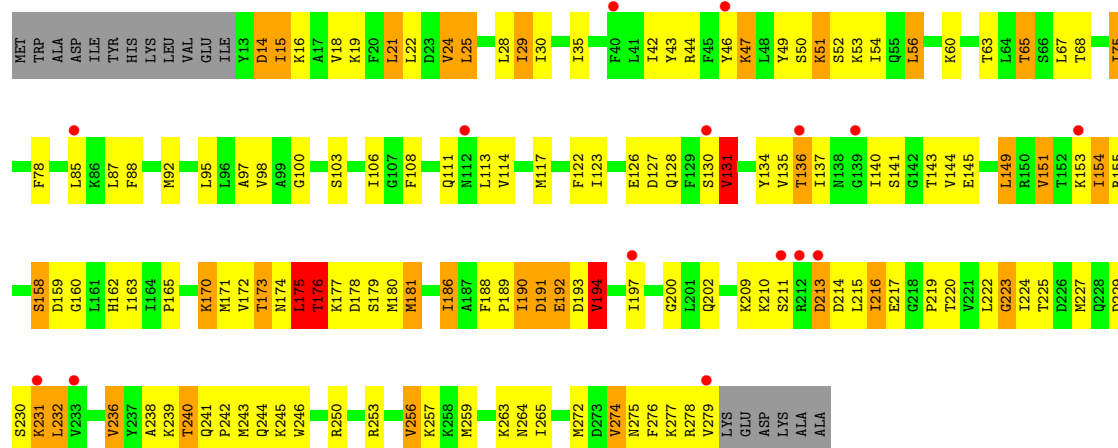
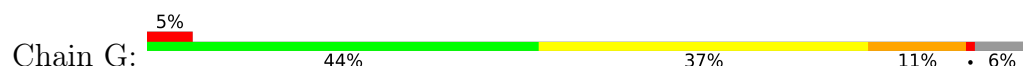




● Molecule 1: Small-conductance mechanosensitive channel, C-terminal peptide from Small-conductance mechanosensitive channel



● Molecule 1: Small-conductance mechanosensitive channel, C-terminal peptide from Small-conductance mechanosensitive channel



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.05Å 139.47Å 224.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.08 – 3.35 42.08 – 3.35	Depositor EDS
% Data completeness (in resolution range)	98.9 (42.08-3.35) 98.9 (42.08-3.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 3.32Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.248 , 0.274 0.240 , 0.267	Depositor DCC
R_{free} test set	1878 reflections (4.32%)	wwPDB-VP
Wilson B-factor (Å ²)	111.9	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 77.9	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	0.92	EDS
Total number of atoms	14903	wwPDB-VP
Average B, all atoms (Å ²)	141.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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

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	0.61	0/2165	0.93	1/2915 (0.0%)
1	B	0.60	0/2165	0.93	2/2915 (0.1%)
1	C	0.63	0/2165	0.95	3/2915 (0.1%)
1	D	0.62	0/2165	0.94	2/2915 (0.1%)
1	E	0.63	0/2165	0.95	3/2915 (0.1%)
1	F	0.62	0/2165	0.95	1/2915 (0.0%)
1	G	0.63	0/2165	0.95	3/2915 (0.1%)
All	All	0.62	0/15155	0.94	15/20405 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	192	GLU	N-CA-C	7.38	120.05	110.53
1	C	192	GLU	N-CA-C	7.27	119.90	110.53
1	G	192	GLU	N-CA-C	7.23	119.86	110.53
1	E	192	GLU	N-CA-C	7.14	119.74	110.53
1	F	192	GLU	N-CA-C	6.84	119.79	110.35
1	A	192	GLU	N-CA-C	6.72	119.62	110.35
1	B	192	GLU	N-CA-C	6.58	119.02	110.53
1	C	194	VAL	N-CA-C	6.09	116.27	110.42
1	G	194	VAL	N-CA-C	5.89	116.08	110.42
1	B	194	VAL	N-CA-C	5.35	115.56	110.53
1	E	194	VAL	N-CA-C	5.13	115.35	110.53
1	D	194	VAL	N-CA-C	5.12	115.89	110.72
1	C	27	ILE	CB-CA-C	-5.07	105.30	112.14
1	E	59	ARG	N-CA-C	-5.05	106.81	113.12
1	G	211	SER	N-CA-C	5.00	119.14	113.19

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	2129	0	2223	136	1
1	B	2129	0	2223	121	0
1	C	2129	0	2223	132	0
1	D	2129	0	2223	125	0
1	E	2129	0	2223	131	0
1	F	2129	0	2223	131	0
1	G	2129	0	2223	126	1
All	All	14903	0	15561	741	1

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 24.

