Full wwPDB X-ray Structure Validation Report (i)

Jun 13, 2024 – 09:17 AM EDT

PDB ID	:	1M3D
Title	:	Structure of Type IV Collagen NC1 Domains
Authors	:	Sundaramoorthy, M.; Meiyappan, M.; Todd, P.; Hudson, B.G.
Deposited on	:	2002-06-27
Resolution	:	2.00 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 (i) 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 (i)) were used in the production of this report:

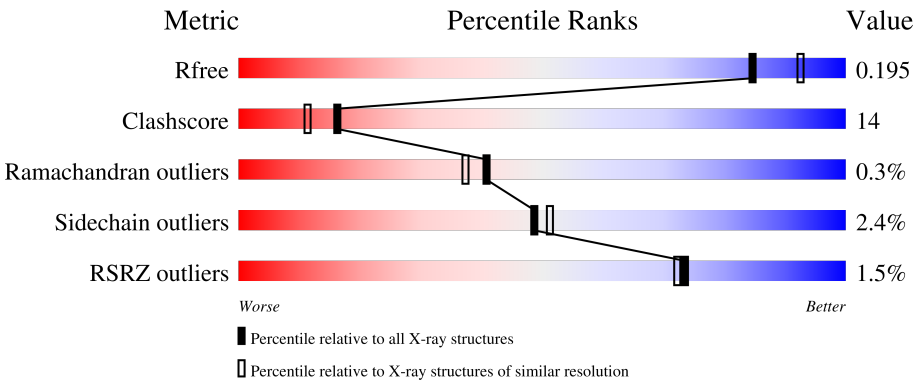
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 <=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	229	72% 23% • •
1	B	229	3% 73% 24% •
1	D	229	2% 70% 27% • •
1	E	229	% 79% 18% • •
1	G	229	71% 26% • •

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Mol	Chain	Length	Quality of chain
1	H	229	2% 71% 27%
1	J	229	% 73% 23%
1	K	229	3% 74% 24%
2	C	227	% 73% 23%
2	F	227	% 72% 25%
2	I	227	3% 71% 24%
2	L	227	79% 18%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BR	A	3005	-	-	X	-
3	BR	B	3012	-	-	X	-
3	BR	B	3028	-	-	X	-
3	BR	E	3036	-	-	X	-
3	BR	H	3006	-	-	X	-
3	BR	J	3008	-	-	X	-
3	BR	K	3033	-	-	X	-
4	GOL	A	4001	-	X	-	-
4	GOL	B	4002	-	X	-	-
4	GOL	D	4003	-	X	-	-
4	GOL	E	4004	-	X	-	-
4	GOL	G	4005	-	X	-	-
4	GOL	H	4006	-	X	-	-
4	GOL	J	4007	-	X	-	-
4	GOL	K	4008	-	X	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 22023 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 Type IV Collagen Noncollagenous Domain- Alpha1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	223	1735	1093	303	318	21	0	2	0
1	B	224	1747	1098	307	321	21	0	2	0
1	D	225	1743	1098	304	320	21	0	1	0
1	E	224	1734	1091	303	319	21	0	0	0
1	G	225	1748	1102	305	320	21	0	2	0
1	H	224	1738	1095	303	319	21	0	1	0
1	J	223	1724	1085	300	318	21	0	0	0
1	K	224	1738	1093	304	320	21	0	0	0

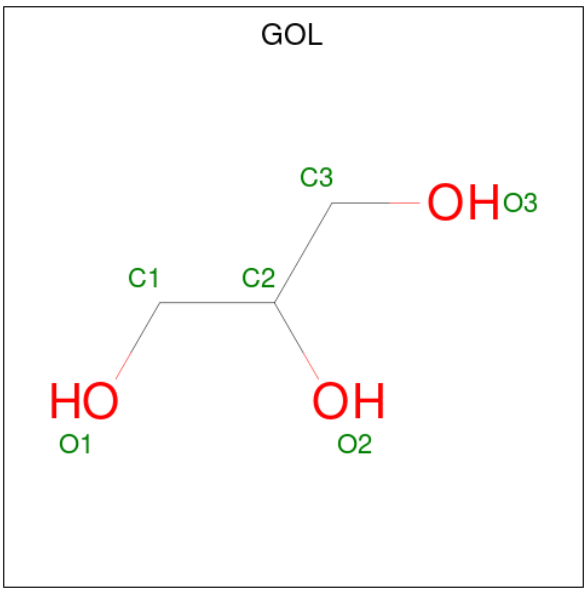
- Molecule 2 is a protein called Type IV Collagen Noncollagenous Domain- Alpha2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	222	1720	1089	291	321	19	0	0	0
2	F	223	1724	1091	292	322	19	0	0	0
2	I	222	1720	1089	291	321	19	0	0	0
2	L	222	1726	1093	293	321	19	0	1	0

- Molecule 3 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Br		
3	A	4	4	4	0	0
3	B	5	5	5	0	0
3	C	4	4	4	0	0
3	D	1	1	1	0	0
3	E	2	2	2	0	0
3	F	2	2	2	0	0
3	G	3	3	3	0	0
3	H	4	4	4	0	0
3	I	3	3	3	0	0
3	J	2	2	2	0	0
3	K	3	3	3	0	0
3	L	3	3	3	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	6	3	3	0	0
4	B	1	6	3	3	0	0
4	D	1	6	3	3	0	0
4	E	1	6	3	3	0	0
4	G	1	6	3	3	0	0
4	H	1	6	3	3	0	0
4	J	1	6	3	3	0	0
4	K	1	6	3	3	0	0

- Molecule 5 is LUTETIUM (III) ION (three-letter code: LU) (formula: Lu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Lu		
5	C	1	1	1	0	0
5	F	1	1	1	0	0
5	I	1	1	1	0	0
5	L	1	1	1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	108	108	108	0	0
6	B	87	87	87	0	0
6	C	103	103	103	0	0
6	D	103	103	103	0	0
6	E	83	83	83	0	0
6	F	111	111	111	0	0

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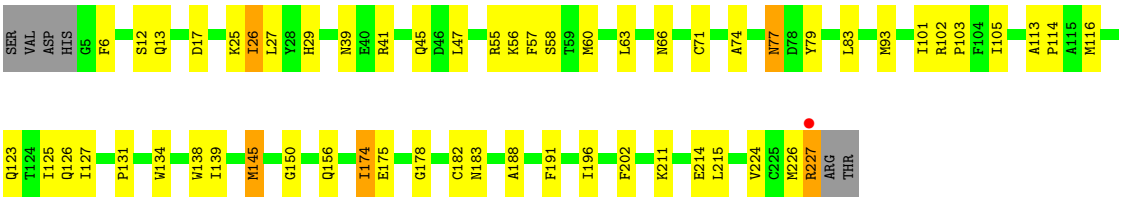
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	G	85	85	85	0	0
			Total	O		
6	H	88	88	88	0	0
			Total	O		
6	I	99	99	99	0	0
			Total	O		
6	J	94	94	94	0	0
			Total	O		
6	K	85	85	85	0	0
			Total	O		
6	L	92	92	92	0	0

3 Residue-property plots (i)

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

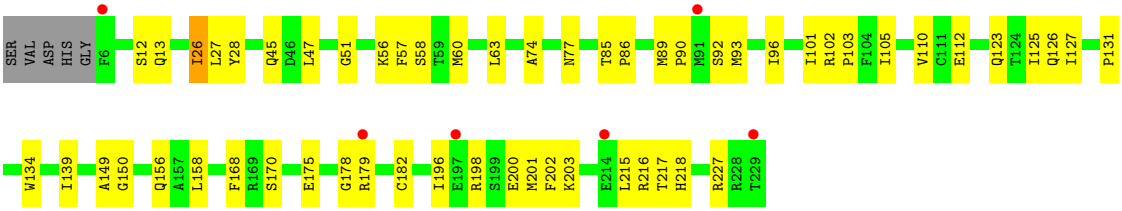
• Molecule 1: Type IV Collagen Noncollagenous Domain- Alpha1

Chain A:



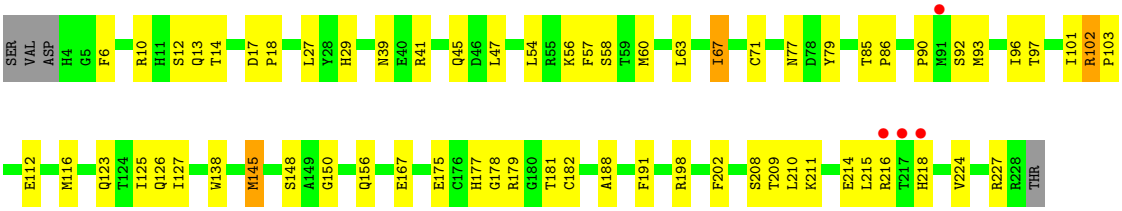
• Molecule 1: Type IV Collagen Noncollagenous Domain- Alpha1

Chain B:



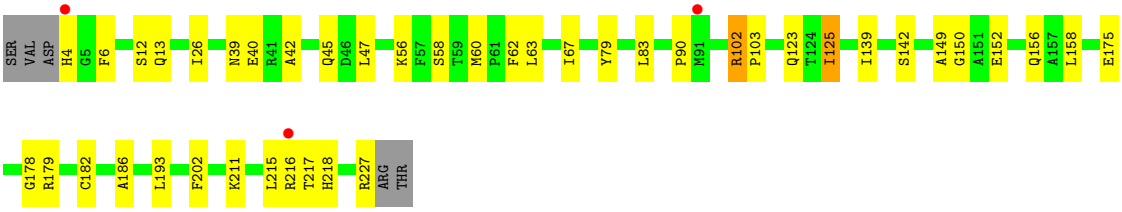
• Molecule 1: Type IV Collagen Noncollagenous Domain- Alpha1

Chain D:



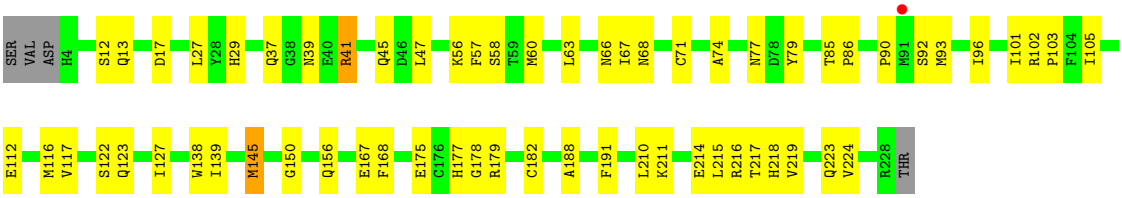
• Molecule 1: Type IV Collagen Noncollagenous Domain- Alpha1

Chain E:



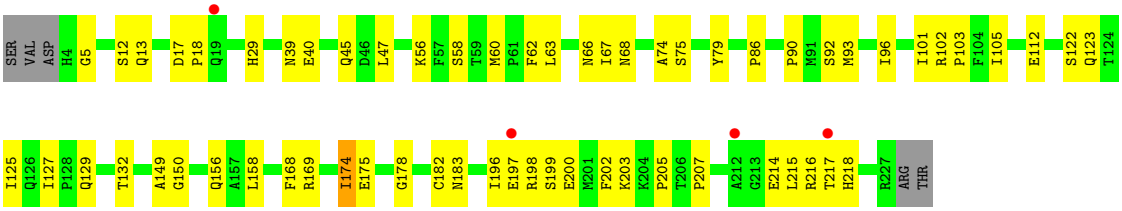
• Molecule 1: Type IV Collagen Noncollagenous Domain- Alpha1