All (741) 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:162:HIS:HD2	1:E:173:THR:HB	1.19	1.04
1:A:173:THR:HB	1:B:162:HIS:HD2	1.24	1.02
1:A:162:HIS:HD2	1:D:173:THR:HB	1.24	1.02
1:G:217:GLU:HB3	1:G:239:LYS:HB2	1.43	1.00
1:C:173:THR:HB	1:F:162:HIS:HD2	1.24	0.99
1:E:162:HIS:HD2	1:F:173:THR:HB	1.23	0.99
1:A:217:GLU:HB3	1:A:239:LYS:HB2	1.44	0.97
1:B:217:GLU:HB3	1:B:239:LYS:HB2	1.47	0.97
1:D:217:GLU:HB3	1:D:239:LYS:HB2	1.45	0.97
1:C:217:GLU:HB3	1:C:239:LYS:HB2	1.44	0.96
1:B:173:THR:HB	1:G:162:HIS:HD2	1.30	0.95
1:F:217:GLU:HB3	1:F:239:LYS:HB2	1.50	0.94
1:D:158:SER:HA	1:E:181:MET:HB3	1.49	0.94
1:E:217:GLU:HB3	1:E:239:LYS:HB2	1.50	0.92
1:D:162:HIS:CD2	1:E:173:THR:HB	2.06	0.91
1:C:162:HIS:HD2	1:G:173:THR:HB	1.35	0.89
1:E:162:HIS:CD2	1:F:173:THR:HB	2.10	0.86
1:C:173:THR:HB	1:F:162:HIS:CD2	2.09	0.86
1:B:277:LYS:HE2	1:G:275:ASN:OD1	1.75	0.85
1:A:173:THR:HB	1:B:162:HIS:CD2	2.11	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:14:ASP:HA	1:E:16:LYS:HZ1	1.42	0.85
1:A:162:HIS:CD2	1:D:173:THR:HB	2.10	0.84
1:C:158:SER:HA	1:G:181:MET:HB3	1.59	0.84
1:D:134:TYR:CD2	1:D:175:LEU:HD23	2.13	0.83
1:C:134:TYR:CD2	1:C:175:LEU:HD23	2.14	0.83
1:G:134:TYR:CD2	1:G:175:LEU:HD23	2.13	0.83
1:G:14:ASP:HA	1:G:16:LYS:HZ3	1.40	0.83
1:B:134:TYR:CD2	1:B:175:LEU:HD23	2.14	0.82
1:B:14:ASP:HA	1:B:16:LYS:HZ1	1.45	0.82
1:C:14:ASP:HA	1:C:16:LYS:HZ3	1.43	0.82
1:A:134:TYR:CD2	1:A:175:LEU:HD23	2.14	0.82
1:C:134:TYR:HD2	1:C:175:LEU:HD23	1.45	0.81
1:A:14:ASP:HA	1:A:16:LYS:HZ3	1.44	0.81
1:F:14:ASP:HA	1:F:16:LYS:HZ3	1.44	0.81
1:B:173:THR:HB	1:G:162:HIS:CD2	2.16	0.81
1:E:134:TYR:CD2	1:E:175:LEU:HD23	2.16	0.81
1:E:275:ASN:OD1	1:F:277:LYS:HE2	1.81	0.80
1:D:275:ASN:OD1	1:E:277:LYS:HE2	1.80	0.80
1:E:88:PHE:CD1	1:F:30:ILE:HB	2.17	0.80
1:F:134:TYR:CD2	1:F:175:LEU:HD23	2.17	0.79
1:D:14:ASP:HA	1:D:16:LYS:HZ3	1.45	0.79
1:G:134:TYR:HD2	1:G:175:LEU:HD23	1.45	0.78
1:A:134:TYR:HD2	1:A:175:LEU:HD23	1.48	0.78
1:E:134:TYR:HD2	1:E:175:LEU:HD23	1.48	0.78
1:D:215:LEU:HD22	1:D:219:PRO:HD3	1.66	0.78
1:D:272:MET:HE2	1:E:272:MET:SD	2.25	0.76
1:A:277:LYS:HE2	1:B:275:ASN:OD1	1.86	0.76
1:D:134:TYR:HD2	1:D:175:LEU:HD23	1.48	0.76
1:E:180:MET:HE2	1:E:245:LYS:HD2	1.66	0.76
1:A:158:SER:HA	1:D:181:MET:HB3	1.66	0.76
1:A:217:GLU:CB	1:A:239:LYS:HB2	2.17	0.74
1:E:88:PHE:HD1	1:F:30:ILE:HB	1.51	0.74
1:B:181:MET:HB3	1:G:158:SER:HA	1.69	0.74
1:B:190:ILE:O	1:G:257:LYS:NZ	2.21	0.74
1:D:217:GLU:CB	1:D:239:LYS:HB2	2.18	0.74
1:B:176:THR:OG1	1:B:177:LYS:N	2.20	0.74
1:A:30:ILE:HB	1:B:88:PHE:CD1	2.23	0.74
1:A:92:MET:HA	1:A:92:MET:HE2	1.68	0.73
1:G:217:GLU:CB	1:G:239:LYS:HB2	2.17	0.73
1:B:134:TYR:HD2	1:B:175:LEU:HD23	1.51	0.73
1:B:217:GLU:CB	1:B:239:LYS:HB2	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:HIS:CD2	1:G:173:THR:HB	2.21	0.72
1:F:134:TYR:HD2	1:F:175:LEU:HD23	1.51	0.72
1:G:215:LEU:HD22	1:G:219:PRO:HD3	1.71	0.72
1:A:272:MET:HE2	1:D:272:MET:SD	2.30	0.71
1:E:176:THR:OG1	1:E:177:LYS:N	2.18	0.71
1:E:215:LEU:HD22	1:E:219:PRO:HD3	1.72	0.71
1:D:180:MET:HE2	1:D:245:LYS:HD2	1.72	0.70
1:F:176:THR:OG1	1:F:177:LYS:N	2.23	0.70
1:C:176:THR:OG1	1:C:177:LYS:N	2.23	0.70
1:A:272:MET:SD	1:B:272:MET:HE2	2.31	0.70
1:A:180:MET:HE2	1:A:245:LYS:HD2	1.73	0.70
1:C:181:MET:HB3	1:F:158:SER:HA	1.73	0.70
1:C:92:MET:HE2	1:C:92:MET:HA	1.74	0.69
1:C:30:ILE:HB	1:F:88:PHE:CD1	2.27	0.69
1:C:180:MET:HE2	1:C:245:LYS:HD2	1.74	0.69
1:D:92:MET:HA	1:D:92:MET:HE2	1.74	0.69
1:C:272:MET:HE2	1:G:272:MET:SD	2.33	0.69
1:G:213:ASP:OD2	1:G:213:ASP:N	2.25	0.69
1:E:272:MET:HE2	1:F:272:MET:SD	2.33	0.69
1:F:92:MET:HA	1:F:92:MET:HE2	1.74	0.69
1:C:277:LYS:HE2	1:F:275:ASN:OD1	1.93	0.69
1:C:217:GLU:CB	1:C:239:LYS:HB2	2.18	0.68
1:C:30:ILE:HB	1:F:88:PHE:HD1	1.58	0.68
1:F:215:LEU:HD22	1:F:219:PRO:HD3	1.73	0.68
1:A:173:THR:CB	1:B:162:HIS:HD2	2.04	0.68
1:E:186:ILE:HG21	1:E:256:VAL:HG11	1.75	0.68
1:F:217:GLU:CB	1:F:239:LYS:HB2	2.23	0.67
1:C:215:LEU:HD22	1:C:219:PRO:HD3	1.77	0.67
1:C:190:ILE:O	1:F:257:LYS:NZ	2.26	0.67
1:E:92:MET:HE2	1:E:92:MET:HA	1.75	0.67
1:F:180:MET:HE2	1:F:245:LYS:HD2	1.75	0.67
1:G:176:THR:OG1	1:G:177:LYS:N	2.21	0.67
1:B:215:LEU:HD22	1:B:219:PRO:HD3	1.76	0.67
1:E:213:ASP:N	1:E:213:ASP:OD2	2.28	0.67
1:D:46:TYR:HD1	1:D:65:THR:HG21	1.61	0.66
1:A:257:LYS:NZ	1:D:190:ILE:O	2.27	0.66
1:F:135:VAL:HG12	1:F:174:ASN:HA	1.77	0.66
1:A:275:ASN:OD1	1:D:277:LYS:HE2	1.95	0.66
1:D:176:THR:OG1	1:D:177:LYS:N	2.27	0.66
1:A:30:ILE:HB	1:B:88:PHE:HD1	1.60	0.66
1:C:257:LYS:HE2	1:G:194:VAL:HG22	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:213:ASP:OD2	1:F:213:ASP:N	2.27	0.66
1:G:217:GLU:HB3	1:G:239:LYS:CB	2.25	0.66
1:G:189:PRO:HD2	1:G:192:GLU:HG3	1.77	0.65
1:C:213:ASP:N	1:C:213:ASP:OD2	2.28	0.65
1:A:215:LEU:HD22	1:A:219:PRO:HD3	1.76	0.65
1:A:217:GLU:HB3	1:A:239:LYS:CB	2.22	0.65
1:C:173:THR:CB	1:F:162:HIS:HD2	2.03	0.65
1:E:162:HIS:HD2	1:F:173:THR:CB	2.04	0.65
1:E:189:PRO:HD2	1:E:192:GLU:HG3	1.78	0.65
1:B:213:ASP:OD2	1:B:213:ASP:N	2.30	0.65
1:C:88:PHE:HD1	1:G:30:ILE:HB	1.61	0.65
1:C:117:MET:HG2	1:C:149:LEU:HD13	1.80	0.64
1:D:162:HIS:HD2	1:E:173:THR:CB	2.03	0.64
1:C:217:GLU:HB3	1:C:239:LYS:CB	2.24	0.64
1:D:257:LYS:NZ	1:E:190:ILE:O	2.29	0.64
1:D:213:ASP:OD2	1:D:213:ASP:N	2.29	0.64
1:E:46:TYR:HD1	1:E:65:THR:HG21	1.62	0.64
1:A:25:LEU:O	1:A:29:ILE:HG23	1.98	0.64
1:C:275:ASN:OD1	1:G:277:LYS:HE2	1.98	0.64
1:A:176:THR:OG1	1:A:177:LYS:N	2.29	0.63
1:D:217:GLU:HB3	1:D:239:LYS:CB	2.25	0.63
1:B:137:ILE:HD12	1:B:154:ILE:CD1	2.27	0.63
1:C:88:PHE:CD1	1:G:30:ILE:HB	2.33	0.63
1:G:92:MET:HE2	1:G:92:MET:HA	1.79	0.63
1:A:117:MET:HG2	1:A:149:LEU:HD13	1.81	0.63
1:B:25:LEU:O	1:B:29:ILE:HG23	1.98	0.63
1:B:46:TYR:HD1	1:B:65:THR:HG21	1.64	0.63
1:B:173:THR:CB	1:G:162:HIS:HD2	2.08	0.63
1:A:46:TYR:HD1	1:A:65:THR:HG21	1.64	0.63
1:B:186:ILE:HG21	1:B:256:VAL:HG11	1.80	0.63
1:F:137:ILE:HD12	1:F:154:ILE:CD1	2.29	0.63
1:G:186:ILE:HG21	1:G:256:VAL:HG11	1.80	0.63
1:B:180:MET:HE2	1:B:245:LYS:HD2	1.81	0.62
1:E:257:LYS:NZ	1:F:190:ILE:O	2.31	0.62
1:B:92:MET:HE2	1:B:92:MET:HA	1.81	0.62
1:E:46:TYR:CD1	1:E:65:THR:HG21	2.35	0.62
1:A:103:SER:OG	1:B:97:ALA:O	2.16	0.62
1:D:200:GLY:C	1:D:259:MET:HE2	2.24	0.62
1:E:217:GLU:CB	1:E:239:LYS:HB2	2.25	0.62
1:G:46:TYR:HD1	1:G:65:THR:HG21	1.64	0.62
1:A:181:MET:HB3	1:B:158:SER:HA	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:VAL:HG12	1:B:174:ASN:HA	1.81	0.62
1:B:75:ILE:HD13	1:G:98:VAL:HG11	1.79	0.62
1:D:113:LEU:HD11	1:E:122:PHE:CZ	2.35	0.62
1:E:158:SER:HA	1:F:181:MET:HB3	1.80	0.62
1:F:25:LEU:O	1:F:29:ILE:HG23	2.00	0.62
1:A:189:PRO:HD2	1:A:192:GLU:HG3	1.82	0.61
1:D:46:TYR:CD1	1:D:65:THR:HG21	2.35	0.61
1:F:46:TYR:HD1	1:F:65:THR:HG21	1.64	0.61
1:E:175:LEU:O	1:E:176:THR:C	2.43	0.61
1:G:175:LEU:O	1:G:176:THR:C	2.43	0.61
1:C:43:TYR:O	1:C:46:TYR:HB3	2.00	0.61
1:A:162:HIS:HD2	1:D:173:THR:CB	2.07	0.61
1:B:219:PRO:HA	1:B:238:ALA:HB2	1.83	0.61
1:E:160:GLY:HA3	1:F:175:LEU:HD12	1.83	0.61
1:F:46:TYR:CD1	1:F:65:THR:HG21	2.35	0.61
1:A:92:MET:HG3	1:B:91:ASP:OD2	2.01	0.61
1:G:117:MET:HG2	1:G:149:LEU:HD13	1.82	0.61
1:C:186:ILE:HG21	1:C:256:VAL:HG11	1.83	0.60
1:E:25:LEU:O	1:E:29:ILE:HG23	2.01	0.60
1:E:91:ASP:OD2	1:F:92:MET:HG3	2.01	0.60
1:D:186:ILE:HG21	1:D:256:VAL:HG11	1.83	0.60
1:E:117:MET:HG2	1:E:149:LEU:HD13	1.83	0.60
1:C:46:TYR:HD1	1:C:65:THR:HG21	1.66	0.60
1:A:213:ASP:OD2	1:A:213:ASP:N	2.34	0.60
1:A:219:PRO:HA	1:A:238:ALA:HB2	1.84	0.60
1:C:272:MET:SD	1:F:272:MET:HE2	2.42	0.60
1:D:88:PHE:HD1	1:E:30:ILE:HB	1.66	0.60
1:E:135:VAL:HG12	1:E:174:ASN:HA	1.84	0.60
1:B:200:GLY:C	1:B:259:MET:HE2	2.26	0.60
1:A:46:TYR:CD1	1:A:65:THR:HG21	2.37	0.59
1:B:175:LEU:O	1:B:176:THR:C	2.43	0.59
1:G:219:PRO:HA	1:G:238:ALA:HB2	1.84	0.59
1:C:257:LYS:NZ	1:G:190:ILE:O	2.36	0.59
1:D:25:LEU:O	1:D:29:ILE:HG23	2.02	0.59
1:A:43:TYR:O	1:A:46:TYR:HB3	2.02	0.59
1:B:189:PRO:HD2	1:B:192:GLU:HG3	1.84	0.59
1:D:253:ARG:HD2	1:E:224:ILE:O	2.02	0.59
1:E:189:PRO:HB2	1:E:191:ASP:HB3	1.85	0.59
1:C:219:PRO:HA	1:C:238:ALA:HB2	1.84	0.59
1:F:186:ILE:HG21	1:F:256:VAL:HG11	1.83	0.59
1:A:186:ILE:HG21	1:A:256:VAL:HG11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:175:LEU:O	1:F:176:THR:C	2.46	0.59
1:G:180:MET:HE2	1:G:245:LYS:HD2	1.84	0.59
1:B:46:TYR:CD1	1:B:65:THR:HG21	2.37	0.59
1:B:117:MET:HG2	1:B:149:LEU:HD13	1.84	0.59
1:C:175:LEU:O	1:C:176:THR:C	2.46	0.59
1:D:216:ILE:HG12	1:D:239:LYS:HB3	1.84	0.59
1:G:43:TYR:O	1:G:46:TYR:HB3	2.03	0.59
1:D:135:VAL:HG12	1:D:174:ASN:HA	1.84	0.59
1:D:276:PHE:CZ	1:E:276:PHE:CE1	2.91	0.59
1:C:46:TYR:CD1	1:C:65:THR:HG21	2.38	0.58
1:D:219:PRO:HA	1:D:238:ALA:HB2	1.83	0.58
1:G:200:GLY:C	1:G:259:MET:HE2	2.28	0.58
1:C:200:GLY:C	1:C:259:MET:HE2	2.29	0.58
1:D:175:LEU:O	1:D:176:THR:C	2.46	0.58
1:D:189:PRO:HD2	1:D:192:GLU:HG3	1.85	0.58
1:E:136:THR:HB	1:E:141:SER:OG	2.04	0.58
1:C:273:ASP:HB2	1:G:275:ASN:HB2	1.85	0.58
1:G:25:LEU:O	1:G:29:ILE:HG23	2.03	0.58
1:G:46:TYR:CD1	1:G:65:THR:HG21	2.37	0.58
1:A:276:PHE:CE1	1:B:276:PHE:CZ	2.92	0.58
1:D:216:ILE:HD11	1:D:239:LYS:HD2	1.85	0.58
1:A:200:GLY:C	1:A:259:MET:HE2	2.29	0.58
1:E:43:TYR:O	1:E:46:TYR:HB3	2.04	0.58
1:D:160:GLY:HA3	1:E:175:LEU:HD12	1.84	0.58
1:C:272:MET:O	1:G:274:VAL:HA	2.03	0.57
1:F:200:GLY:C	1:F:259:MET:HE2	2.29	0.57
1:C:137:ILE:HD12	1:C:154:ILE:CD1	2.34	0.57
1:E:47:LYS:HB2	1:E:47:LYS:NZ	2.18	0.57
1:F:117:MET:HG2	1:F:149:LEU:HD13	1.86	0.57
1:D:43:TYR:O	1:D:46:TYR:HB3	2.05	0.57
1:F:189:PRO:HD2	1:F:192:GLU:HG3	1.86	0.57
1:D:108:PHE:O	1:D:111:GLN:HG2	2.04	0.57
1:C:135:VAL:HG12	1:C:174:ASN:HA	1.87	0.57
1:B:175:LEU:HD12	1:G:160:GLY:HA3	1.86	0.57
1:B:217:GLU:HB3	1:B:239:LYS:CB	2.29	0.57
1:C:117:MET:HG2	1:C:149:LEU:CD1	2.35	0.57
1:C:175:LEU:HD12	1:F:160:GLY:HA3	1.85	0.57
1:B:47:LYS:HB2	1:B:47:LYS:NZ	2.19	0.57
1:C:25:LEU:O	1:C:29:ILE:HG23	2.05	0.57
1:A:190:ILE:O	1:B:257:LYS:NZ	2.38	0.57
1:C:180:MET:HE1	1:C:246:TRP:CH2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:PRO:HB2	1:A:191:ASP:HB3	1.86	0.57
1:C:189:PRO:HD2	1:C:192:GLU:HG3	1.87	0.57
1:E:42:ILE:HD11	1:E:68:THR:HG22	1.87	0.56
1:G:189:PRO:HB2	1:G:191:ASP:HB3	1.87	0.56
1:B:103:SER:OG	1:G:97:ALA:O	2.21	0.56
1:C:108:PHE:O	1:C:111:GLN:HG2	2.05	0.56
1:D:88:PHE:CD1	1:E:30:ILE:HB	2.41	0.56
1:E:97:ALA:O	1:F:103:SER:OG	2.22	0.56
1:G:136:THR:HB	1:G:141:SER:OG	2.05	0.56
1:E:217:GLU:HB3	1:E:239:LYS:CB	2.29	0.56
1:B:43:TYR:O	1:B:46:TYR:HB3	2.05	0.56
1:C:188:PHE:CE2	1:C:197:ILE:HG21	2.40	0.56
1:F:43:TYR:O	1:F:46:TYR:HB3	2.06	0.56
1:F:217:GLU:HB3	1:F:239:LYS:CB	2.31	0.56
1:C:97:ALA:O	1:G:103:SER:OG	2.23	0.56
1:C:103:SER:OG	1:F:97:ALA:O	2.20	0.56
1:E:188:PHE:HE2	1:E:234:ILE:HG13	1.71	0.56
1:D:117:MET:HG2	1:D:149:LEU:HD13	1.88	0.55
1:E:188:PHE:CG	1:E:197:ILE:HD13	2.42	0.55
1:G:180:MET:HE1	1:G:246:TRP:CH2	2.41	0.55
1:A:136:THR:HB	1:A:141:SER:OG	2.06	0.55
1:F:188:PHE:CG	1:F:197:ILE:HD13	2.42	0.55
1:F:219:PRO:HA	1:F:238:ALA:HB2	1.88	0.55
1:A:135:VAL:HG12	1:A:174:ASN:HA	1.87	0.55
1:G:135:VAL:HG12	1:G:174:ASN:HA	1.88	0.55
1:A:137:ILE:HD12	1:A:154:ILE:CD1	2.37	0.55
1:A:47:LYS:HB2	1:A:47:LYS:NZ	2.22	0.55
1:A:188:PHE:CG	1:A:197:ILE:HD13	2.42	0.55
1:F:47:LYS:HB2	1:F:47:LYS:NZ	2.21	0.55
1:G:47:LYS:HB2	1:G:47:LYS:NZ	2.22	0.55
1:C:189:PRO:HB2	1:C:191:ASP:HB3	1.89	0.54
1:D:188:PHE:CG	1:D:197:ILE:HD13	2.42	0.54
1:D:188:PHE:HE2	1:D:234:ILE:HG13	1.72	0.54
1:A:175:LEU:O	1:A:176:THR:C	2.48	0.54
1:F:180:MET:HE1	1:F:246:TRP:CH2	2.42	0.54
1:B:30:ILE:HB	1:G:88:PHE:HD1	1.71	0.54
1:D:47:LYS:HB2	1:D:47:LYS:NZ	2.23	0.54
1:F:188:PHE:CE2	1:F:197:ILE:HG21	2.41	0.54
1:C:257:LYS:CE	1:G:194:VAL:HG22	2.38	0.54
1:B:189:PRO:HB2	1:B:191:ASP:HB3	1.89	0.54
1:F:216:ILE:HD11	1:F:239:LYS:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:PHE:O	1:A:111:GLN:HG2	2.08	0.54
1:A:216:ILE:HG12	1:A:239:LYS:HB3	1.88	0.54
1:A:253:ARG:HD2	1:D:224:ILE:O	2.07	0.54
1:B:153:LYS:HG2	1:B:163:ILE:HG12	1.90	0.54
1:C:21:LEU:O	1:C:25:LEU:HB2	2.08	0.54
1:G:188:PHE:CG	1:G:197:ILE:HD13	2.43	0.54
1:D:153:LYS:HG2	1:D:163:ILE:HG12	1.88	0.54
1:E:200:GLY:C	1:E:259:MET:HE2	2.32	0.54
1:C:136:THR:HB	1:C:141:SER:OG	2.09	0.53
1:D:136:THR:HB	1:D:141:SER:OG	2.09	0.53
1:D:98:VAL:HG11	1:E:75:ILE:HD13	1.90	0.53
1:B:188:PHE:CG	1:B:197:ILE:HD13	2.44	0.53
1:F:189:PRO:HB2	1:F:191:ASP:HB3	1.90	0.53
1:A:188:PHE:CE2	1:A:197:ILE:HG21	2.44	0.53
1:F:151:VAL:HG23	1:F:165:PRO:HA	1.91	0.53
1:F:216:ILE:HG12	1:F:239:LYS:HB3	1.90	0.53
1:G:154:ILE:HG22	1:G:154:ILE:O	2.08	0.53
1:C:253:ARG:HD2	1:G:224:ILE:O	2.08	0.53
1:C:273:ASP:CB	1:G:275:ASN:HB2	2.39	0.53
1:D:257:LYS:CE	1:E:194:VAL:HG22	2.39	0.53
1:G:108:PHE:O	1:G:111:GLN:HG2	2.09	0.53
1:A:21:LEU:O	1:A:25:LEU:HB2	2.08	0.52
1:B:136:THR:HB	1:B:141:SER:OG	2.09	0.52
1:C:91:ASP:OD2	1:G:92:MET:HG3	2.09	0.52
1:E:98:VAL:CG1	1:F:75:ILE:HD13	2.40	0.52
1:E:134:TYR:H	1:E:176:THR:HG21	1.74	0.52
1:F:188:PHE:HE2	1:F:234:ILE:HG13	1.75	0.52
1:D:180:MET:HE1	1:D:246:TRP:CH2	2.44	0.52
1:B:272:MET:SD	1:G:272:MET:HE2	2.49	0.52
1:D:189:PRO:HB2	1:D:191:ASP:HB3	1.91	0.52
1:B:21:LEU:O	1:B:25:LEU:HB2	2.10	0.52
1:D:98:VAL:CG1	1:E:75:ILE:HD13	2.40	0.52
1:D:250:ARG:CZ	1:E:222:LEU:HD12	2.40	0.52
1:E:117:MET:HG2	1:E:149:LEU:CD1	2.40	0.52
1:B:30:ILE:HB	1:G:88:PHE:CD1	2.45	0.52
1:E:180:MET:HE1	1:E:246:TRP:CH2	2.45	0.52
1:E:221:VAL:HG22	1:E:236:VAL:HG12	1.92	0.52
1:A:113:LEU:HD11	1:D:122:PHE:CZ	2.44	0.51
1:B:216:ILE:HG12	1:B:239:LYS:HB3	1.92	0.51
1:G:186:ILE:HD12	1:G:256:VAL:HG21	1.91	0.51
1:C:47:LYS:HB2	1:C:47:LYS:NZ	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:153:LYS:HG2	1:F:163:ILE:HG12	1.91	0.51
1:E:219:PRO:HA	1:E:238:ALA:HB2	1.92	0.51
1:A:151:VAL:HG23	1:A:165:PRO:HA	1.91	0.51
1:A:190:ILE:O	1:A:192:GLU:N	2.42	0.51
1:C:188:PHE:CG	1:C:197:ILE:HD13	2.45	0.51
1:D:21:LEU:O	1:D:25:LEU:HB2	2.10	0.51
1:C:276:PHE:CZ	1:G:276:PHE:CE1	2.98	0.51
1:E:56:LEU:HD12	1:E:60:LYS:CB	2.41	0.51
1:A:134:TYR:H	1:A:176:THR:HG21	1.75	0.51
1:A:241:GLN:HG3	1:A:242:PRO:HD2	1.93	0.51
1:C:153:LYS:HG2	1:C:163:ILE:HG12	1.93	0.51
1:B:134:TYR:H	1:B:176:THR:HG21	1.76	0.50
1:B:75:ILE:HD13	1:G:98:VAL:CG1	2.41	0.50
1:C:224:ILE:O	1:F:253:ARG:HD2	2.11	0.50
1:F:136:THR:HB	1:F:141:SER:OG	2.11	0.50
1:G:216:ILE:HG12	1:G:239:LYS:HB3	1.93	0.50
1:D:134:TYR:H	1:D:176:THR:HG21	1.77	0.50
1:G:188:PHE:CE2	1:G:197:ILE:HG21	2.47	0.50
1:C:162:HIS:HD2	1:G:173:THR:CB	2.15	0.50
1:G:21:LEU:O	1:G:25:LEU:HB2	2.11	0.50
1:E:108:PHE:O	1:E:111:GLN:HG2	2.12	0.50
1:F:134:TYR:H	1:F:176:THR:HG21	1.76	0.50
1:A:257:LYS:HE2	1:D:194:VAL:HG22	1.94	0.50
1:B:108:PHE:O	1:B:111:GLN:HG2	2.11	0.50
1:C:276:PHE:CZ	1:G:276:PHE:CZ	3.00	0.50
1:D:113:LEU:CD1	1:E:122:PHE:CE2	2.95	0.50
1:D:113:LEU:HD13	1:E:122:PHE:CE2	2.46	0.50
1:A:153:LYS:HG2	1:A:163:ILE:HG12	1.94	0.50
1:B:188:PHE:HE2	1:B:234:ILE:HG13	1.77	0.50
1:C:188:PHE:HE2	1:C:234:ILE:HG13	1.76	0.50
1:E:188:PHE:CE2	1:E:197:ILE:HG21	2.47	0.50
1:E:197:ILE:HG12	1:E:265:ILE:HD13	1.94	0.50
1:B:137:ILE:HD12	1:B:154:ILE:HD12	1.94	0.49
1:B:214:ASP:HB2	1:B:244:GLN:HG3	1.94	0.49
1:E:98:VAL:HG11	1:F:75:ILE:HD13	1.93	0.49
1:G:181:MET:O	1:G:245:LYS:HE2	2.12	0.49
1:C:106:ILE:HA	1:G:114:VAL:HG11	1.93	0.49
1:G:117:MET:HG2	1:G:149:LEU:CD1	2.42	0.49
1:E:21:LEU:O	1:E:25:LEU:HB2	2.11	0.49
1:F:21:LEU:O	1:F:25:LEU:HB2	2.11	0.49
1:G:151:VAL:HG23	1:G:165:PRO:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:PHE:CZ	1:G:113:LEU:HD11	2.47	0.49
1:D:188:PHE:CE2	1:D:197:ILE:HG21	2.48	0.49
1:E:153:LYS:HG2	1:E:163:ILE:HG12	1.95	0.49
1:F:190:ILE:O	1:F:192:GLU:N	2.46	0.49
1:A:216:ILE:HD11	1:A:239:LYS:HD2	1.95	0.49
1:A:154:ILE:O	1:A:154:ILE:HG22	2.13	0.49
1:A:180:MET:HE1	1:A:246:TRP:CH2	2.47	0.49
1:D:222:LEU:HD22	1:D:237:TYR:CD1	2.48	0.49
1:E:222:LEU:HD22	1:E:237:TYR:CD1	2.47	0.49
1:B:46:TYR:C	1:B:46:TYR:CD2	2.91	0.49
1:A:214:ASP:HB2	1:A:244:GLN:HG3	1.95	0.48
1:D:257:LYS:HE2	1:E:194:VAL:HG22	1.95	0.48
1:F:15:ILE:H	1:F:16:LYS:NZ	2.11	0.48
1:C:241:GLN:HG3	1:C:242:PRO:HD2	1.94	0.48
1:E:222:LEU:O	1:E:223:GLY:O	2.30	0.48
1:G:134:TYR:H	1:G:176:THR:HG21	1.79	0.48
1:A:278:ARG:HB2	1:A:278:ARG:CZ	2.43	0.48
1:F:154:ILE:O	1:F:154:ILE:HG22	2.13	0.48
1:F:15:ILE:H	1:F:16:LYS:HZ3	1.61	0.48
1:D:154:ILE:O	1:D:154:ILE:HG22	2.14	0.48
1:B:117:MET:HG2	1:B:149:LEU:CD1	2.44	0.48
1:A:51:LYS:HD2	1:A:51:LYS:HA	1.63	0.48
1:A:177:LYS:O	1:A:179:SER:N	2.44	0.48
1:B:177:LYS:O	1:B:179:SER:N	2.45	0.48
1:C:154:ILE:HG22	1:C:154:ILE:O	2.13	0.48
1:D:18:VAL:HG13	1:D:19:LYS:N	2.29	0.48
1:E:130:SER:O	1:E:132:GLY:N	2.47	0.48
1:G:222:LEU:O	1:G:223:GLY:O	2.32	0.48
1:B:151:VAL:HG23	1:B:165:PRO:HA	1.96	0.48
1:B:222:LEU:HD12	1:G:250:ARG:CZ	2.44	0.48
1:D:241:GLN:HG3	1:D:242:PRO:HD2	1.95	0.48
1:E:178:ASP:O	1:E:179:SER:OG	2.29	0.48
1:G:46:TYR:C	1:G:46:TYR:CD2	2.92	0.48
1:C:179:SER:HB2	1:C:240:THR:O	2.14	0.47
1:A:29:ILE:HG13	1:A:30:ILE:N	2.29	0.47
1:A:186:ILE:HG22	1:D:227:MET:HE3	1.94	0.47
1:C:273:ASP:HB3	1:G:275:ASN:ND2	2.29	0.47
1:F:117:MET:HG2	1:F:149:LEU:CD1	2.43	0.47
1:C:134:TYR:H	1:C:176:THR:HG21	1.78	0.47
1:F:241:GLN:HG3	1:F:242:PRO:HD2	1.95	0.47
1:E:188:PHE:CE2	1:E:234:ILE:HG13	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:18:VAL:HG13	1:G:19:LYS:N	2.29	0.47
1:C:214:ASP:HB2	1:C:244:GLN:HG3	1.95	0.47
1:F:179:SER:HB2	1:F:240:THR:O	2.14	0.47
1:G:51:LYS:HD2	1:G:51:LYS:HA	1.64	0.47
1:B:29:ILE:HG13	1:B:30:ILE:N	2.30	0.47
1:E:46:TYR:C	1:E:46:TYR:CD2	2.93	0.47
1:E:95:LEU:HD23	1:F:79:LEU:HD11	1.96	0.47
1:F:181:MET:O	1:F:245:LYS:HE2	2.14	0.47
1:A:52:SER:O	1:A:54:ILE:HG13	2.15	0.47
1:C:100:GLY:O	1:C:104:LEU:HG	2.14	0.47
1:C:151:VAL:HG23	1:C:165:PRO:HA	1.96	0.47
1:D:186:ILE:HG22	1:E:227:MET:HE3	1.97	0.47
1:D:214:ASP:HB2	1:D:244:GLN:HG3	1.95	0.47
1:F:108:PHE:O	1:F:111:GLN:HG2	2.14	0.47
1:G:197:ILE:HG12	1:G:265:ILE:HD13	1.95	0.47
1:A:222:LEU:O	1:A:223:GLY:O	2.33	0.47
1:C:18:VAL:HG13	1:C:19:LYS:N	2.30	0.47
1:G:242:PRO:O	1:G:243:MET:HB2	2.14	0.47
1:A:181:MET:HE2	1:A:181:MET:HB2	1.62	0.47
1:A:257:LYS:CE	1:D:194:VAL:HG22	2.44	0.47
1:E:51:LYS:HD2	1:E:51:LYS:HA	1.59	0.47
1:B:154:ILE:O	1:B:154:ILE:HG22	2.14	0.47
1:B:181:MET:O	1:B:245:LYS:HE2	2.15	0.47
1:B:224:ILE:O	1:G:253:ARG:HD2	2.15	0.47
1:B:222:LEU:HD22	1:B:237:TYR:CD1	2.49	0.46
1:E:154:ILE:HG22	1:E:154:ILE:O	2.14	0.46
1:A:194:VAL:O	1:A:198:ILE:HG13	2.16	0.46
1:G:60:LYS:O	1:G:63:THR:HG22	2.15	0.46
1:G:153:LYS:HG2	1:G:163:ILE:HG12	1.97	0.46
1:G:60:LYS:HA	1:G:60:LYS:HD3	1.81	0.46
1:G:257:LYS:HD3	1:G:257:LYS:C	2.41	0.46
1:G:177:LYS:O	1:G:179:SER:N	2.43	0.46
1:A:194:VAL:HG22	1:B:257:LYS:HE2	1.97	0.46
1:C:98:VAL:HG11	1:G:75:ILE:HD13	1.98	0.46
1:C:177:LYS:HD2	1:C:177:LYS:HA	1.80	0.46
1:E:193:ASP:C	1:E:193:ASP:OD1	2.58	0.46
1:A:172:VAL:O	1:A:172:VAL:HG22	2.16	0.46
1:A:186:ILE:HD12	1:A:256:VAL:HG21	1.98	0.46
1:C:46:TYR:C	1:C:46:TYR:CD2	2.94	0.46
1:E:56:LEU:HD12	1:E:60:LYS:HB2	1.98	0.46
1:E:151:VAL:HG23	1:E:165:PRO:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:190:ILE:H	1:F:190:ILE:HG12	1.44	0.46
1:G:42:ILE:HD11	1:G:68:THR:HG22	1.97	0.46
1:C:186:ILE:HD12	1:C:256:VAL:HG21	1.97	0.46
1:C:190:ILE:HG12	1:C:230:SER:C	2.41	0.46
1:G:231:LYS:HB2	1:G:231:LYS:NZ	2.31	0.46
1:B:179:SER:HB2	1:B:240:THR:O	2.16	0.46
1:C:51:LYS:HD2	1:C:51:LYS:HA	1.64	0.46
1:A:175:LEU:HD12	1:B:160:GLY:HA3	1.98	0.45
1:A:224:ILE:O	1:B:253:ARG:HD2	2.16	0.45
1:B:188:PHE:CE2	1:B:197:ILE:HG21	2.52	0.45
1:E:276:PHE:CZ	1:F:276:PHE:CE1	3.03	0.45
1:F:194:VAL:O	1:F:198:ILE:HG13	2.15	0.45
1:C:194:VAL:HG22	1:F:257:LYS:HE2	1.98	0.45
1:B:18:VAL:HG13	1:B:19:LYS:N	2.31	0.45
1:C:216:ILE:HG12	1:C:239:LYS:HB3	1.97	0.45
1:A:18:VAL:HG13	1:A:19:LYS:N	2.31	0.45
1:A:46:TYR:C	1:A:46:TYR:CD2	2.95	0.45
1:A:145:GLU:OE2	1:A:155:ARG:HD2	2.16	0.45
1:F:197:ILE:HG12	1:F:265:ILE:HD13	1.98	0.45
1:B:42:ILE:HD11	1:B:68:THR:HG22	1.99	0.45
1:C:190:ILE:O	1:C:192:GLU:N	2.49	0.45
1:F:137:ILE:HD12	1:F:154:ILE:HD12	1.98	0.45
1:F:222:LEU:O	1:F:223:GLY:O	2.35	0.45
1:A:113:LEU:HD13	1:D:122:PHE:CE2	2.52	0.45
1:B:114:VAL:HG11	1:G:106:ILE:HA	1.98	0.45
1:D:130:SER:O	1:D:132:GLY:N	2.49	0.45
1:A:75:ILE:HD13	1:B:98:VAL:HG11	1.99	0.45
1:A:117:MET:HG2	1:A:149:LEU:CD1	2.46	0.45
1:B:186:ILE:H	1:B:186:ILE:HG12	1.63	0.45
1:B:145:GLU:OE2	1:B:155:ARG:HD2	2.16	0.45
1:D:258:LYS:HD3	1:D:258:LYS:HA	1.86	0.45
1:F:181:MET:HE2	1:F:181:MET:HB2	1.62	0.45
1:A:250:ARG:CZ	1:D:222:LEU:HD12	2.46	0.45
1:A:275:ASN:HB2	1:B:273:ASP:HB2	1.99	0.45
1:B:222:LEU:O	1:B:223:GLY:O	2.35	0.45
1:E:250:ARG:CZ	1:F:222:LEU:HD12	2.46	0.45
1:F:177:LYS:HD2	1:F:177:LYS:HA	1.75	0.45
1:F:190:ILE:HG12	1:F:230:SER:C	2.42	0.45
1:G:47:LYS:HA	1:G:50:SER:HB3	1.98	0.45
1:A:122:PHE:CZ	1:B:113:LEU:HD11	2.51	0.45
1:B:222:LEU:HD22	1:B:237:TYR:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:ILE:HD12	1:C:154:ILE:HD12	1.98	0.45
1:C:145:GLU:OE2	1:C:155:ARG:HD2	2.17	0.45
1:C:187:ALA:HB2	1:C:233:VAL:HG22	1.98	0.45
1:D:42:ILE:O	1:D:46:TYR:HB2	2.17	0.45
1:E:177:LYS:HA	1:E:177:LYS:HD2	1.75	0.45
1:F:186:ILE:HD12	1:F:256:VAL:HG21	1.99	0.45
1:G:181:MET:HE2	1:G:181:MET:HB2	1.66	0.45
1:G:190:ILE:HG12	1:G:230:SER:C	2.42	0.45
1:A:130:SER:O	1:A:132:GLY:N	2.51	0.44
1:C:114:VAL:HG11	1:F:106:ILE:HA	1.98	0.44
1:D:15:ILE:H	1:D:16:LYS:NZ	2.15	0.44
1:A:75:ILE:HD13	1:B:98:VAL:CG1	2.47	0.44
1:B:190:ILE:O	1:B:192:GLU:N	2.50	0.44
1:D:46:TYR:C	1:D:46:TYR:CD2	2.96	0.44
1:G:190:ILE:O	1:G:192:GLU:N	2.51	0.44
1:F:56:LEU:HD12	1:F:60:LYS:CB	2.47	0.44
1:A:179:SER:HB2	1:A:240:THR:O	2.18	0.44
1:B:180:MET:HE1	1:B:246:TRP:CH2	2.53	0.44
1:A:92:MET:HE2	1:A:92:MET:CA	2.42	0.44
1:D:51:LYS:HD2	1:D:51:LYS:HA	1.65	0.44
1:D:188:PHE:CE2	1:D:234:ILE:HG13	2.52	0.44