Chain G:



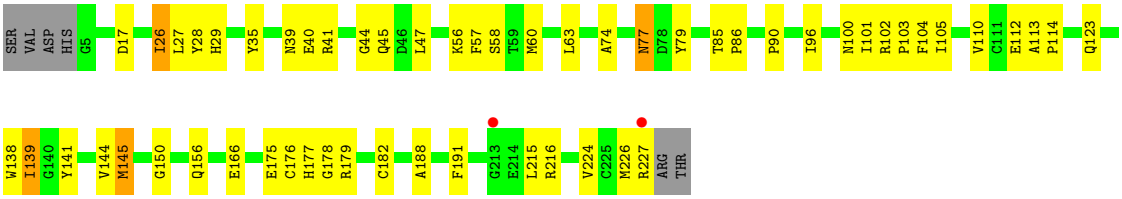
• Molecule 1: Type IV Collagen Noncollagenous Domain- Alpha1

Chain H:



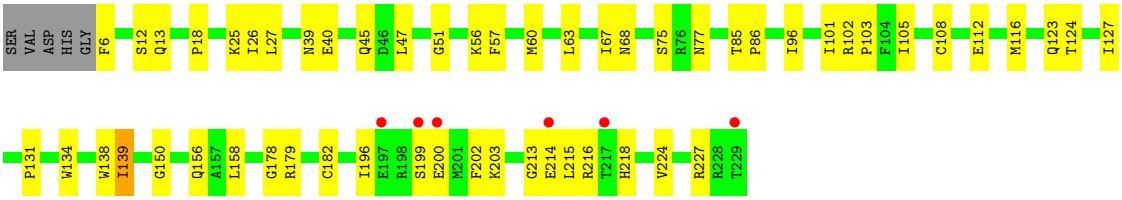
• Molecule 1: Type IV Collagen Noncollagenous Domain- Alpha1

Chain J:



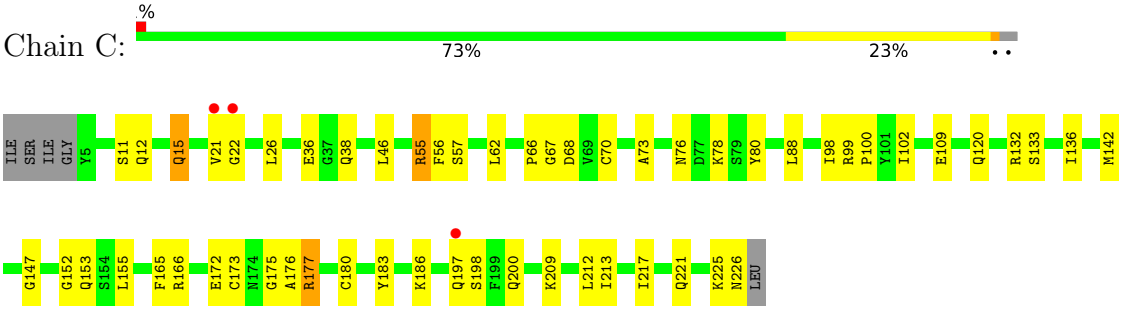
• Molecule 1: Type IV Collagen Noncollagenous Domain- Alpha1

Chain K:



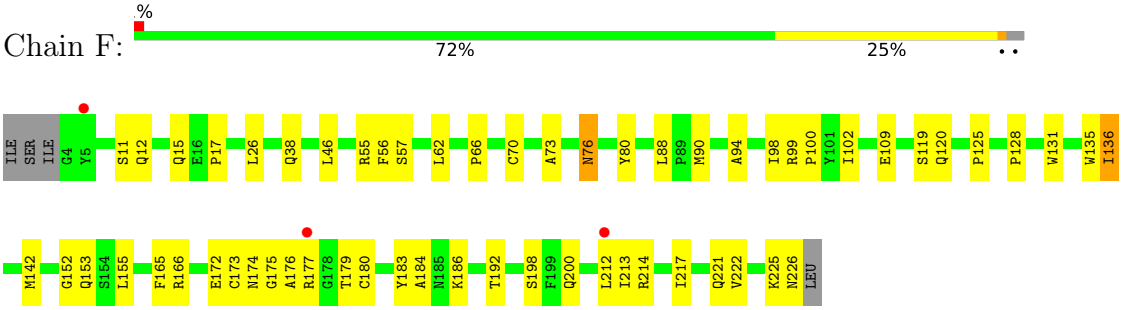
• Molecule 2: Type IV Collagen Noncollagenous Domain- Alpha2

Chain C:



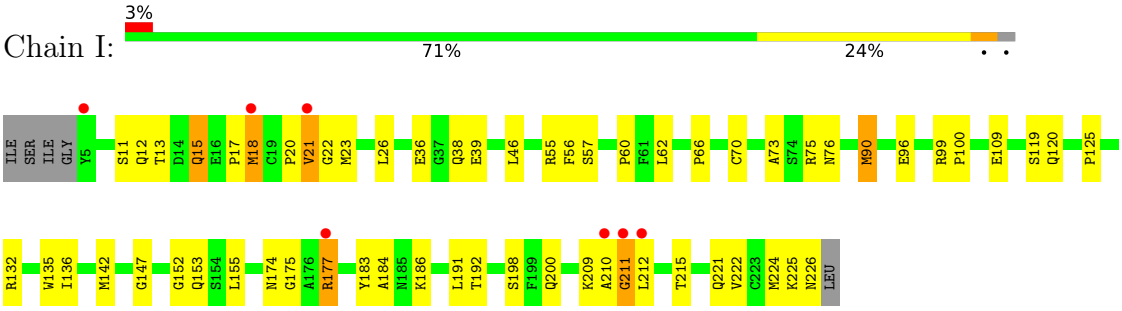
• Molecule 2: Type IV Collagen Noncollagenous Domain- Alpha2

Chain F:



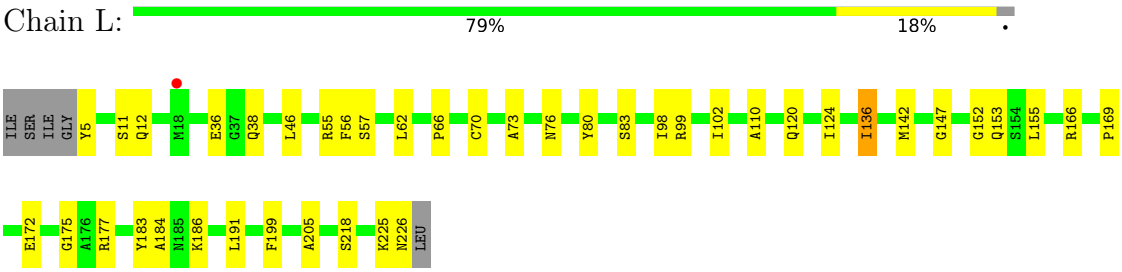
• Molecule 2: Type IV Collagen Noncollagenous Domain- Alpha2

Chain I:



• Molecule 2: Type IV Collagen Noncollagenous Domain- Alpha2

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	80.07Å 137.96Å 127.13Å 90.00° 90.31° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00 93.49 – 1.99	Depositor EDS
% Data completeness (in resolution range)	95.9 (8.00-2.00) 97.2 (93.49-1.99)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	10.45 (at 2.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.169 , 0.197 0.169 , 0.195	Depositor DCC
R_{free} test set	9172 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	14.8	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 62.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	22023	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, LU, BR

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	0.33	0/1793	0.60	0/2435
1	B	0.32	0/1805	0.59	0/2452
1	D	0.32	0/1798	0.59	0/2443
1	E	0.32	0/1785	0.59	0/2425
1	G	0.31	0/1806	0.59	0/2453
1	H	0.31	0/1793	0.58	0/2436
1	J	0.31	0/1774	0.58	0/2410
1	K	0.31	0/1788	0.59	0/2429
2	C	0.31	0/1771	0.61	0/2410
2	F	0.32	0/1775	0.62	0/2415
2	I	0.30	0/1771	0.61	0/2410
2	L	0.31	0/1782	0.61	0/2425
All	All	0.31	0/21441	0.60	0/29143

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1735	0	1657	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1747	0	1668	70	0
1	D	1743	0	1657	63	0
1	E	1734	0	1648	50	0
1	G	1748	0	1670	54	0
1	H	1738	0	1655	73	0
1	J	1724	0	1641	55	0
1	K	1738	0	1658	71	0
2	C	1720	0	1629	61	0
2	F	1724	0	1632	65	0
2	I	1720	0	1629	59	0
2	L	1726	0	1632	43	0
3	A	4	0	0	3	0
3	B	5	0	0	5	0
3	C	4	0	0	1	0
3	D	1	0	0	0	0
3	E	2	0	0	3	0
3	F	2	0	0	1	0
3	G	3	0	0	2	0
3	H	4	0	0	2	0
3	I	3	0	0	1	0
3	J	2	0	0	2	0
3	K	3	0	0	4	0
3	L	3	0	0	1	0
4	A	6	0	4	0	0
4	B	6	0	4	0	0
4	D	6	0	4	0	0
4	E	6	0	4	0	0
4	G	6	0	4	0	0
4	H	6	0	4	0	0
4	J	6	0	4	0	0
4	K	6	0	4	0	0
5	C	1	0	0	0	0
5	F	1	0	0	0	0
5	I	1	0	0	0	0
5	L	1	0	0	0	0
6	A	108	0	0	1	0
6	B	87	0	0	4	0
6	C	103	0	0	3	0
6	D	103	0	0	1	0
6	E	83	0	0	3	0
6	F	111	0	0	2	0
6	G	85	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	88	0	0	3	0
6	I	99	0	0	2	0
6	J	94	0	0	1	0
6	K	85	0	0	1	0
6	L	92	0	0	2	0
All	All	22023	0	19808	588	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 14.