1:E:47:LYS:HA	1:E:50:SER:HB3	1.99	0.44
1:E:90:ILE:HA	1:F:83:SER:OG	2.18	0.44
1:E:190:ILE:O	1:E:192:GLU:N	2.51	0.44
1:G:214:ASP:HB2	1:G:244:GLN:HG3	1.99	0.44
1:B:186:ILE:HD12	1:B:256:VAL:HG21	1.99	0.44
1:A:60:LYS:HA	1:A:60:LYS:HD3	1.80	0.44
1:A:20:PHE:O	1:A:24:VAL:HG12	2.18	0.44
1:B:53:LYS:HB3	1:B:53:LYS:HE2	1.78	0.44
1:E:181:MET:HE2	1:E:181:MET:HB2	1.58	0.44
1:F:188:PHE:CE2	1:F:234:ILE:HG13	2.52	0.44
1:A:138:ASN:ND2	1:A:168:GLU:O	2.50	0.44
1:A:197:ILE:HG12	1:A:265:ILE:HD13	2.00	0.44
1:C:79:LEU:HD23	1:C:79:LEU:HA	1.72	0.44
1:F:20:PHE:O	1:F:24:VAL:HG12	2.18	0.44
1:F:79:LEU:HA	1:F:79:LEU:HD23	1.61	0.44
1:C:53:LYS:HB3	1:C:53:LYS:HE2	1.76	0.43
1:C:138:ASN:ND2	1:C:168:GLU:O	2.51	0.43
1:D:47:LYS:HA	1:D:50:SER:HB3	1.99	0.43
1:D:186:ILE:H	1:D:186:ILE:HG12	1.69	0.43
1:F:137:ILE:HD12	1:F:154:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:244:GLN:O	1:F:245:LYS:C	2.60	0.43
1:G:100:GLY:HA2	1:G:103:SER:HB2	1.99	0.43
1:G:241:GLN:HG3	1:G:242:PRO:HD2	1.99	0.43
1:A:15:ILE:H	1:A:16:LYS:NZ	2.16	0.43
1:D:87:LEU:HD12	1:D:87:LEU:HA	1.69	0.43
1:F:18:VAL:HG13	1:F:19:LYS:N	2.33	0.43
1:F:60:LYS:HA	1:F:60:LYS:HD3	1.86	0.43
1:G:56:LEU:HD12	1:G:60:LYS:HB2	2.00	0.43
1:E:42:ILE:O	1:E:46:TYR:HB2	2.18	0.43
1:F:46:TYR:C	1:F:46:TYR:CD2	2.96	0.43
1:G:15:ILE:H	1:G:16:LYS:NZ	2.17	0.43
1:B:56:LEU:HD12	1:B:60:LYS:CB	2.48	0.43
1:C:56:LEU:HD12	1:C:60:LYS:CB	2.49	0.43
1:C:122:PHE:CZ	1:F:113:LEU:HD11	2.54	0.43
1:D:179:SER:HB2	1:D:240:THR:O	2.19	0.43
1:E:123:ILE:HA	1:E:128:GLN:HG3	2.00	0.43
1:B:42:ILE:O	1:B:46:TYR:HB2	2.18	0.43
1:E:126:GLU:O	1:E:127:ASP:C	2.62	0.43
1:F:257:LYS:HD3	1:F:257:LYS:C	2.44	0.43
1:C:160:GLY:HA3	1:G:175:LEU:HD12	2.01	0.43
1:C:177:LYS:O	1:C:179:SER:N	2.46	0.43
1:F:29:ILE:HG13	1:F:30:ILE:N	2.33	0.43
1:A:190:ILE:HG12	1:A:230:SER:C	2.44	0.43
1:D:222:LEU:O	1:D:223:GLY:O	2.37	0.43
1:E:18:VAL:HG13	1:E:19:LYS:N	2.33	0.43
1:F:16:LYS:HB2	1:F:16:LYS:HE2	1.89	0.43
1:F:87:LEU:HD12	1:F:87:LEU:HA	1.79	0.43
1:F:186:ILE:H	1:F:186:ILE:HG12	1.63	0.43
1:C:216:ILE:HD11	1:C:239:LYS:HD2	2.01	0.43
1:C:276:PHE:CE1	1:F:276:PHE:CZ	3.07	0.43
1:D:42:ILE:HD11	1:D:68:THR:HG22	2.00	0.43
1:A:47:LYS:HA	1:A:50:SER:HB3	2.00	0.43
1:A:275:ASN:HB2	1:B:273:ASP:CB	2.49	0.43
1:B:64:LEU:HD23	1:B:64:LEU:C	2.44	0.43
1:C:16:LYS:HE2	1:C:16:LYS:HB2	1.84	0.43
1:C:257:LYS:HD3	1:C:257:LYS:C	2.44	0.43
1:D:100:GLY:O	1:D:104:LEU:HG	2.19	0.43
1:D:138:ASN:ND2	1:D:168:GLU:O	2.52	0.43
1:E:61:ILE:O	1:E:65:THR:HB	2.19	0.43
1:E:216:ILE:HG12	1:E:239:LYS:HB3	1.99	0.43
1:F:129:PHE:CD2	1:F:147:ILE:HD11	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:SER:O	1:B:54:ILE:N	2.50	0.43
1:C:61:ILE:O	1:C:65:THR:HB	2.19	0.43
1:C:222:LEU:O	1:C:223:GLY:O	2.37	0.43
1:G:137:ILE:HD12	1:G:154:ILE:CD1	2.49	0.43
1:G:216:ILE:HD11	1:G:239:LYS:HD2	1.99	0.43
1:A:56:LEU:HA	1:A:57:PRO:HD3	1.92	0.42
1:A:181:MET:O	1:A:245:LYS:HE2	2.19	0.42
1:C:78:PHE:CE2	1:F:94:SER:HB3	2.54	0.42
1:D:177:LYS:HD2	1:D:177:LYS:HA	1.74	0.42
1:E:108:PHE:HB3	1:F:111:GLN:OE1	2.18	0.42
1:F:123:ILE:HA	1:F:128:GLN:HG3	1.99	0.42
1:A:275:ASN:HD22	1:B:273:ASP:HB3	1.84	0.42
1:C:18:VAL:HG13	1:C:19:LYS:H	1.83	0.42
1:C:47:LYS:HA	1:C:50:SER:HB3	2.01	0.42
1:C:222:LEU:HD22	1:C:237:TYR:CD1	2.54	0.42
1:E:87:LEU:HD12	1:E:87:LEU:HA	1.77	0.42
1:E:145:GLU:OE2	1:E:155:ARG:HD2	2.18	0.42
1:E:190:ILE:HG12	1:E:230:SER:C	2.43	0.42
1:B:60:LYS:HA	1:B:60:LYS:HD3	1.84	0.42
1:B:123:ILE:HA	1:B:128:GLN:HG3	2.02	0.42
1:B:244:GLN:O	1:B:245:LYS:C	2.62	0.42
1:D:123:ILE:HA	1:D:128:GLN:HG3	2.02	0.42
1:D:190:ILE:HG12	1:D:230:SER:C	2.43	0.42
1:G:197:ILE:CG1	1:G:265:ILE:HD13	2.49	0.42
1:A:126:GLU:O	1:A:127:ASP:C	2.62	0.42
1:A:177:LYS:HA	1:A:177:LYS:HD2	1.77	0.42
1:B:15:ILE:H	1:B:16:LYS:NZ	2.18	0.42
1:C:273:ASP:HB3	1:G:275:ASN:HD22	1.84	0.42
1:D:174:ASN:ND2	1:D:177:LYS:HD3	2.35	0.42
1:E:186:ILE:HD12	1:E:256:VAL:HG21	2.01	0.42
1:G:16:LYS:HB2	1:G:16:LYS:HE2	1.87	0.42
1:A:42:ILE:O	1:A:46:TYR:HB2	2.19	0.42
1:A:52:SER:O	1:A:54:ILE:N	2.52	0.42
1:B:47:LYS:HA	1:B:50:SER:HB3	2.01	0.42
1:B:216:ILE:HD11	1:B:239:LYS:HD2	2.00	0.42
1:D:187:ALA:HB2	1:D:233:VAL:HG22	2.02	0.42
1:F:222:LEU:HD22	1:F:237:TYR:CD1	2.53	0.42
1:G:42:ILE:O	1:G:46:TYR:HB2	2.20	0.42
1:A:88:PHE:HD1	1:D:30:ILE:HB	1.84	0.42
1:A:113:LEU:CD1	1:D:122:PHE:CE2	3.03	0.42
1:A:134:TYR:H	1:A:176:THR:CG2	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:LEU:C	1:C:64:LEU:HD23	2.44	0.42
1:C:227:MET:HE3	1:F:186:ILE:HG22	2.02	0.42
1:E:94:SER:HB3	1:F:78:PHE:CE2	2.54	0.42
1:E:253:ARG:HD2	1:F:224:ILE:O	2.19	0.42
1:G:179:SER:HB2	1:G:240:THR:O	2.19	0.42
1:A:190:ILE:C	1:A:192:GLU:N	2.77	0.42
1:C:24:VAL:O	1:C:28:LEU:HG	2.19	0.42
1:C:42:ILE:O	1:C:46:TYR:HB2	2.20	0.42
1:C:113:LEU:HD11	1:G:122:PHE:CZ	2.55	0.42
1:E:244:GLN:O	1:E:245:LYS:C	2.62	0.42
1:G:131:VAL:HG12	1:G:131:VAL:O	2.20	0.42
1:B:177:LYS:HD2	1:B:177:LYS:HA	1.76	0.42
1:C:188:PHE:CE2	1:C:234:ILE:HG13	2.54	0.42
1:C:194:VAL:O	1:C:198:ILE:HG13	2.20	0.42
1:C:231:LYS:NZ	1:C:231:LYS:HB2	2.35	0.42
1:D:190:ILE:HG12	1:D:190:ILE:H	1.51	0.42
1:E:131:VAL:HG12	1:E:131:VAL:O	2.20	0.42
1:F:100:GLY:HA2	1:F:103:SER:HB2	2.02	0.42
1:F:145:GLU:OE2	1:F:155:ARG:HD2	2.18	0.42
1:G:123:ILE:HA	1:G:128:GLN:HG3	2.02	0.42
1:A:182:ALA:HB1	1:A:249:GLU:HG3	2.02	0.42
1:A:188:PHE:HE2	1:A:234:ILE:HG13	1.85	0.42
1:D:131:VAL:HG12	1:D:131:VAL:O	2.20	0.42
1:E:93:THR:CG2	1:F:96:LEU:HB2	2.50	0.42
1:F:172:VAL:O	1:F:172:VAL:HG22	2.20	0.42
1:A:276:PHE:CZ	1:D:276:PHE:CE1	3.07	0.42
1:C:180:MET:HE1	1:C:246:TRP:CZ3	2.55	0.42
1:C:193:ASP:OD1	1:C:193:ASP:C	2.63	0.42
1:D:250:ARG:NE	1:E:222:LEU:HD12	2.34	0.42
1:E:51:LYS:N	1:E:51:LYS:HD3	2.34	0.42
1:F:47:LYS:HA	1:F:50:SER:HB3	2.01	0.42
1:G:145:GLU:OE2	1:G:155:ARG:HD2	2.20	0.42
1:A:24:VAL:O	1:A:28:LEU:HG	2.19	0.41
1:A:83:SER:OG	1:B:90:ILE:HA	2.19	0.41
1:C:134:TYR:H	1:C:176:THR:CG2	2.33	0.41
1:D:117:MET:HG2	1:D:149:LEU:CD1	2.48	0.41
1:F:14:ASP:HA	1:F:16:LYS:NZ	2.26	0.41
1:G:56:LEU:HD12	1:G:60:LYS:CB	2.49	0.41
1:A:96:LEU:HD12	1:B:97:ALA:HB2	2.02	0.41
1:D:18:VAL:HG13	1:D:19:LYS:H	1.83	0.41
1:E:29:ILE:HG13	1:E:30:ILE:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:241:GLN:HG3	1:E:242:PRO:HD2	2.02	0.41
1:F:121:PHE:CD2	1:F:121:PHE:C	2.99	0.41
1:G:29:ILE:HG13	1:G:30:ILE:N	2.34	0.41
1:G:278:ARG:HB2	1:G:278:ARG:CZ	2.50	0.41
1:B:56:LEU:HD12	1:B:60:LYS:HB2	2.02	0.41
1:B:129:PHE:CE1	1:B:172:VAL:HG21	2.56	0.41
1:B:130:SER:O	1:B:132:GLY:N	2.53	0.41
1:C:250:ARG:CZ	1:G:222:LEU:HD12	2.50	0.41
1:D:151:VAL:HG23	1:D:165:PRO:HA	2.01	0.41
1:E:20:PHE:O	1:E:24:VAL:HG12	2.20	0.41
1:E:257:LYS:C	1:E:257:LYS:HD3	2.44	0.41
1:F:53:LYS:HE2	1:F:53:LYS:HB3	1.75	0.41
1:F:56:LEU:HD12	1:F:60:LYS:HB2	2.01	0.41
1:A:257:LYS:HD3	1:A:257:LYS:C	2.45	0.41
1:B:190:ILE:HG12	1:B:230:SER:C	2.45	0.41
1:C:249:GLU:O	1:C:253:ARG:HG3	2.20	0.41
1:E:106:ILE:HA	1:F:114:VAL:HG11	2.02	0.41
1:C:244:GLN:O	1:C:245:LYS:C	2.63	0.41
1:E:15:ILE:H	1:E:16:LYS:NZ	2.19	0.41
1:F:177:LYS:O	1:F:179:SER:N	2.48	0.41
1:F:209:LYS:HB2	1:F:209:LYS:HE3	1.81	0.41
1:A:19:LYS:HE3	1:A:19:LYS:HB3	1.78	0.41
1:A:79:LEU:HA	1:A:79:LEU:HD23	1.70	0.41
1:B:56:LEU:HA	1:B:57:PRO:HD3	1.93	0.41
1:B:138:ASN:ND2	1:B:168:GLU:O	2.54	0.41
1:C:52:SER:O	1:C:54:ILE:N	2.53	0.41
1:C:218:GLY:HA3	1:C:219:PRO:HA	1.91	0.41
1:E:222:LEU:HD22	1:E:237:TYR:CE1	2.56	0.41
1:E:258:LYS:HD3	1:E:258:LYS:HA	1.89	0.41
1:A:78:PHE:CE2	1:B:94:SER:HB3	2.56	0.41
1:A:222:LEU:HD22	1:A:237:TYR:CD1	2.56	0.41
1:A:275:ASN:ND2	1:B:273:ASP:HB3	2.35	0.41
1:C:186:ILE:HG22	1:G:227:MET:HE3	2.03	0.41
1:D:19:LYS:HB3	1:D:19:LYS:HE3	1.80	0.41
1:D:92:MET:HE2	1:D:92:MET:CA	2.48	0.41
1:E:121:PHE:CD2	1:E:121:PHE:C	2.98	0.41
1:E:216:ILE:HD11	1:E:239:LYS:HD2	2.02	0.41
1:F:138:ASN:ND2	1:F:168:GLU:O	2.54	0.41
1:G:190:ILE:C	1:G:192:GLU:N	2.79	0.41
1:A:137:ILE:HD12	1:A:154:ILE:HD12	2.03	0.41
1:A:190:ILE:C	1:A:192:GLU:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:PHE:CZ	1:B:276:PHE:CZ	3.09	0.41
1:B:181:MET:HB2	1:B:181:MET:HE2	1.61	0.41
1:C:92:MET:HE2	1:C:92:MET:CA	2.48	0.41
1:C:181:MET:HB2	1:C:181:MET:HE2	1.62	0.41
1:C:222:LEU:HD12	1:F:250:ARG:CZ	2.51	0.41
1:D:215:LEU:HD12	1:D:215:LEU:O	2.20	0.41
1:A:130:SER:C	1:A:132:GLY:H	2.29	0.41
1:B:51:LYS:HD2	1:B:51:LYS:HA	1.67	0.41
1:B:126:GLU:O	1:B:127:ASP:C	2.64	0.41
1:C:56:LEU:HD12	1:C:60:LYS:HB2	2.02	0.41
1:C:94:SER:HB3	1:G:78:PHE:CE2	2.56	0.41
1:D:186:ILE:HD12	1:D:256:VAL:HG21	2.02	0.41
1:D:194:VAL:O	1:D:198:ILE:HG13	2.20	0.41
1:E:214:ASP:HB2	1:E:244:GLN:HG3	2.02	0.41
1:E:257:LYS:HE2	1:F:194:VAL:HG22	2.03	0.41
1:F:42:ILE:O	1:F:46:TYR:HB2	2.21	0.41
1:F:193:ASP:OD1	1:F:193:ASP:C	2.63	0.41
1:G:24:VAL:O	1:G:28:LEU:HG	2.21	0.41
1:G:193:ASP:OD1	1:G:193:ASP:C	2.64	0.41
1:A:244:GLN:O	1:A:245:LYS:C	2.63	0.41
1:A:267:PHE:HB3	1:A:268:PRO:HD2	2.03	0.41
1:B:241:GLN:HG3	1:B:242:PRO:HD2	2.02	0.41
1:D:20:PHE:O	1:D:24:VAL:HG12	2.21	0.41
1:D:24:VAL:O	1:D:28:LEU:HG	2.21	0.41
1:E:177:LYS:O	1:E:179:SER:N	2.49	0.41
1:F:61:ILE:O	1:F:65:THR:HB	2.21	0.41
1:G:126:GLU:O	1:G:127:ASP:C	2.64	0.41
1:A:88:PHE:CD1	1:D:30:ILE:HB	2.56	0.40
1:A:123:ILE:HA	1:A:128:GLN:HG3	2.03	0.40
1:A:227:MET:HE3	1:B:186:ILE:HG22	2.03	0.40
1:B:257:LYS:HD3	1:B:257:LYS:C	2.47	0.40
1:C:257:LYS:HD3	1:C:257:LYS:O	2.21	0.40
1:D:222:LEU:HD22	1:D:237:TYR:CE1	2.56	0.40
1:F:19:LYS:HB3	1:F:19:LYS:HE3	1.78	0.40
1:G:52:SER:O	1:G:54:ILE:N	2.51	0.40
1:G:220:THR:O	1:G:236:VAL:HA	2.21	0.40
1:G:232:LEU:O	1:G:232:LEU:HD23	2.21	0.40
1:A:160:GLY:HA3	1:D:175:LEU:HD12	2.03	0.40
1:A:180:MET:HE1	1:A:246:TRP:CZ3	2.57	0.40
1:C:106:ILE:HG22	1:F:101:ILE:HG23	2.02	0.40
1:C:131:VAL:HA	1:C:144:VAL:CG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:LEU:C	1:D:64:LEU:HD23	2.46	0.40
1:D:134:TYR:H	1:D:176:THR:CG2	2.34	0.40
1:D:181:MET:O	1:D:245:LYS:HE2	2.22	0.40
1:E:208:VAL:CG2	1:E:255:ARG:HD2	2.50	0.40
1:F:60:LYS:O	1:F:63:THR:HG22	2.21	0.40
1:A:56:LEU:HD12	1:A:60:LYS:CB	2.51	0.40
1:A:97:ALA:O	1:D:103:SER:OG	2.33	0.40
1:A:205:CYS:SG	1:A:219:PRO:HB2	2.62	0.40
1:D:162:HIS:HA	1:E:173:THR:HA	2.04	0.40
1:E:130:SER:C	1:E:132:GLY:H	2.28	0.40
1:E:267:PHE:HB3	1:E:268:PRO:HD2	2.03	0.40
1:G:44:ARG:C	1:G:46:TYR:N	2.78	0.40
1:G:177:LYS:HD2	1:G:177:LYS:HA	1.74	0.40
1:D:149:LEU:O	1:D:166:ASN:ND2	2.53	0.40
1:E:134:TYR:H	1:E:176:THR:CG2	2.34	0.40
1:A:18:VAL:HG13	1:A:19:LYS:H	1.86	0.40
1:C:101:ILE:HD13	1:G:106:ILE:HG21	2.04	0.40
1:D:52:SER:O	1:D:54:ILE:N	2.52	0.40
1:D:174:ASN:C	1:D:175:LEU:O	2.65	0.40
1:D:220:THR:O	1:D:236:VAL:HA	2.21	0.40
1:D:242:PRO:O	1:D:243:MET:HB2	2.21	0.40
1:D:273:ASP:HB3	1:E:275:ASN:ND2	2.37	0.40
1:E:52:SER:O	1:E:54:ILE:N	2.55	0.40
1:E:186:ILE:H	1:E:186:ILE:HG12	1.66	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ARG:NH2	1:G:210:LYS:C[4_455]	2.06	0.14

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	265/285 (93%)	233 (88%)	20 (8%)	12 (4%)	2	12
1	B	265/285 (93%)	236 (89%)	17 (6%)	12 (4%)	2	12
1	C	265/285 (93%)	233 (88%)	21 (8%)	11 (4%)	2	13
1	D	265/285 (93%)	233 (88%)	20 (8%)	12 (4%)	2	12
1	E	265/285 (93%)	234 (88%)	20 (8%)	11 (4%)	2	13
1	F	265/285 (93%)	234 (88%)	19 (7%)	12 (4%)	2	12
1	G	265/285 (93%)	235 (89%)	19 (7%)	11 (4%)	2	13
All	All	1855/1995 (93%)	1638 (88%)	136 (7%)	81 (4%)	2	12

All (81) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	ASP
1	A	191	ASP
1	A	223	GLY
1	B	14	ASP
1	B	191	ASP
1	B	223	GLY
1	C	14	ASP
1	C	191	ASP
1	C	223	GLY
1	D	14	ASP
1	D	191	ASP
1	D	223	GLY
1	E	14	ASP
1	E	191	ASP
1	E	223	GLY
1	F	14	ASP
1	F	191	ASP
1	F	223	GLY
1	G	14	ASP
1	G	191	ASP
1	G	223	GLY
1	A	131	VAL
1	A	170	LYS
1	A	175	LEU
1	A	229	ASP
1	B	131	VAL
1	B	170	LYS