All (588) 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)
2:L:98:ILE:HG22	2:L:102:ILE:HD11	1.29	1.10
1:J:101:ILE:HG22	1:J:105:ILE:HD11	1.37	1.04
2:F:214:ARG:HA	2:F:217:ILE:HD12	1.43	1.00
1:B:90:PRO:HG2	1:B:96:ILE:HD11	1.44	0.99
1:D:10:ARG:HH12	1:H:129:GLN:NE2	1.62	0.95
1:D:10:ARG:HH12	1:H:129:GLN:HE22	0.97	0.94
2:F:213:ILE:HG22	2:F:217:ILE:HD11	1.51	0.93
1:A:174:ILE:HD13	1:A:175:GLU:N	1.86	0.90
1:H:174:ILE:HD13	1:H:175:GLU:N	1.89	0.87
2:I:136:ILE:HG22	2:I:221:GLN:HG2	1.59	0.84
1:G:123:GLN:HE22	2:I:55:ARG:H	1.27	0.83
2:F:136:ILE:HG22	2:F:221:GLN:HG2	1.60	0.83
1:D:27:LEU:HD11	1:D:112:GLU:HB2	1.61	0.83
1:J:123:GLN:HE22	2:L:55:ARG:H	1.26	0.82
1:A:123:GLN:HE22	2:C:55:ARG:H	1.27	0.81
1:K:12:SER:HB3	1:K:18:PRO:HG3	1.63	0.81
1:E:42:ALA:HB2	1:E:152:GLU:HG3	1.62	0.80
1:K:63:LEU:HD23	6:L:3117:HOH:O	1.82	0.80
1:D:123:GLN:HE22	2:F:55:ARG:H	1.28	0.79
1:B:179[B]:ARG:NH2	2:F:76:ASN:HD22	1.80	0.79
2:F:11:SER:HB3	2:F:17:PRO:HG3	1.65	0.79
1:G:27:LEU:HD11	1:G:112:GLU:HB2	1.62	0.79
1:A:45:GLN:HE22	1:B:158:LEU:H	1.29	0.79
1:A:174:ILE:HD11	1:A:183:ASN:N	1.98	0.78
1:G:45:GLN:HE22	1:H:158:LEU:H	1.28	0.78
2:I:183:TYR:H	2:I:186:LYS:HZ2	1.31	0.78
1:D:10:ARG:NH1	1:H:129:GLN:HE22	1.79	0.77
1:H:174:ILE:HD11	1:H:183:ASN:N	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:LEU:H	1:A:156:GLN:HE22	1.33	0.77
1:K:216:ARG:HD2	3:K:3033:BR:BR	2.40	0.77
1:H:101:ILE:HG22	1:H:105:ILE:HD11	1.67	0.76
2:I:11:SER:HB3	2:I:17:PRO:HG3	1.67	0.76
1:B:47:LEU:H	1:B:156:GLN:HE22	1.34	0.76
1:J:139:ILE:HD13	1:J:139:ILE:H	1.50	0.76
1:K:139:ILE:HD13	6:K:4034:HOH:O	1.85	0.76
1:B:179[B]:ARG:HH21	2:F:76:ASN:HA	1.51	0.75
2:I:177:ARG:HH12	2:L:205:ALA:HB2	1.51	0.75
1:K:45:GLN:HE22	2:L:155:LEU:H	1.33	0.75
1:H:45:GLN:HE22	2:I:155:LEU:H	1.34	0.75
2:I:174:ASN:HD22	1:K:77:ASN:ND2	1.83	0.75
1:B:45:GLN:HE22	2:C:155:LEU:H	1.34	0.75
1:G:47:LEU:H	1:G:156:GLN:HE22	1.33	0.74
1:J:45:GLN:HE22	1:K:158:LEU:H	1.32	0.74
1:E:45:GLN:HE22	2:F:155:LEU:H	1.36	0.74
2:C:183:TYR:H	2:C:186:LYS:HZ2	1.36	0.74
1:J:27:LEU:HD11	1:J:112:GLU:HB2	1.69	0.73
2:C:12:GLN:HE21	2:C:166:ARG:HH11	1.36	0.73
1:H:174:ILE:HD12	1:H:182:CYS:HB3	1.69	0.73
1:D:47:LEU:H	1:D:156:GLN:HE22	1.36	0.73
2:I:20:PRO:HB2	2:I:23:MET:HE3	1.70	0.73
1:D:45:GLN:HE22	1:E:158:LEU:H	1.37	0.73
1:B:90:PRO:HG2	1:B:96:ILE:CD1	2.17	0.73
1:D:85:THR:HB	1:D:86:PRO:HD2	1.70	0.72
2:F:26:LEU:HD11	2:F:109:GLU:HB2	1.71	0.72
1:A:174:ILE:HD12	1:A:182:CYS:HB3	1.72	0.71
1:J:56:LYS:H	1:K:123:GLN:HE22	1.34	0.71
1:D:56:LYS:H	1:E:123:GLN:HE22	1.38	0.71
1:D:127:ILE:HD11	1:H:125:ILE:HD12	1.73	0.71
2:L:183:TYR:H	2:L:186:LYS:HZ2	1.38	0.71
1:B:150:GLY:H	2:F:38:GLN:NE2	1.89	0.71
1:J:101:ILE:CG2	1:J:105:ILE:HD11	2.19	0.71
1:K:47:LEU:H	1:K:156:GLN:HE22	1.37	0.70
1:H:47:LEU:H	1:H:156:GLN:HE22	1.36	0.70
1:B:179[B]:ARG:NH2	6:B:4010:HOH:O	2.25	0.69
1:H:174:ILE:HD13	1:H:175:GLU:H	1.58	0.69
1:J:47:LEU:H	1:J:156:GLN:HE22	1.40	0.69
1:B:90:PRO:CG	1:B:96:ILE:HD11	2.21	0.68
2:F:225:LYS:O	2:F:226:ASN:HB2	1.93	0.68
1:B:77:ASN:OD1	1:B:179[B]:ARG:NH2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179[B]:ARG:HG2	1:B:179[B]:ARG:HH11	1.58	0.68
1:G:13:GLN:OE1	1:G:167:GLU:HG2	1.93	0.68
1:B:27:LEU:HD11	1:B:112:GLU:HB2	1.75	0.68
1:H:12:SER:HB3	1:H:18:PRO:HG3	1.75	0.68
1:H:150:GLY:H	2:L:38:GLN:NE2	1.92	0.68
1:A:56:LYS:H	1:B:123:GLN:HE22	1.40	0.68
1:G:105:ILE:HD12	1:H:202:PHE:HE2	1.60	0.67
1:A:101:ILE:HG22	1:A:105:ILE:HD11	1.75	0.67
1:H:217:THR:HG23	1:H:218:HIS:ND1	2.09	0.67
1:A:150:GLY:H	1:D:39:ASN:ND2	1.92	0.67
1:E:42:ALA:CB	1:E:152:GLU:HG3	2.25	0.67
1:K:101:ILE:HG22	1:K:105:ILE:HD11	1.77	0.66
1:A:174:ILE:HD13	1:A:175:GLU:H	1.61	0.66
2:C:38:GLN:NE2	1:E:150:GLY:H	1.93	0.66
2:I:183:TYR:H	2:I:186:LYS:NZ	1.94	0.66
1:E:217:THR:HG23	1:E:218:HIS:ND1	2.12	0.65
2:L:225:LYS:O	2:L:226:ASN:HB2	1.97	0.65
1:B:217:THR:HG23	1:B:218:HIS:ND1	2.12	0.65
1:K:214:GLU:HG2	1:K:218:HIS:CE1	2.32	0.64
1:B:89:MET:HE2	1:B:93:MET:HG2	1.80	0.64
1:E:47:LEU:H	1:E:156:GLN:HE22	1.43	0.64
1:D:216:ARG:CZ	1:H:197:GLU:HG2	2.27	0.64
1:G:39:ASN:ND2	1:J:150:GLY:H	1.95	0.64
1:A:45:GLN:NE2	1:B:158:LEU:H	1.94	0.64
1:A:211:LYS:O	1:A:214:GLU:HG2	1.98	0.63
2:C:183:TYR:H	2:C:186:LYS:NZ	1.96	0.63
1:E:67:ILE:HG12	2:F:184:ALA:HA	1.80	0.63
2:F:183:TYR:H	2:F:186:LYS:HZ2	1.45	0.63
2:F:136:ILE:HD13	2:F:136:ILE:H	1.63	0.63
1:G:85:THR:HB	1:G:86:PRO:HD2	1.81	0.63
1:G:56:LYS:H	1:H:123:GLN:HE22	1.44	0.63
2:I:26:LEU:HD11	2:I:109:GLU:HB2	1.80	0.63
1:G:217:THR:HG23	1:G:218:HIS:ND1	2.13	0.63
1:B:127:ILE:HD13	1:B:139:ILE:HG21	1.79	0.63
2:I:38:GLN:NE2	1:K:150:GLY:H	1.97	0.63
2:F:136:ILE:HD13	6:F:3089:HOH:O	1.98	0.63
1:K:56:LYS:H	2:L:120:GLN:HE22	1.46	0.62
2:I:21:VAL:HG13	2:I:22:GLY:H	1.63	0.62
2:C:225:LYS:O	2:C:226:ASN:HB2	1.99	0.62
1:B:200:GLU:HA	1:B:203:LYS:HE2	1.81	0.62
1:B:168:PHE:HB3	1:B:216:ARG:HH11	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:98:ILE:HG22	2:F:102:ILE:HD11	1.82	0.62
1:H:102:ARG:HB3	1:H:103:PRO:HD3	1.80	0.61
1:J:85:THR:HB	1:J:86:PRO:HD2	1.82	0.61
1:G:45:GLN:NE2	1:H:158:LEU:H	1.97	0.61
1:J:141:TYR:CE2	1:J:216:ARG:HG3	2.36	0.61
1:E:216:ARG:HG3	3:E:3036:BR:BR	2.55	0.61
1:K:214:GLU:HG2	1:K:218:HIS:HE1	1.63	0.60
1:B:56:LYS:H	2:C:120:GLN:HE22	1.48	0.60
1:G:217:THR:HG23	1:G:218:HIS:CE1	2.35	0.60
1:H:96:ILE:O	1:H:101:ILE:HD11	2.01	0.60
1:K:27:LEU:HD11	1:K:112:GLU:HB2	1.84	0.60
1:B:168:PHE:HB3	1:B:216:ARG:NH1	2.16	0.60
2:C:88:LEU:HD23	6:C:3098:HOH:O	2.01	0.60
1:G:150:GLY:H	1:J:39:ASN:ND2	1.99	0.59
1:G:47:LEU:H	1:G:156:GLN:NE2	2.00	0.59
1:G:211:LYS:O	1:G:214:GLU:HG2	2.01	0.59
1:H:67:ILE:HG12	2:I:184:ALA:HA	1.84	0.59
1:A:105:ILE:HD12	1:B:202:PHE:HE2	1.67	0.59
1:D:216:ARG:NH1	1:H:197:GLU:HG2	2.16	0.59
1:A:39:ASN:ND2	1:D:150:GLY:H	1.99	0.59
1:A:125:ILE:HD11	1:A:126:GLN:NE2	2.17	0.59
1:B:26:ILE:HD13	1:B:27:LEU:N	2.17	0.59
1:H:60:MET:HB2	1:H:178:GLY:HA2	1.85	0.59
1:A:174:ILE:CD1	1:A:182:CYS:HB3	2.33	0.59
1:E:215:LEU:HB2	3:E:3036:BR:BR	2.58	0.59
2:I:18:MET:SD	2:I:18:MET:N	2.67	0.59
1:A:26:ILE:HD13	1:A:27:LEU:N	2.18	0.59
2:F:15:GLN:HE21	2:F:15:GLN:HA	1.68	0.59
1:H:39:ASN:ND2	2:L:147:GLY:H	2.00	0.59
2:L:136:ILE:HD13	6:L:3050:HOH:O	2.02	0.59
2:I:225:LYS:O	2:I:226:ASN:HB2	2.03	0.59
1:J:105:ILE:HD13	1:K:202:PHE:HE2	1.67	0.59
1:K:139:ILE:HD13	1:K:139:ILE:H	1.68	0.59
1:H:56:LYS:H	2:I:120:GLN:HE22	1.49	0.58
2:L:102:ILE:N	2:L:102:ILE:HD12	2.18	0.58
2:I:11:SER:O	2:I:12:GLN:HB2	2.03	0.58
1:B:57:PHE:CD1	1:B:105:ILE:HD13	2.38	0.58
1:J:26:ILE:HD13	1:J:27:LEU:N	2.19	0.58
1:G:71:CYS:SG	1:H:215:LEU:HD22	2.43	0.58
1:E:60:MET:HB2	1:E:178:GLY:HA2	1.85	0.58
2:C:177:ARG:HG2	2:C:177:ARG:HH21	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:57:PHE:CD1	1:K:105:ILE:HD13	2.38	0.58
2:L:183:TYR:H	2:L:186:LYS:NZ	2.02	0.58
1:D:67:ILE:CD1	1:E:186:ALA:HA	2.33	0.58
1:A:56:LYS:H	1:B:123:GLN:NE2	2.02	0.58
1:D:56:LYS:H	1:E:123:GLN:NE2	2.00	0.58
1:D:214:GLU:O	1:D:218:HIS:HD2	1.87	0.57
2:C:98:ILE:HG22	2:C:102:ILE:HD11	1.86	0.57
2:C:99:ARG:HB2	2:C:100:PRO:HD3	1.86	0.57
1:H:39:ASN:HD21	2:L:147:GLY:H	1.52	0.57
1:G:216:ARG:HG3	3:G:3031:BR:BR	2.59	0.57
2:C:165:PHE:CD2	2:C:217:ILE:HD13	2.39	0.57
1:J:45:GLN:NE2	1:K:158:LEU:H	2.01	0.57
1:A:71:CYS:SG	1:B:215:LEU:HG	2.45	0.57
1:K:60:MET:HB2	1:K:178:GLY:HA2	1.87	0.56
1:B:101:ILE:HG22	1:B:105:ILE:HD11	1.87	0.56
2:C:55:ARG:HD3	6:C:3126:HOH:O	2.05	0.56
1:G:127:ILE:N	1:G:127:ILE:HD12	2.20	0.56
1:H:127:ILE:N	1:H:127:ILE:HD12	2.20	0.56
2:F:46:LEU:H	2:F:153:GLN:HE22	1.53	0.56
1:B:178:GLY:HA3	3:B:3012:BR:BR	2.61	0.56
1:G:37:GLN:NE2	1:J:40:GLU:OE1	2.38	0.56
1:G:41:ARG:HD3	6:H:4059:HOH:O	2.06	0.56
1:G:56:LYS:H	1:H:123:GLN:NE2	2.03	0.56
2:I:21:VAL:HG13	2:I:22:GLY:N	2.20	0.56
1:J:101:ILE:HG22	1:J:105:ILE:CD1	2.23	0.56
1:A:150:GLY:H	1:D:39:ASN:HD21	1.53	0.56
1:H:174:ILE:CD1	1:H:182:CYS:HB3	2.35	0.56
2:C:46:LEU:H	2:C:153:GLN:HE22	1.52	0.56
1:D:102:ARG:HB3	1:D:103:PRO:HD3	1.88	0.56
1:K:96:ILE:O	1:K:101:ILE:HD11	2.05	0.56
2:L:102:ILE:HD12	2:L:102:ILE:H	1.71	0.55
1:G:13:GLN:CD	1:G:167:GLU:HG2	2.26	0.55
2:I:39:GLU:HG3	1:K:40:GLU:HG2	1.88	0.55
1:B:217:THR:HG23	1:B:218:HIS:CE1	2.42	0.55
1:H:199:SER:O	1:H:203:LYS:HE2	2.07	0.55
1:A:93:MET:CE	1:E:211:LYS:HE2	2.37	0.55
2:I:13:THR:OG1	2:I:15:GLN:HG2	2.06	0.55
1:J:56:LYS:H	1:K:123:GLN:NE2	2.02	0.55
1:A:202:PHE:HE2	2:C:102:ILE:HD12	1.72	0.55
1:H:45:GLN:NE2	2:I:155:LEU:H	2.03	0.55
2:C:176:ALA:HB3	1:E:179:ARG:HD3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:212:LEU:N	2:C:212:LEU:HD22	2.22	0.54
1:G:101:ILE:HG22	1:G:105:ILE:HD11	1.87	0.54
1:H:47:LEU:H	1:H:156:GLN:NE2	2.05	0.54
1:H:67:ILE:HD12	1:H:68:ASN:N	2.23	0.54
1:K:45:GLN:NE2	2:L:155:LEU:H	2.05	0.54
1:B:47:LEU:H	1:B:156:GLN:NE2	2.05	0.54
2:L:83:SER:O	2:L:166:ARG:NH1	2.41	0.54
1:B:179[B]:ARG:HG2	1:B:179[B]:ARG:NH1	2.23	0.54
1:B:216:ARG:NH1	3:B:3028:BR:BR	2.95	0.54
1:K:57:PHE:CE1	1:K:105:ILE:HD13	2.42	0.54
1:G:145:MET:HG2	1:G:191:PHE:HB2	1.90	0.54
1:A:55:ARG:NH1	6:A:4068:HOH:O	2.34	0.53
1:E:45:GLN:NE2	2:F:155:LEU:H	2.01	0.53
1:K:96:ILE:CG2	1:K:101:ILE:HD13	2.38	0.53
2:I:20:PRO:CB	2:I:23:MET:HE3	2.37	0.53
2:F:11:SER:O	2:F:12:GLN:HB2	2.08	0.53
2:I:147:GLY:H	1:K:39:ASN:ND2	2.07	0.53
1:K:67:ILE:HG12	2:L:184:ALA:HA	1.91	0.53
1:D:71:CYS:SG	1:E:215:LEU:HG	2.48	0.53
2:I:174:ASN:HD22	1:K:77:ASN:HD22	1.57	0.53
2:I:39:GLU:CG	1:K:40:GLU:HG2	2.38	0.52
1:J:26:ILE:HD13	1:J:26:ILE:C	2.29	0.52
1:K:56:LYS:H	2:L:120:GLN:NE2	2.07	0.52
1:A:47:LEU:H	1:A:156:GLN:NE2	2.05	0.52
1:D:211:LYS:O	1:D:214:GLU:HG2	2.08	0.52
1:K:47:LEU:H	1:K:156:GLN:NE2	2.05	0.52
1:A:102:ARG:HB3	1:A:103:PRO:HD3	1.91	0.52
1:A:105:ILE:CD1	1:B:202:PHE:HE2	2.22	0.52
1:G:67:ILE:C	1:G:67:ILE:HD12	2.28	0.52
1:K:179:ARG:HG3	1:K:179:ARG:HH11	1.75	0.52
2:C:56:PHE:CE2	2:C:102:ILE:HD13	2.44	0.52
2:I:46:LEU:H	2:I:153:GLN:HE22	1.55	0.52
2:C:21:VAL:HG13	2:C:22:GLY:N	2.25	0.52
1:E:56:LYS:H	2:F:120:GLN:HE22	1.56	0.52
1:E:125:ILE:HD12	6:E:4037:HOH:O	2.09	0.52
1:G:150:GLY:H	1:J:39:ASN:HD21	1.58	0.52
2:I:90:MET:HE2	2:I:90:MET:HA	1.92	0.52
1:J:101:ILE:O	1:J:105:ILE:HD12	2.10	0.52
1:K:102:ARG:HB3	1:K:103:PRO:HD3	1.92	0.52
1:B:60:MET:HB2	1:B:178:GLY:HA2	1.92	0.52
1:J:90:PRO:HD2	6:J:4083:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:LEU:H	1:D:156:GLN:NE2	2.06	0.52
1:H:96:ILE:HD12	1:H:96:ILE:N	2.25	0.52
2:I:90:MET:HA	2:I:90:MET:CE	2.40	0.52
2:I:177:ARG:HG2	2:I:177:ARG:HH21	1.75	0.51
1:A:26:ILE:HD13	1:A:26:ILE:C	2.31	0.51
2:F:56:PHE:CE2	2:F:102:ILE:HD13	2.45	0.51
1:B:56:LYS:H	2:C:120:GLN:NE2	2.08	0.51
1:J:17:ASP:HB3	1:J:29:HIS:CD2	2.46	0.51
1:B:57:PHE:CE1	1:B:105:ILE:HD13	2.46	0.51
2:L:56:PHE:CD1	2:L:57:SER:N	2.79	0.51
1:A:58:SER:HB2	1:B:196:ILE:HD13	1.92	0.51
1:A:139:ILE:C	1:A:139:ILE:HD12	2.31	0.51
1:B:45:GLN:NE2	2:C:155:LEU:H	2.04	0.51
2:F:214:ARG:CA	2:F:217:ILE:HD12	2.28	0.51
1:A:123:GLN:NE2	2:C:55:ARG:H	2.03	0.51
1:A:6:PHE:CE2	1:A:116:MET:HG2	2.46	0.51
1:G:116:MET:HE2	1:G:117:VAL:H	1.76	0.51
1:A:93:MET:HE3	1:E:211:LYS:HE2	1.91	0.50
1:B:179[B]:ARG:NH2	2:F:76:ASN:ND2	2.56	0.50
2:F:136:ILE:HG22	2:F:221:GLN:CG	2.38	0.50
1:G:39:ASN:HD21	1:J:150:GLY:H	1.59	0.50
1:J:58:SER:HB2	1:K:196:ILE:HD13	1.93	0.50
2:F:214:ARG:HA	2:F:217:ILE:CD1	2.28	0.50
2:L:124:ILE:HD12	2:L:124:ILE:N	2.26	0.50
2:I:147:GLY:H	1:K:39:ASN:HD21	1.59	0.50
1:A:127:ILE:HD12	1:A:127:ILE:N	2.26	0.50
1:B:26:ILE:HD13	1:B:27:LEU:C	2.32	0.50
1:G:58:SER:HB2	1:H:196[B]:ILE:HD13	1.93	0.50
2:I:212:LEU:HG	2:I:215:THR:HG23	1.92	0.50
2:F:73:ALA:HA	3:F:3013:BR:BR	2.67	0.50
2:F:99:ARG:HB3	2:F:100:PRO:HD3	1.94	0.50
1:J:114:PRO:HD2	1:J:226:MET:SD	2.52	0.50
2:I:209:LYS:C	2:I:211:GLY:H	2.15	0.49
1:K:96:ILE:HG22	1:K:101:ILE:HD13	1.94	0.49
1:G:175:GLU:O	1:G:182:CYS:HA	2.11	0.49
1:D:97:THR:HG22	1:D:181:THR:HG22	1.94	0.49
1:E:63:LEU:HD12	1:E:63:LEU:C	2.33	0.49
1:K:63:LEU:C	1:K:63:LEU:HD12	2.33	0.49
2:I:75:ARG:O	1:K:179:ARG:NH1	2.44	0.49
1:J:28:TYR:CZ	1:J:110:VAL:HG21	2.47	0.49
1:K:215:LEU:HB3	3:K:3033:BR:BR	2.67	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:147:GLY:H	1:E:39:ASN:ND2	2.10	0.49
1:H:90:PRO:HD2	6:H:4090:HOH:O	2.11	0.49
1:J:102:ARG:HB3	1:J:103:PRO:HD3	1.95	0.49
1:A:114:PRO:HD2	1:A:226:MET:SD	2.52	0.49
1:B:102:ARG:HB3	1:B:103:PRO:HD3	1.95	0.49
1:D:67:ILE:HD11	1:E:186:ALA:HA	1.94	0.49
2:F:174:ASN:ND2	6:F:3090:HOH:O	2.40	0.49
2:F:62:LEU:HD12	2:F:62:LEU:C	2.33	0.48
1:D:67:ILE:HD12	1:E:186:ALA:HA	1.94	0.48
1:H:58:SER:HA	2:I:200:GLN:O	2.13	0.48
1:A:138:TRP:CE2	1:A:224:VAL:HG21	2.48	0.48
1:H:96:ILE:CG2	1:H:101:ILE:HD13	2.43	0.48
2:I:135:TRP:CZ2	2:I:222:VAL:HG21	2.48	0.48
2:L:225:LYS:O	2:L:226:ASN:CB	2.62	0.48
1:B:125:ILE:C	1:B:125:ILE:HD12	2.34	0.48
2:F:119:SER:HB3	2:F:125:PRO:HD3	1.96	0.48
2:I:36:GLU:OE1	1:K:40:GLU:OE2	2.32	0.48
2:I:62:LEU:HD12	2:I:62:LEU:C	2.34	0.48
1:J:139:ILE:HD13	1:J:139:ILE:N	2.23	0.48
1:K:213:GLY:O	1:K:214:GLU:HB3	2.13	0.48
2:I:73:ALA:HA	3:I:3014:BR:BR	2.68	0.48
2:L:11:SER:O	2:L:12:GLN:HB2	2.13	0.48
2:L:46:LEU:H	2:L:153:GLN:HE22	1.61	0.48
2:F:142:MET:HA	2:F:152:GLY:HA2	1.96	0.48
1:K:214:GLU:HG2	1:K:214:GLU:O	2.14	0.48
2:C:36:GLU:OE1	1:E:40:GLU:OE2	2.32	0.48
1:D:45:GLN:NE2	1:E:158:LEU:H	2.06	0.48
1:D:96:ILE:O	1:D:101:ILE:HD11	2.13	0.48
1:E:56:LYS:H	2:F:120:GLN:NE2	2.12	0.48
1:G:116:MET:CE	1:G:117:VAL:H	2.27	0.48
1:H:40:GLU:OE2	2:L:36:GLU:OE1	2.31	0.48
1:H:62:PHE:HA	2:I:192:THR:HG23	1.96	0.48
2:I:209:LYS:O	2:I:211:GLY:N	2.47	0.48
1:J:101:ILE:HD13	1:J:182:CYS:SG	2.54	0.48
1:D:202:PHE:HE2	2:F:102:ILE:HD12	1.80	0.47
2:I:57:SER:O	2:I:60:PRO:HD3	2.14	0.47
1:A:101:ILE:CG2	1:A:105:ILE:HD11	2.44	0.47
1:B:63:LEU:C	1:B:63:LEU:HD12	2.34	0.47
1:K:101:ILE:HD12	1:K:182:CYS:HB2	1.95	0.47
1:A:188:ALA:O	2:C:66:PRO:HD3	2.13	0.47
1:B:139:ILE:HD12	1:B:139:ILE:C	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:TRP:CE2	1:D:224:VAL:HG21	2.50	0.47
1:K:67:ILE:HD12	1:K:68:ASN:N	2.29	0.47
1:A:227:ARG:HD3	1:A:227:ARG:C	2.34	0.47
1:J:178:GLY:HA3	3:J:3008:BR:BR	2.70	0.47
2:L:191:LEU:HB3	2:L:218:SER:HB3	1.96	0.47
1:B:179[A]:ARG:HD3	2:F:176:ALA:HB3	1.97	0.47
2:C:56:PHE:CD1	2:C:57:SER:N	2.83	0.47
2:C:73:ALA:HA	3:C:3007:BR:BR	2.70	0.47
2:C:213:ILE:HG22	2:C:217:ILE:HD11	1.95	0.47
1:E:47:LEU:H	1:E:156:GLN:NE2	2.09	0.47
2:F:183:TYR:H	2:F:186:LYS:NZ	2.13	0.47
1:G:63:LEU:C	1:G:63:LEU:HD12	2.35	0.47
1:G:90:PRO:HD2	6:G:4054:HOH:O	2.13	0.47
2:I:135:TRP:CE2	2:I:222:VAL:HG21	2.50	0.47
1:A:26:ILE:HD13	1:A:27:LEU:C	2.35	0.47
1:A:227:ARG:NH1	2:C:109:GLU:OE1	2.47	0.47
1:J:100:ASN:O	1:J:103:PRO:HD2	2.15	0.47
2:L:5:TYR:HD1	2:L:110:ALA:HB3	1.80	0.47
2:C:98:ILE:CG2	2:C:102:ILE:HD11	2.44	0.47
2:C:225:LYS:O	2:C:226:ASN:CB	2.62	0.47
1:E:12:SER:O	1:E:13:GLN:HB2	2.15	0.47
1:A:125:ILE:HD12	1:A:125:ILE:C	2.35	0.47
2:C:38:GLN:HE22	1:E:149:ALA:HA	1.80	0.47
1:K:178:GLY:HA3	3:K:3009:BR:BR	2.70	0.47
1:B:139:ILE:HD12	1:B:139:ILE:O	2.16	0.46
1:D:6:PHE:CE2	1:D:116:MET:HG2	2.50	0.46
1:K:199:SER:O	1:K:203:LYS:HE2	2.15	0.46
1:B:90:PRO:HD2	6:B:4053:HOH:O	2.15	0.46
1:B:179[B]:ARG:CZ	2:F:76:ASN:HD22	2.28	0.46
1:B:217:THR:HG23	1:B:218:HIS:HD1	1.77	0.46
1:G:188:ALA:O	2:I:66:PRO:HD3	2.15	0.46
6:H:4054:HOH:O	2:L:177:ARG:HD2	2.15	0.46
1:K:131:PRO:HB2	1:K:134:TRP:CD1	2.50	0.46
2:L:136:ILE:HD13	2:L:136:ILE:H	1.80	0.46
2:F:135:TRP:CZ2	2:F:222:VAL:HG21	2.50	0.46
1:J:138:TRP:CE2	1:J:224:VAL:HG21	2.50	0.46
1:A:17:ASP:HB3	1:A:29:HIS:CD2	2.50	0.46
1:D:14:THR:CG2	1:H:198:ARG:NH1	2.79	0.46
2:I:119:SER:HB3	2:I:125:PRO:HD3	1.97	0.46
1:K:215:LEU:CB	3:K:3033:BR:BR	3.18	0.46
2:L:73:ALA:HA	3:L:3010:BR:BR	2.70	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:225:LYS:O	2:F:226:ASN:CB	2.63	0.46
1:K:12:SER:O	1:K:13:GLN:HB2	2.16	0.46
2:L:80:TYR:CE1	2:L:172:GLU:HB2	2.50	0.46
1:B:125:ILE:HD12	1:B:126:GLN:N	2.31	0.46
1:D:125:ILE:HG13	1:D:126:GLN:NE2	2.31	0.46
1:D:175:GLU:O	1:D:182:CYS:HA	2.15	0.46
1:H:175:GLU:O	1:H:182:CYS:HA	2.16	0.46
1:A:57:PHE:CG	1:A:58:SER:N	2.83	0.46
1:D:67:ILE:HD13	1:D:67:ILE:N	2.31	0.46
2:F:56:PHE:CD1	2:F:57:SER:N	2.84	0.46
1:G:177:HIS:HB2	1:G:179:ARG:HG2	1.97	0.46
1:D:12:SER:O	1:D:13:GLN:HB2	2.16	0.46
1:G:215:LEU:HD22	2:I:70:CYS:SG	2.56	0.46
3:A:3004:BR:BR	1:D:178:GLY:HA3	2.70	0.46
2:C:56:PHE:CG	2:C:57:SER:N	2.84	0.46
1:H:56:LYS:H	2:I:120:GLN:NE2	2.12	0.46
2:L:98:ILE:O	2:L:102:ILE:CD1	2.64	0.46
1:A:101:ILE:HG22	1:A:105:ILE:CD1	2.46	0.45
1:D:67:ILE:HD13	1:D:67:ILE:H	1.80	0.45
1:E:4:HIS:HB3	1:E:6:PHE:CE1	2.51	0.45
1:E:139:ILE:HD12	1:E:139:ILE:C	2.35	0.45
1:J:144:VAL:HG13	1:J:145:MET:SD	2.56	0.45
1:A:63:LEU:C	1:A:63:LEU:HD12	2.36	0.45
1:A:83:LEU:HD12	1:A:83:LEU:HA	1.86	0.45
1:A:131:PRO:HB3	2:C:26:LEU:HD22	1.99	0.45
1:A:174:ILE:HD11	1:A:183:ASN:H	1.76	0.45
2:I:132:ARG:HH22	2:I:224:MET:CE	2.29	0.45
1:J:145:MET:HG2	1:J:191:PHE:HB2	1.98	0.45
2:L:166:ARG:O	2:L:169:PRO:HD3	2.16	0.45
1:A:215:LEU:HD22	2:C:70:CYS:SG	2.57	0.45
2:I:177:ARG:CD	1:K:179:ARG:HG2	2.46	0.45
1:A:77:ASN:HD22	1:A:77:ASN:HA	1.58	0.45
2:C:177:ARG:CD	1:E:179:ARG:HG2	2.47	0.45
1:G:60:MET:HB2	1:G:178:GLY:HA2	1.98	0.45
1:J:26:ILE:HD13	1:J:27:LEU:C	2.36	0.45
1:J:175:GLU:O	1:J:182:CYS:HA	2.16	0.45
1:K:67:ILE:HD12	1:K:67:ILE:C	2.36	0.45
1:K:200:GLU:HA	1:K:203:LYS:CE	2.47	0.45
2:L:56:PHE:CG	2:L:57:SER:N	2.84	0.45
1:A:145:MET:HG2	1:A:191:PHE:HB2	1.97	0.45
2:I:96:GLU:HG2	6:I:3114:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:62:LEU:C	2:L:62:LEU:HD12	2.37	0.45
1:H:96:ILE:HG22	1:H:101:ILE:HD13	1.98	0.45
1:J:96:ILE:HD13	1:J:104:PHE:CE1	2.52	0.45