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Mol	Chain	Res	Type
1	B	175	LEU
1	B	229	ASP
1	C	170	LYS
1	C	175	LEU
1	C	229	ASP
1	D	131	VAL
1	D	170	LYS
1	D	175	LEU
1	D	229	ASP
1	E	131	VAL
1	E	170	LYS
1	E	175	LEU
1	E	229	ASP
1	F	131	VAL
1	F	170	LYS
1	F	175	LEU
1	F	229	ASP
1	G	170	LYS
1	G	175	LEU
1	G	229	ASP
1	A	178	ASP
1	B	53	LYS
1	C	53	LYS
1	C	131	VAL
1	C	178	ASP
1	D	53	LYS
1	E	53	LYS
1	E	178	ASP
1	F	53	LYS
1	F	245	LYS
1	G	53	LYS
1	G	178	ASP
1	A	53	LYS
1	B	176	THR
1	B	178	ASP
1	C	176	THR
1	D	176	THR
1	D	178	ASP
1	E	176	THR
1	F	176	THR
1	F	178	ASP
1	G	131	VAL

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Mol	Chain	Res	Type
1	G	176	THR
1	A	176	THR
1	A	245	LYS
1	A	264	ASN
1	B	245	LYS
1	C	245	LYS
1	D	245	LYS
1	D	264	ASN
1	E	245	LYS
1	F	264	ASN
1	G	264	ASN
1	B	264	ASN