1:K:12:SER:CB	1:K:18:PRO:HG3	2.39	0.45
1:K:105:ILE:HD12	2:L:199:PHE:HE1	1.81	0.45
1:E:90:PRO:HD2	6:E:4063:HOH:O	2.17	0.45
1:G:138:TRP:CE2	1:G:224:VAL:HG21	2.51	0.45
1:H:74:ALA:HA	3:H:3006:BR:BR	2.72	0.45
1:A:178:GLY:HA3	3:A:3005:BR:BR	2.71	0.45
1:B:216:ARG:HG3	3:B:3034:BR:BR	2.71	0.45
2:C:62:LEU:C	2:C:62:LEU:HD12	2.37	0.45
2:C:78:LYS:HB2	2:C:173:CYS:O	2.17	0.45
1:D:210:LEU:N	1:D:210:LEU:CD1	2.80	0.45
1:B:149:ALA:HA	2:F:38:GLN:HE22	1.81	0.45
1:D:57:PHE:CG	1:D:58:SER:N	2.84	0.45
1:D:90:PRO:HD2	6:D:4006:HOH:O	2.16	0.45
1:D:188:ALA:O	2:F:66:PRO:HD3	2.17	0.45
2:F:128:PRO:HB2	2:F:131:TRP:CD1	2.52	0.45
1:H:63:LEU:HD12	1:H:63:LEU:C	2.37	0.45
1:H:214:GLU:O	1:H:214:GLU:HG2	2.17	0.45
1:H:101:ILE:HG22	1:H:105:ILE:CD1	2.41	0.44
2:L:98:ILE:O	2:L:102:ILE:HD12	2.17	0.44
2:C:147:GLY:H	1:E:39:ASN:HD21	1.64	0.44
2:F:26:LEU:N	2:F:26:LEU:HD12	2.32	0.44
1:G:57:PHE:CD2	1:G:105:ILE:HD13	2.52	0.44
1:D:208:SER:OG	1:D:210:LEU:HD11	2.17	0.44
1:D:210:LEU:N	1:D:210:LEU:HD12	2.33	0.44
2:I:142:MET:HA	2:I:152:GLY:HA2	2.00	0.44
1:J:188:ALA:O	2:L:66:PRO:HD3	2.18	0.44
1:G:74:ALA:HA	3:G:3016:BR:BR	2.73	0.44
1:G:92:SER:O	1:G:93:MET:HB2	2.18	0.44
1:J:177:HIS:HB2	1:J:179:ARG:HG2	1.99	0.44
2:L:142:MET:HA	2:L:152:GLY:HA2	1.98	0.44
1:H:17:ASP:HB3	1:H:29:HIS:CD2	2.53	0.44
1:J:57:PHE:CG	1:J:58:SER:N	2.85	0.44
1:J:74:ALA:HA	3:J:3008:BR:BR	2.73	0.44
1:B:131:PRO:HB2	1:B:134:TRP:CD1	2.53	0.44
2:C:56:PHE:CD2	2:C:102:ILE:HD13	2.53	0.44
1:E:58:SER:HA	2:F:200:GLN:O	2.18	0.44
2:F:56:PHE:CD2	2:F:102:ILE:HD13	2.52	0.44
1:H:178:GLY:HA3	3:H:3006:BR:BR	2.73	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:56:PHE:CG	2:I:57:SER:N	2.86	0.44
1:B:12:SER:O	1:B:13:GLN:HB2	2.16	0.44
1:D:167:GLU:OE1	1:H:198:ARG:CZ	2.65	0.44
2:F:15:GLN:HA	2:F:15:GLN:NE2	2.33	0.44
1:G:105:ILE:CD1	1:H:202:PHE:HE2	2.27	0.44
1:J:63:LEU:HD12	1:J:63:LEU:C	2.38	0.44
1:K:45:GLN:HE21	1:K:51:GLY:HA3	1.83	0.44
2:C:21:VAL:HG13	2:C:22:GLY:H	1.82	0.44
1:D:17:ASP:HB3	1:D:29:HIS:CD2	2.52	0.44
1:D:101:ILE:HD12	1:D:182:CYS:SG	2.58	0.44
2:F:80:TYR:CE1	2:F:172:GLU:HB2	2.53	0.44
1:H:174:ILE:HD11	1:H:183:ASN:H	1.81	0.44
1:K:138:TRP:CE2	1:K:224:VAL:HG21	2.53	0.44
2:C:142:MET:HA	2:C:152:GLY:HA2	1.99	0.43
2:F:56:PHE:CG	2:F:57:SER:N	2.86	0.43
1:H:217:THR:HG23	1:H:218:HIS:CE1	2.53	0.43
1:B:45:GLN:HE21	1:B:51:GLY:HA3	1.82	0.43
2:F:88:LEU:CD2	2:F:88:LEU:H	2.32	0.43
1:H:149:ALA:HA	2:L:38:GLN:HE22	1.82	0.43
1:J:47:LEU:H	1:J:156:GLN:NE2	2.13	0.43
1:B:200:GLU:HG2	1:B:203:LYS:CE	2.48	0.43
1:D:102:ARG:HA	1:E:202:PHE:CE2	2.53	0.43
1:E:178:GLY:HA3	3:E:3003:BR:BR	2.74	0.43
1:H:92:SER:O	1:H:93:MET:HB2	2.18	0.43
2:C:136:ILE:HD12	2:C:136:ILE:C	2.38	0.43
1:D:63:LEU:C	1:D:63:LEU:HD12	2.39	0.43
2:F:88:LEU:N	2:F:88:LEU:HD22	2.33	0.43
1:G:12:SER:O	1:G:13:GLN:HB2	2.18	0.43
2:I:15:GLN:HE21	2:I:15:GLN:HB3	1.57	0.43
2:I:26:LEU:HD12	2:I:26:LEU:N	2.34	0.43
1:B:179[B]:ARG:HH21	2:F:76:ASN:HD22	1.62	0.43
1:B:198:ARG:NH2	6:B:4085:HOH:O	2.51	0.43
1:K:127:ILE:HD13	1:K:139:ILE:HG21	2.00	0.43
2:L:98:ILE:CG2	2:L:102:ILE:HD11	2.22	0.43
1:A:66:ASN:HB2	6:B:4019:HOH:O	2.18	0.43
1:D:215:LEU:HD22	2:F:70:CYS:SG	2.59	0.43
2:C:80:TYR:CE1	2:C:172:GLU:HB2	2.54	0.43
1:E:139:ILE:HD12	1:E:139:ILE:O	2.17	0.43
1:G:57:PHE:CG	1:G:58:SER:N	2.86	0.43
2:C:88:LEU:H	2:C:88:LEU:CD2	2.32	0.43
1:E:175:GLU:O	1:E:182:CYS:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:165:PHE:O	2:F:166:ARG:HG3	2.18	0.43
1:H:56:LYS:HG2	2:I:198:SER:HA	2.00	0.43
1:B:198:ARG:HA	1:B:201:MET:HG3	1.99	0.43
1:E:83:LEU:HD12	1:E:83:LEU:HA	1.94	0.43
2:I:177:ARG:HH22	1:K:75:SER:HA	1.84	0.43
1:J:227:ARG:HH11	1:J:227:ARG:HG3	1.84	0.43
1:D:209:THR:C	1:D:210:LEU:HD12	2.39	0.42
1:E:142:SER:HB2	1:E:193:LEU:HB2	2.00	0.42
1:A:12:SER:O	1:A:13:GLN:HB2	2.19	0.42
1:D:60:MET:HB2	1:D:178:GLY:HA2	2.01	0.42
1:D:67:ILE:HD12	6:E:4027:HOH:O	2.18	0.42
1:E:125:ILE:HD13	1:E:125:ILE:H	1.84	0.42
1:G:17:ASP:HB3	1:G:29:HIS:CD2	2.54	0.42
2:L:99:ARG:HA	2:L:102:ILE:HD13	2.00	0.42
2:I:209:LYS:C	2:I:211:GLY:N	2.72	0.42
1:J:56:LYS:HE3	1:K:124:THR:CG2	2.49	0.42
1:J:105:ILE:HD13	1:K:202:PHE:CE2	2.52	0.42
1:B:85:THR:HB	1:B:86:PRO:CD	2.49	0.42
1:B:175:GLU:O	1:B:182:CYS:HA	2.19	0.42
1:H:101:ILE:CG2	1:H:105:ILE:HD11	2.42	0.42
2:F:165:PHE:CD2	2:F:217:ILE:HD13	2.55	0.42
1:H:101:ILE:HD12	1:H:182:CYS:SG	2.60	0.42
1:J:96:ILE:HD13	1:J:104:PHE:CZ	2.55	0.42
1:J:138:TRP:CD1	1:J:166:GLU:HG2	2.55	0.42
1:A:60:MET:HB2	1:A:178:GLY:HA2	2.02	0.42
1:A:202:PHE:CE2	2:C:102:ILE:HD12	2.53	0.42
2:C:88:LEU:N	2:C:88:LEU:HD22	2.34	0.42
1:D:92:SER:O	1:D:93:MET:HB2	2.19	0.42
2:I:174:ASN:HB3	1:K:77:ASN:HD21	1.85	0.42
1:B:92:SER:O	1:B:93:MET:HB2	2.20	0.42
1:E:125:ILE:H	1:E:125:ILE:CD1	2.33	0.42
1:B:74:ALA:HA	3:B:3012:BR:BR	2.74	0.42
2:C:209:LYS:NZ	2:F:90:MET:SD	2.80	0.42
1:E:125:ILE:HD13	1:E:125:ILE:N	2.34	0.42
1:G:122:SER:O	1:G:123:GLN:HB2	2.19	0.42
1:H:200:GLU:HA	1:H:203:LYS:HE2	2.00	0.42
2:C:173:CYS:HA	2:C:180:CYS:HA	2.01	0.42
1:D:101:ILE:HD12	1:D:182:CYS:HB2	2.01	0.42
1:E:62:PHE:HA	2:F:192:THR:HG23	2.02	0.42
2:I:99:ARG:HB3	2:I:100:PRO:HD3	2.02	0.42
1:J:35:TYR:CB	1:J:44:GLY:HA2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:77:ASN:HD22	1:J:77:ASN:HA	1.57	0.42
1:K:26:ILE:HG12	1:K:27:LEU:N	2.34	0.42
1:D:57:PHE:CD1	1:D:58:SER:N	2.88	0.41
1:D:67:ILE:CD1	1:D:67:ILE:H	2.33	0.41
1:G:139:ILE:HD11	1:G:223:GLN:OE1	2.19	0.41
1:B:28:TYR:CZ	1:B:110:VAL:HG21	2.55	0.41
1:E:102:ARG:HB3	1:E:103:PRO:HD3	2.02	0.41
2:I:56:PHE:CD1	2:I:57:SER:N	2.87	0.41
2:C:132:ARG:HG2	2:C:132:ARG:HH11	1.86	0.41
1:D:12:SER:HB3	1:D:18:PRO:HD3	2.03	0.41
2:C:213:ILE:HG22	2:C:217:ILE:CD1	2.50	0.41
2:F:94:ALA:HB2	2:F:179:THR:HG22	2.02	0.41
1:G:67:ILE:HD12	1:G:68:ASN:N	2.34	0.41
1:G:168:PHE:CE2	1:G:219:VAL:HG21	2.55	0.41
1:K:18:PRO:HG2	1:K:108:CYS:HA	2.01	0.41
1:K:85:THR:HB	1:K:86:PRO:CD	2.50	0.41
2:C:67:GLY:O	2:C:68:ASP:HB2	2.21	0.41
1:H:66:ASN:HB2	6:I:3025:HOH:O	2.20	0.41
1:A:39:ASN:HD21	1:D:150:GLY:H	1.64	0.41
1:B:58:SER:HA	2:C:200:GLN:O	2.21	0.41
1:B:179[A]:ARG:HH11	2:F:176:ALA:HB1	1.85	0.41
1:G:96:ILE:N	1:G:96:ILE:HD12	2.35	0.41
1:H:101:ILE:HD12	1:H:182:CYS:HB2	2.03	0.41
1:J:60:MET:HB2	1:J:178:GLY:HA2	2.03	0.41
1:H:75:SER:HA	2:L:177:ARG:NH2	2.35	0.41
1:A:175:GLU:O	1:A:182:CYS:HA	2.19	0.41
1:B:179[B]:ARG:CZ	2:F:76:ASN:ND2	2.83	0.41
2:C:133:SER:OG	2:C:221:GLN:NE2	2.52	0.41
1:H:205:PRO:O	1:H:207:PRO:HD3	2.21	0.41
1:K:67:ILE:HD12	1:K:68:ASN:OD1	2.20	0.41
2:C:177:ARG:HD2	1:E:179:ARG:HG2	2.03	0.41
2:C:177:ARG:HD3	6:C:3066:HOH:O	2.21	0.41
1:D:54:LEU:HD12	1:D:54:LEU:N	2.36	0.41
1:D:198:ARG:HG3	2:F:55:ARG:CZ	2.51	0.41
1:E:56:LYS:HG2	2:F:198:SER:HA	2.03	0.41
2:F:173:CYS:HA	2:F:180:CYS:HA	2.03	0.41
1:G:102:ARG:HB3	1:G:103:PRO:HD3	2.03	0.41
1:H:86:PRO:HG3	1:H:169:ARG:NH2	2.36	0.41
1:K:101:ILE:HD12	1:K:182:CYS:SG	2.61	0.41
1:K:200:GLU:HA	1:K:203:LYS:HE2	2.02	0.41
1:A:74:ALA:HA	3:A:3005:BR:BR	2.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:11:SER:O	2:C:12:GLN:HB2	2.21	0.41
1:K:6:PHE:CD2	1:K:116:MET:HG2	2.55	0.41
1:A:131:PRO:HB2	1:A:134:TRP:CD1	2.56	0.40
1:G:57:PHE:CD1	1:G:58:SER:N	2.89	0.40
1:H:5:GLY:HA3	1:H:112:GLU:OE1	2.21	0.40
1:H:168:PHE:CD1	1:H:216:ARG:HG2	2.56	0.40
1:J:176:CYS:HA	1:J:182:CYS:HA	2.03	0.40
1:J:215:LEU:HD22	2:L:70:CYS:SG	2.61	0.40
1:B:101:ILE:HD13	1:B:182:CYS:SG	2.61	0.40
2:C:15:GLN:HE21	2:C:15:GLN:HA	1.86	0.40
1:D:145:MET:HG2	1:D:191:PHE:HB2	2.02	0.40
2:F:136:ILE:HD13	2:F:136:ILE:N	2.33	0.40
1:H:122:SER:O	1:H:123:GLN:HB2	2.21	0.40
1:H:200:GLU:HG2	1:H:203:LYS:CE	2.51	0.40
1:K:25:LYS:HG2	1:K:112:GLU:HB3	2.03	0.40
1:A:196[A]:ILE:HD13	2:C:57:SER:HB2	2.03	0.40
1:B:216:ARG:CZ	3:B:3028:BR:BR	3.24	0.40
1:D:216:ARG:CZ	1:H:197:GLU:CG	2.98	0.40
2:F:135:TRP:CE2	2:F:222:VAL:HG21	2.56	0.40
1:A:113:ALA:HA	1:A:114:PRO:HD3	1.88	0.40
2:C:12:GLN:NE2	2:C:166:ARG:HD3	2.36	0.40
1:H:12:SER:O	1:H:13:GLN:HB2	2.20	0.40
1:K:139:ILE:HD13	1:K:139:ILE:N	2.34	0.40
1:D:177:HIS:HB2	1:D:179:ARG:HG2	2.03	0.40
1:G:66:ASN:HB2	6:G:4022:HOH:O	2.21	0.40
1:J:113:ALA:HA	1:J:114:PRO:HD3	1.89	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	223/229 (97%)	215 (96%)	8 (4%)	0	100	100
1	B	224/229 (98%)	216 (96%)	8 (4%)	0	100	100
1	D	224/229 (98%)	216 (96%)	7 (3%)	1 (0%)	34	30
1	E	222/229 (97%)	214 (96%)	8 (4%)	0	100	100
1	G	225/229 (98%)	216 (96%)	9 (4%)	0	100	100
1	H	223/229 (97%)	213 (96%)	10 (4%)	0	100	100
1	J	221/229 (96%)	213 (96%)	8 (4%)	0	100	100
1	K	222/229 (97%)	215 (97%)	7 (3%)	0	100	100
2	C	220/227 (97%)	209 (95%)	9 (4%)	2 (1%)	17	11
2	F	221/227 (97%)	211 (96%)	9 (4%)	1 (0%)	29	23
2	I	220/227 (97%)	207 (94%)	9 (4%)	4 (2%)	8	3
2	L	221/227 (97%)	210 (95%)	10 (4%)	1 (0%)	29	23
All	All	2666/2740 (97%)	2555 (96%)	102 (4%)	9 (0%)	41	37

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	175	GLY
2	I	21	VAL
2	I	211	GLY
2	L	175	GLY
2	I	175	GLY
2	I	210	ALA
2	C	175	GLY
2	C	198	SER
1	D	148	SER

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	191/195 (98%)	183 (96%)	8 (4%)	30	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	193/195 (99%)	190 (98%)	3 (2%)	62	67
1	D	191/195 (98%)	184 (96%)	7 (4%)	34	32
1	E	190/195 (97%)	185 (97%)	5 (3%)	46	48
1	G	192/195 (98%)	188 (98%)	4 (2%)	53	57
1	H	191/195 (98%)	188 (98%)	3 (2%)	62	67
1	J	189/195 (97%)	183 (97%)	6 (3%)	39	38
1	K	191/195 (98%)	189 (99%)	2 (1%)	76	81
2	C	187/191 (98%)	182 (97%)	5 (3%)	44	46
2	F	187/191 (98%)	183 (98%)	4 (2%)	53	57
2	I	187/191 (98%)	181 (97%)	6 (3%)	39	38
2	L	188/191 (98%)	186 (99%)	2 (1%)	73	78
All	All	2277/2324 (98%)	2222 (98%)	55 (2%)	49	51

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LYS
1	A	26	ILE
1	A	41	ARG
1	A	77	ASN
1	A	79	TYR
1	A	145	MET
1	A	174	ILE
1	A	227	ARG
1	B	26	ILE
1	B	170	SER
1	B	227	ARG
2	C	15	GLN
2	C	55	ARG
2	C	76	ASN
2	C	177	ARG
2	C	197	GLN
1	D	41	ARG
1	D	67	ILE
1	D	77	ASN
1	D	79	TYR
1	D	102	ARG
1	D	145	MET