5.3.2 Protein sidechains [i](#)

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	236/251 (94%)	186 (79%)	50 (21%)	1	3
1	B	236/251 (94%)	188 (80%)	48 (20%)	1	4
1	C	236/251 (94%)	186 (79%)	50 (21%)	1	3
1	D	236/251 (94%)	187 (79%)	49 (21%)	1	4
1	E	236/251 (94%)	186 (79%)	50 (21%)	1	3
1	F	236/251 (94%)	185 (78%)	51 (22%)	1	3
1	G	236/251 (94%)	185 (78%)	51 (22%)	1	3
All	All	1652/1757 (94%)	1303 (79%)	349 (21%)	1	4

All (349) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ILE
1	A	21	LEU
1	A	22	LEU
1	A	24	VAL
1	A	25	LEU

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Mol	Chain	Res	Type
1	A	29	ILE
1	A	35	ILE
1	A	42	ILE
1	A	47	LYS
1	A	49	TYR
1	A	51	LYS
1	A	53	LYS
1	A	54	ILE
1	A	56	LEU
1	A	65	THR
1	A	67	LEU
1	A	85	LEU
1	A	87	LEU
1	A	95	LEU
1	A	130	SER
1	A	131	VAL
1	A	136	THR
1	A	140	ILE
1	A	143	THR
1	A	144	VAL
1	A	149	LEU
1	A	151	VAL
1	A	154	ILE
1	A	159	ASP
1	A	170	LYS
1	A	171	MET
1	A	172	VAL
1	A	173	THR
1	A	175	LEU
1	A	176	THR
1	A	186	ILE
1	A	190	ILE
1	A	194	VAL
1	A	202	GLN
1	A	213	ASP
1	A	216	ILE
1	A	225	THR
1	A	231	LYS
1	A	232	LEU
1	A	236	VAL
1	A	240	THR
1	A	256	VAL

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Mol	Chain	Res	Type
1	A	263	LYS
1	A	274	VAL
1	A	279	VAL
1	B	15	ILE
1	B	21	LEU
1	B	22	LEU
1	B	24	VAL
1	B	25	LEU
1	B	29	ILE
1	B	35	ILE
1	B	47	LYS
1	B	49	TYR
1	B	51	LYS
1	B	56	LEU
1	B	65	THR
1	B	67	LEU
1	B	75	ILE
1	B	85	LEU
1	B	87	LEU
1	B	95	LEU
1	B	130	SER
1	B	131	VAL
1	B	136	THR
1	B	140	ILE
1	B	143	THR
1	B	144	VAL
1	B	149	LEU
1	B	151	VAL
1	B	154	ILE
1	B	159	ASP
1	B	170	LYS
1	B	171	MET
1	B	172	VAL
1	B	173	THR
1	B	175	LEU
1	B	176	THR
1	B	181	MET
1	B	186	ILE
1	B	190	ILE
1	B	194	VAL
1	B	213	ASP
1	B	216	ILE

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Mol	Chain	Res	Type
1	B	225	THR
1	B	231	LYS
1	B	232	LEU
1	B	236	VAL
1	B	240	THR
1	B	256	VAL
1	B	263	LYS
1	B	274	VAL
1	B	279	VAL
1	C	15	ILE
1	C	21	LEU
1	C	22	LEU
1	C	24	VAL
1	C	25	LEU
1	C	29	ILE
1	C	35	ILE
1	C	47	LYS
1	C	49	TYR
1	C	51	LYS
1	C	53	LYS
1	C	56	LEU
1	C	65	THR
1	C	67	LEU
1	C	85	LEU
1	C	87	LEU
1	C	95	LEU
1	C	130	SER
1	C	131	VAL
1	C	136	THR
1	C	140	ILE
1	C	143	THR
1	C	144	VAL
1	C	149	LEU
1	C	151	VAL
1	C	154	ILE
1	C	159	ASP
1	C	170	LYS
1	C	171	MET
1	C	172	VAL
1	C	173	THR
1	C	175	LEU
1	C	176	THR

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Mol	Chain	Res	Type
1	C	186	ILE
1	C	190	ILE
1	C	194	VAL
1	C	202	GLN
1	C	213	ASP
1	C	215	LEU
1	C	216	ILE
1	C	225	THR
1	C	231	LYS
1	C	232	LEU
1	C	234	ILE
1	C	236	VAL
1	C	240	THR
1	C	256	VAL
1	C	263	LYS
1	C	274	VAL
1	C	279	VAL
1	D	15	ILE
1	D	21	LEU
1	D	22	LEU
1	D	24	VAL
1	D	25	LEU
1	D	29	ILE
1	D	35	ILE
1	D	47	LYS
1	D	49	TYR
1	D	51	LYS
1	D	53	LYS
1	D	56	LEU
1	D	65	THR
1	D	67	LEU
1	D	75	ILE
1	D	85	LEU
1	D	87	LEU
1	D	95	LEU
1	D	130	SER
1	D	131	VAL
1	D	136	THR
1	D	140	ILE
1	D	143	THR
1	D	144	VAL
1	D	149	LEU

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Mol	Chain	Res	Type
1	D	151	VAL
1	D	154	ILE
1	D	159	ASP
1	D	170	LYS
1	D	171	MET
1	D	172	VAL
1	D	173	THR
1	D	175	LEU
1	D	176	THR
1	D	186	ILE
1	D	190	ILE
1	D	194	VAL
1	D	202	GLN
1	D	213	ASP
1	D	216	ILE
1	D	225	THR
1	D	231	LYS
1	D	232	LEU
1	D	234	ILE
1	D	236	VAL
1	D	240	THR
1	D	263	LYS
1	D	274	VAL
1	D	279	VAL
1	E	15	ILE
1	E	21	LEU
1	E	22	LEU
1	E	24	VAL
1	E	25	LEU
1	E	29	ILE
1	E	35	ILE
1	E	47	LYS
1	E	49	TYR
1	E	51	LYS
1	E	56	LEU
1	E	65	THR
1	E	67	LEU
1	E	75	ILE
1	E	85	LEU
1	E	87	LEU
1	E	95	LEU
1	E	130	SER

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Mol	Chain	Res	Type
1	E	131	VAL
1	E	136	THR
1	E	140	ILE
1	E	143	THR
1	E	144	VAL
1	E	149	LEU
1	E	151	VAL
1	E	154	ILE
1	E	158	SER
1	E	159	ASP
1	E	170	LYS
1	E	171	MET
1	E	172	VAL
1	E	173	THR
1	E	175	LEU
1	E	176	THR
1	E	181	MET
1	E	186	ILE
1	E	190	ILE
1	E	194	VAL
1	E	202	GLN
1	E	213	ASP
1	E	216	ILE
1	E	225	THR
1	E	231	LYS
1	E	232	LEU
1	E	234	ILE
1	E	236	VAL
1	E	240	THR
1	E	263	LYS
1	E	274	VAL
1	E	279	VAL
1	F	15	ILE
1	F	21	LEU
1	F	22	LEU
1	F	24	VAL
1	F	25	LEU
1	F	29	ILE
1	F	35	ILE
1	F	47	LYS
1	F	49	TYR
1	F	51	LYS

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Mol	Chain	Res	Type
1	F	56	LEU
1	F	65	THR
1	F	67	LEU
1	F	85	LEU
1	F	87	LEU
1	F	95	LEU
1	F	130	SER
1	F	131	VAL
1	F	136	THR
1	F	140	ILE
1	F	143	THR
1	F	144	VAL
1	F	149	LEU
1	F	151	VAL
1	F	154	ILE
1	F	159	ASP
1	F	170	LYS
1	F	171	MET
1	F	172	VAL
1	F	173	THR
1	F	175	LEU
1	F	176	THR
1	F	181	MET
1	F	186	ILE
1	F	190	ILE
1	F	194	VAL
1	F	202	GLN
1	F	209	LYS
1	F	213	ASP
1	F	215	LEU
1	F	216	ILE
1	F	225	THR
1	F	231	LYS
1	F	232	LEU
1	F	234	ILE
1	F	236	VAL
1	F	240	THR
1	F	256	VAL
1	F	263	LYS
1	F	274	VAL
1	F	279	VAL
1	G	15	ILE

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Mol	Chain	Res	Type
1	G	21	LEU
1	G	22	LEU
1	G	24	VAL
1	G	25	LEU
1	G	29	ILE
1	G	35	ILE
1	G	47	LYS
1	G	49	TYR
1	G	51	LYS
1	G	56	LEU
1	G	65	THR
1	G	67	LEU
1	G	75	ILE
1	G	85	LEU
1	G	87	LEU
1	G	95	LEU
1	G	130	SER
1	G	131	VAL
1	G	136	THR
1	G	140	ILE
1	G	143	THR
1	G	144	VAL
1	G	149	LEU
1	G	151	VAL
1	G	154	ILE
1	G	158	SER
1	G	159	ASP
1	G	170	LYS
1	G	171	MET
1	G	172	VAL
1	G	173	THR
1	G	175	LEU
1	G	176	THR
1	G	181	MET
1	G	186	ILE
1	G	190	ILE
1	G	194	VAL
1	G	202	GLN
1	G	209	LYS
1	G	213	ASP
1	G	216	ILE
1	G	225	THR

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Mol	Chain	Res	Type
1	G	231	LYS
1	G	232	LEU
1	G	236	VAL
1	G	240	THR
1	G	256	VAL
1	G	263	LYS
1	G	274	VAL
1	G	279	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	162	HIS
1	B	162	HIS
1	B	241	GLN
1	C	241	GLN
1	D	162	HIS
1	E	162	HIS
1	F	162	HIS
1	F	241	GLN
1	G	162	HIS
1	G	241	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	267/285 (93%)	0.26	12 (4%) 38 27	98, 136, 200, 250	0
1	B	267/285 (93%)	0.24	4 (1%) 72 57	99, 133, 200, 249	0
1	C	267/285 (93%)	0.31	11 (4%) 41 29	94, 131, 198, 249	0
1	D	267/285 (93%)	0.25	19 (7%) 22 17	100, 135, 200, 252	0
1	E	267/285 (93%)	0.40	10 (3%) 45 32	98, 134, 199, 266	0
1	F	267/285 (93%)	0.30	12 (4%) 38 27	94, 134, 200, 248	0
1	G	267/285 (93%)	0.36	15 (5%) 30 22	90, 131, 199, 249	0
All	All	1869/1995 (93%)	0.30	83 (4%) 39 28	90, 134, 200, 266	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	211	SER	8.0
1	D	23	ASP	5.4
1	C	40	PHE	4.8
1	E	48	LEU	4.8
1	E	215	LEU	4.8
1	E	40	PHE	4.6
1	F	129	PHE	4.5
1	G	279	VAL	4.4
1	A	276	PHE	4.3
1	G	231	LYS	4.3
1	G	139	GLY	4.2
1	D	94	SER	4.1
1	G	136	THR	4.0
1	D	244	GLN	4.0
1	E	201	LEU	3.8
1	F	260	PHE	3.8
1	E	234	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	243	MET	3.6
1	D	265	ILE	3.6
1	F	172	VAL	3.6
1	F	89	ASN	3.6
1	C	129	PHE	3.6
1	G	211	SER	3.5
1	C	39	ASP	3.5
1	C	175	LEU	3.4
1	C	42	ILE	3.3
1	D	164	ILE	3.3
1	G	212	ARG	3.3
1	D	204	ILE	3.2
1	G	233	VAL	3.2
1	B	208	VAL	3.0
1	B	58	GLN	3.0
1	C	242	PRO	3.0
1	D	89	ASN	3.0
1	F	33	ILE	3.0
1	C	179	SER	2.9
1	E	164	ILE	2.9
1	C	119	SER	2.8
1	F	128	GLN	2.7
1	A	134	TYR	2.7
1	D	146	GLU	2.7
1	D	149	LEU	2.7
1	A	180	MET	2.7
1	A	143	THR	2.7
1	A	242	PRO	2.7
1	A	74	TYR	2.6
1	G	213	ASP	2.6
1	A	246	TRP	2.6
1	D	91	ASP	2.5
1	D	163	ILE	2.5
1	F	90	ILE	2.5
1	B	243	MET	2.5
1	E	236	VAL	2.5
1	D	206	GLU	2.4
1	G	197	ILE	2.4
1	E	150	ARG	2.4
1	F	115	LYS	2.3
1	E	112	ASN	2.3
1	D	78	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	85	LEU	2.3
1	A	32	PHE	2.3
1	G	40	PHE	2.3
1	G	112	ASN	2.3
1	D	22	LEU	2.2
1	F	67	LEU	2.2
1	A	198	ILE	2.2
1	C	130	SER	2.2
1	B	277	LYS	2.2
1	F	209	LYS	2.1
1	G	130	SER	2.1
1	G	46	TYR	2.1
1	D	207	GLU	2.1
1	F	100	GLY	2.1
1	D	26	LYS	2.1
1	F	265	ILE	2.1
1	E	188	PHE	2.1
1	G	153	LYS	2.0
1	D	56	LEU	2.0
1	G	85	LEU	2.0
1	D	153	LYS	2.0
1	D	151	VAL	2.0
1	A	252	ILE	2.0
1	C	123	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.