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Mol	Chain	Res	Type
1	D	227	ARG
1	E	26	ILE
1	E	79	TYR
1	E	102	ARG
1	E	125	ILE
1	E	227	ARG
2	F	76	ASN
2	F	136	ILE
2	F	177	ARG
2	F	212	LEU
1	G	41	ARG
1	G	77	ASN
1	G	79	TYR
1	G	145	MET
1	H	79	TYR
1	H	132	THR
1	H	174	ILE
2	I	15	GLN
2	I	18	MET
2	I	76	ASN
2	I	90	MET
2	I	177	ARG
2	I	191	LEU
1	J	26	ILE
1	J	41	ARG
1	J	77	ASN
1	J	79	TYR
1	J	139	ILE
1	J	145	MET
1	K	139	ILE
1	K	227	ARG
2	L	76	ASN
2	L	136	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	37	GLN
1	A	39	ASN
1	A	45	GLN
1	A	77	ASN

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Mol	Chain	Res	Type
1	A	123	GLN
1	A	156	GLN
1	B	37	GLN
1	B	45	GLN
1	B	69	ASN
1	B	123	GLN
1	B	129	GLN
1	B	156	GLN
2	C	12	GLN
2	C	15	GLN
2	C	38	GLN
2	C	76	ASN
2	C	120	GLN
2	C	153	GLN
2	C	174	ASN
2	C	200	GLN
2	C	221	GLN
2	C	226	ASN
1	D	29	HIS
1	D	39	ASN
1	D	45	GLN
1	D	77	ASN
1	D	100	ASN
1	D	123	GLN
1	D	126	GLN
1	D	156	GLN
1	E	4	HIS
1	E	29	HIS
1	E	37	GLN
1	E	39	ASN
1	E	45	GLN
1	E	77	ASN
1	E	123	GLN
1	E	156	GLN
2	F	15	GLN
2	F	38	GLN
2	F	76	ASN
2	F	120	GLN
2	F	153	GLN
2	F	200	GLN
2	F	221	GLN
2	F	226	ASN

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Mol	Chain	Res	Type
1	G	29	HIS
1	G	39	ASN
1	G	45	GLN
1	G	77	ASN
1	G	100	ASN
1	G	123	GLN
1	G	129	GLN
1	G	156	GLN
1	H	29	HIS
1	H	37	GLN
1	H	39	ASN
1	H	45	GLN
1	H	77	ASN
1	H	123	GLN
1	H	129	GLN
1	H	156	GLN
2	I	15	GLN
2	I	38	GLN
2	I	76	ASN
2	I	120	GLN
2	I	153	GLN
2	I	216	HIS
2	I	221	GLN
2	I	226	ASN
1	J	29	HIS
1	J	39	ASN
1	J	45	GLN
1	J	77	ASN
1	J	123	GLN
1	J	126	GLN
1	J	156	GLN
1	K	29	HIS
1	K	37	GLN
1	K	39	ASN
1	K	45	GLN
1	K	69	ASN
1	K	77	ASN
1	K	123	GLN
1	K	156	GLN
1	K	218	HIS
2	L	12	GLN
2	L	15	GLN

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Mol	Chain	Res	Type
2	L	38	GLN
2	L	76	ASN
2	L	120	GLN
2	L	153	GLN
2	L	174	ASN
2	L	200	GLN
2	L	221	GLN
2	L	226	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 48 ligands modelled in this entry, 40 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GOL	K	4008	-	5,5,5	4.55	5 (100%)	5,5,5	5.75	3 (60%)
4	GOL	J	4007	-	5,5,5	4.58	5 (100%)	5,5,5	5.77	3 (60%)
4	GOL	H	4006	-	5,5,5	4.55	5 (100%)	5,5,5	5.77	3 (60%)
4	GOL	E	4004	-	5,5,5	4.53	5 (100%)	5,5,5	5.79	3 (60%)
4	GOL	G	4005	-	5,5,5	4.53	5 (100%)	5,5,5	5.75	3 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GOL	A	4001	-	5,5,5	4.55	5 (100%)	5,5,5	5.75	3 (60%)
4	GOL	B	4002	-	5,5,5	4.53	5 (100%)	5,5,5	5.75	3 (60%)
4	GOL	D	4003	-	5,5,5	4.53	5 (100%)	5,5,5	5.78	3 (60%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	K	4008	-	-	2/4/4/4	-
4	GOL	J	4007	-	-	3/4/4/4	-
4	GOL	H	4006	-	-	2/4/4/4	-
4	GOL	E	4004	-	-	2/4/4/4	-
4	GOL	G	4005	-	-	2/4/4/4	-
4	GOL	A	4001	-	-	2/4/4/4	-
4	GOL	B	4002	-	-	2/4/4/4	-
4	GOL	D	4003	-	-	3/4/4/4	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	4007	GOL	C3-C2	-7.56	1.20	1.51
4	K	4008	GOL	C3-C2	-7.53	1.20	1.51
4	E	4004	GOL	C3-C2	-7.47	1.21	1.51
4	H	4006	GOL	C3-C2	-7.47	1.21	1.51
4	A	4001	GOL	C3-C2	-7.46	1.21	1.51
4	B	4002	GOL	C3-C2	-7.45	1.21	1.51
4	D	4003	GOL	C3-C2	-7.42	1.21	1.51
4	G	4005	GOL	C3-C2	-7.42	1.21	1.51
4	J	4007	GOL	O1-C1	4.57	1.61	1.42
4	B	4002	GOL	O1-C1	4.51	1.61	1.42
4	E	4004	GOL	O1-C1	4.51	1.61	1.42
4	D	4003	GOL	O1-C1	4.50	1.61	1.42
4	A	4001	GOL	O1-C1	4.49	1.61	1.42
4	G	4005	GOL	O1-C1	4.47	1.61	1.42
4	K	4008	GOL	O1-C1	4.46	1.61	1.42
4	H	4006	GOL	O1-C1	4.43	1.61	1.42
4	D	4003	GOL	O3-C3	3.43	1.56	1.42
4	B	4002	GOL	O3-C3	3.41	1.56	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	4006	GOL	O3-C3	3.39	1.56	1.42
4	G	4005	GOL	O3-C3	3.37	1.56	1.42
4	A	4001	GOL	O3-C3	3.36	1.56	1.42
4	E	4004	GOL	O3-C3	3.34	1.56	1.42
4	K	4008	GOL	O3-C3	3.34	1.56	1.42
4	J	4007	GOL	O3-C3	3.29	1.56	1.42
4	H	4006	GOL	C1-C2	-2.99	1.39	1.51
4	J	4007	GOL	O2-C2	-2.94	1.34	1.43
4	G	4005	GOL	O2-C2	-2.88	1.34	1.43
4	K	4008	GOL	C1-C2	-2.87	1.39	1.51
4	A	4001	GOL	C1-C2	-2.86	1.39	1.51
4	G	4005	GOL	C1-C2	-2.85	1.40	1.51
4	A	4001	GOL	O2-C2	-2.84	1.34	1.43
4	B	4002	GOL	C1-C2	-2.84	1.40	1.51
4	D	4003	GOL	C1-C2	-2.84	1.40	1.51
4	H	4006	GOL	O2-C2	-2.80	1.35	1.43
4	E	4004	GOL	O2-C2	-2.77	1.35	1.43
4	J	4007	GOL	C1-C2	-2.76	1.40	1.51
4	D	4003	GOL	O2-C2	-2.75	1.35	1.43
4	E	4004	GOL	C1-C2	-2.75	1.40	1.51
4	K	4008	GOL	O2-C2	-2.72	1.35	1.43
4	B	4002	GOL	O2-C2	-2.69	1.35	1.43

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	4003	GOL	O3-C3-C2	10.52	160.63	110.20
4	E	4004	GOL	O3-C3-C2	10.47	160.42	110.20
4	H	4006	GOL	O3-C3-C2	10.43	160.23	110.20
4	K	4008	GOL	O3-C3-C2	10.42	160.14	110.20
4	B	4002	GOL	O3-C3-C2	10.41	160.13	110.20
4	J	4007	GOL	O3-C3-C2	10.41	160.11	110.20
4	G	4005	GOL	O3-C3-C2	10.41	160.09	110.20
4	A	4001	GOL	O3-C3-C2	10.38	159.97	110.20
4	A	4001	GOL	O2-C2-C3	6.83	139.19	109.12
4	E	4004	GOL	O2-C2-C3	6.82	139.15	109.12
4	H	4006	GOL	O2-C2-C3	6.82	139.15	109.12
4	G	4005	GOL	O2-C2-C3	6.80	139.09	109.12
4	J	4007	GOL	O2-C2-C3	6.78	139.00	109.12
4	K	4008	GOL	O2-C2-C3	6.77	138.94	109.12
4	B	4002	GOL	O2-C2-C3	6.73	138.76	109.12
4	D	4003	GOL	O2-C2-C3	6.72	138.72	109.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	J	4007	GOL	O1-C1-C2	3.36	126.29	110.20
4	B	4002	GOL	O1-C1-C2	3.32	126.14	110.20
4	E	4004	GOL	O1-C1-C2	3.32	126.12	110.20
4	D	4003	GOL	O1-C1-C2	3.28	125.93	110.20
4	K	4008	GOL	O1-C1-C2	3.25	125.78	110.20
4	A	4001	GOL	O1-C1-C2	3.23	125.68	110.20
4	H	4006	GOL	O1-C1-C2	3.22	125.64	110.20
4	G	4005	GOL	O1-C1-C2	3.22	125.62	110.20

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	4001	GOL	C1-C2-C3-O3
4	B	4002	GOL	C1-C2-C3-O3
4	D	4003	GOL	C1-C2-C3-O3
4	E	4004	GOL	O1-C1-C2-O2
4	E	4004	GOL	C1-C2-C3-O3
4	G	4005	GOL	O1-C1-C2-O2
4	G	4005	GOL	C1-C2-C3-O3
4	H	4006	GOL	O1-C1-C2-C3
4	H	4006	GOL	C1-C2-C3-O3
4	J	4007	GOL	O1-C1-C2-C3
4	J	4007	GOL	C1-C2-C3-O3
4	K	4008	GOL	O1-C1-C2-C3
4	K	4008	GOL	C1-C2-C3-O3
4	A	4001	GOL	O1-C1-C2-O2
4	B	4002	GOL	O1-C1-C2-O2
4	D	4003	GOL	O1-C1-C2-C3
4	J	4007	GOL	O1-C1-C2-O2
4	D	4003	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	223/229 (97%)	-0.25	1 (0%)	92	92	6, 12, 25, 35	0
1	B	224/229 (97%)	-0.15	6 (2%)	54	53	6, 12, 29, 42	0
1	D	225/229 (98%)	-0.15	4 (1%)	68	66	7, 13, 27, 40	0
1	E	224/229 (97%)	-0.15	3 (1%)	77	76	6, 12, 29, 43	0
1	G	225/229 (98%)	-0.14	1 (0%)	92	92	8, 15, 28, 39	0
1	H	224/229 (97%)	-0.12	4 (1%)	68	66	8, 14, 30, 41	0
1	J	223/229 (97%)	-0.14	2 (0%)	84	83	8, 14, 29, 39	0
1	K	224/229 (97%)	-0.10	6 (2%)	54	53	6, 14, 31, 45	0
2	C	222/227 (97%)	-0.12	3 (1%)	75	74	7, 13, 28, 39	0
2	F	223/227 (98%)	-0.07	3 (1%)	77	76	7, 12, 30, 41	0
2	I	222/227 (97%)	-0.06	7 (3%)	47	46	8, 15, 32, 44	0
2	L	222/227 (97%)	-0.15	1 (0%)	91	90	7, 14, 28, 37	0
All	All	2681/2740 (97%)	-0.13	41 (1%)	73	72	6, 14, 30, 45	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	212	LEU	7.9
2	I	212	LEU	5.5
2	C	22	GLY	4.5
2	C	21	VAL	4.3
1	E	4	HIS	3.9
2	I	18	MET	3.1
1	K	214	GLU	3.1
1	H	19	GLN	3.0
2	C	197	GLN	2.7
1	E	91	MET	2.7
1	K	229	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	6	PHE	2.6
2	I	211	GLY	2.6
1	H	197	GLU	2.6
1	D	216	ARG	2.5
1	D	91	MET	2.5
2	I	21	VAL	2.4
2	I	210	ALA	2.4
1	D	217	THR	2.4
1	B	179[A]	ARG	2.4
1	K	197	GLU	2.4
1	H	217	THR	2.4
1	K	199	SER	2.4
2	I	177	ARG	2.4
2	L	18	MET	2.4
2	I	5	TYR	2.3
1	K	200	GLU	2.3
2	F	5	TYR	2.2
1	G	91	MET	2.2
1	A	227	ARG	2.2
1	K	217	THR	2.2
1	B	197	GLU	2.2
1	H	212	ALA	2.2
1	J	213	GLY	2.2
1	D	218	HIS	2.1
1	B	229	THR	2.1
2	F	177	ARG	2.1
1	J	227	ARG	2.1
1	B	91	MET	2.0
1	B	214	GLU	2.0
1	E	216	ARG	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	K	4008	6/6	0.75	0.24	43,46,46,47	0
4	GOL	D	4003	6/6	0.76	0.19	42,42,42,43	0
4	GOL	E	4004	6/6	0.81	0.25	25,34,35,36	0
4	GOL	G	4005	6/6	0.83	0.22	38,42,44,45	0
4	GOL	B	4002	6/6	0.84	0.18	31,35,36,37	0
4	GOL	J	4007	6/6	0.85	0.19	35,37,38,38	0
4	GOL	H	4006	6/6	0.85	0.25	37,42,43,43	0
4	GOL	A	4001	6/6	0.90	0.18	31,35,36,37	0
3	BR	K	3033	1/1	0.91	0.07	46,46,46,46	1
3	BR	B	3034	1/1	0.92	0.08	43,43,43,43	1
3	BR	E	3036	1/1	0.93	0.07	53,53,53,53	1
3	BR	D	3030	1/1	0.93	0.11	39,39,39,39	1
3	BR	J	3032	1/1	0.95	0.09	37,37,37,37	1
3	BR	G	3031	1/1	0.95	0.08	37,37,37,37	1
3	BR	B	3028	1/1	0.96	0.06	29,29,29,29	1
3	BR	H	3035	1/1	0.97	0.08	53,53,53,53	1
3	BR	C	3029	1/1	0.98	0.07	30,30,30,30	1
3	BR	L	3017	1/1	0.98	0.06	22,22,22,22	1
5	LU	L	2004	1/1	0.98	0.06	34,34,34,34	1
5	LU	F	2002	1/1	0.99	0.05	42,42,42,42	1
5	LU	I	2003	1/1	0.99	0.05	36,36,36,36	1
5	LU	C	2001	1/1	0.99	0.04	37,37,37,37	1
3	BR	H	3011	1/1	1.00	0.06	17,17,17,17	0
3	BR	H	3020	1/1	1.00	0.04	20,20,20,20	1
3	BR	B	3026	1/1	1.00	0.06	32,32,32,32	1
3	BR	I	3014	1/1	1.00	0.06	18,18,18,18	0
3	BR	I	3023	1/1	1.00	0.04	24,24,24,24	1
3	BR	I	3024	1/1	1.00	0.05	23,23,23,23	1
3	BR	J	3008	1/1	1.00	0.06	16,16,16,16	0
3	BR	A	3001	1/1	1.00	0.07	16,16,16,16	0
3	BR	K	3009	1/1	1.00	0.07	18,18,18,18	0
3	BR	K	3027	1/1	1.00	0.05	34,34,34,34	1
3	BR	A	3002	1/1	1.00	0.05	15,15,15,15	0
3	BR	L	3010	1/1	1.00	0.05	18,18,18,18	0
3	BR	C	3007	1/1	1.00	0.05	15,15,15,15	0
3	BR	L	3025	1/1	1.00	0.04	22,22,22,22	1
3	BR	C	3018	1/1	1.00	0.04	21,21,21,21	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	BR	C	3019	1/1	1.00	0.04	19,19,19,19	1
3	BR	A	3004	1/1	1.00	0.07	14,14,14,14	0
3	BR	A	3005	1/1	1.00	0.07	14,14,14,14	0
3	BR	E	3003	1/1	1.00	0.06	16,16,16,16	0
3	BR	B	3012	1/1	1.00	0.06	18,18,18,18	0
3	BR	F	3013	1/1	1.00	0.06	15,15,15,15	0
3	BR	F	3022	1/1	1.00	0.05	20,20,20,20	1
3	BR	G	3015	1/1	1.00	0.06	15,15,15,15	0
3	BR	G	3016	1/1	1.00	0.05	17,17,17,17	0
3	BR	B	3021	1/1	1.00	0.05	23,23,23,23	1
3	BR	H	3006	1/1	1.00	0.07	17,17,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.