Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2023 – 05:48 PM EDT

PDB ID	:	3M7N
Title	:	archaeoglobus fulgidus exosome with RNA bound to the active site
Authors	:	Hartung, S.; Hopfner, K.-P.
Deposited on	:	2010-03-16
Resolution	:	2.40 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:

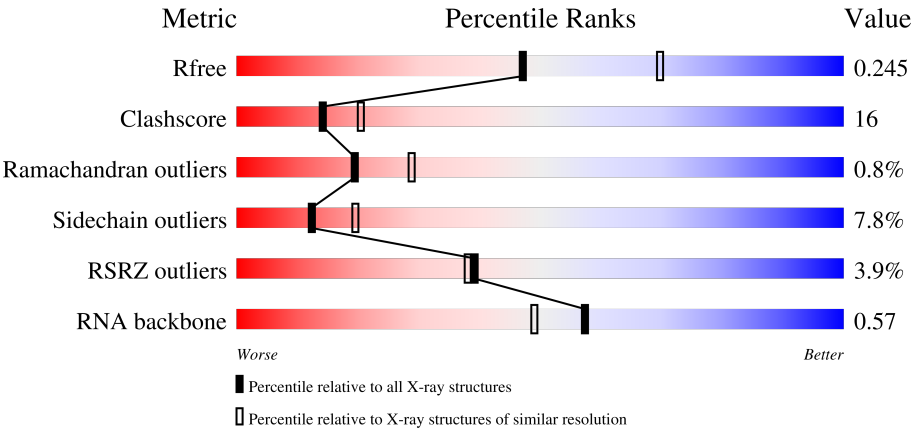
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)
RNA backbone	3102	1174 (2.80-2.00)

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	179	4% 69% 28%
1	B	179	16% 66% 33%
1	C	179	11% 73% 26%
2	D	258	62% 29% 6%

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Mol	Chain	Length	Quality of chain
2	E	258	2% 65% 29%
2	F	258	% 69% 23% 5%
3	G	259	3% 62% 31% 5%
3	H	259	% 69% 25% 5%
3	I	259	2% 66% 30%
4	X	6	17% 67% 17% 17%
4	Y	6	17% 17% 50% 17% 17%
4	Z	6	67% 33%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 16859 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 Putative uncharacterized protein AF_0206.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	179	Total	C	N	O	S	28	0	0
			1371	855	242	266	8			
1	B	179	Total	C	N	O	S	44	0	0
			1371	855	242	266	8			
1	C	179	Total	C	N	O	S	31	0	0
			1371	855	242	266	8			

- Molecule 2 is a protein called Probable exosome complex exonuclease 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	243	Total	C	N	O	S	12	0	0
			1902	1198	334	357	13			
2	E	248	Total	C	N	O	S	7	0	0
			1944	1224	340	367	13			
2	F	246	Total	C	N	O	S	16	0	0
			1926	1213	337	363	13			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	65	GLU	ARG	engineered mutation	UNP O29757
E	65	GLU	ARG	engineered mutation	UNP O29757
F	65	GLU	ARG	engineered mutation	UNP O29757

- Molecule 3 is a protein called Probable exosome complex exonuclease 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	254	Total	C	N	O	S	9	0	0
			1971	1245	327	394	5			
3	H	258	Total	C	N	O	S	14	0	0
			2005	1266	331	403	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	258	Total	C	N	O	S	11	0	0
			2005	1266	331	403	5			

- Molecule 4 is a RNA chain called 5'-R(*C*UP*CP*CP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	X	5	Total	C	N	O	P	0	0	0
			97	45	14	34	4			
4	Y	5	Total	C	N	O	P	0	0	0
			100	45	14	36	5			
4	Z	4	Total	C	N	O	P	0	0	0
			77	36	12	26	3			

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		
5	B	1	Total	Zn	0	0
			1	1		
5	C	1	Total	Zn	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	30	Total	O	0	0
			30	30		
6	B	7	Total	O	0	0
			7	7		
6	C	38	Total	O	0	0
			38	38		
6	D	63	Total	O	0	0
			63	63		
6	E	99	Total	O	0	0
			99	99		
6	F	136	Total	O	0	0
			136	136		
6	G	66	Total	O	0	0
			66	66		
6	H	126	Total	O	0	0
			126	126		

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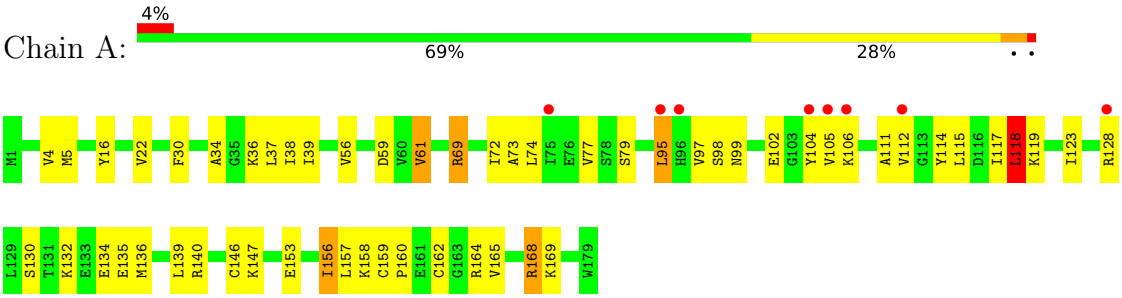
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	I	136	Total O 136 136	0	0
6	X	5	Total O 5 5	0	0
6	Y	7	Total O 7 7	0	0
6	Z	3	Total O 3 3	0	0

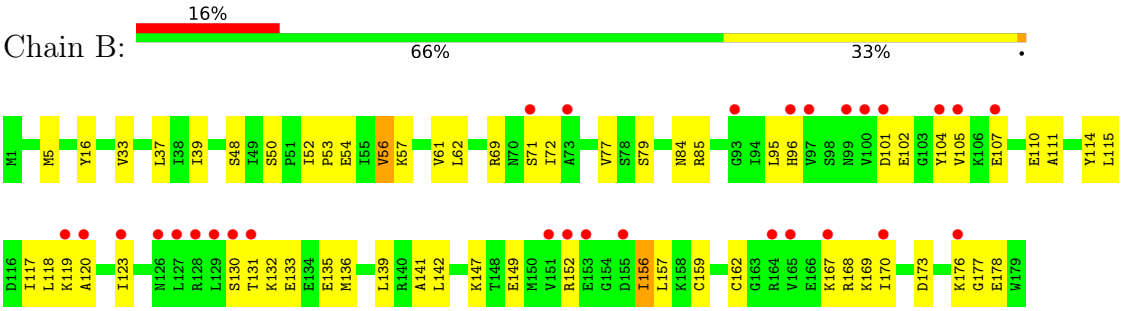
3 Residue-property plots (i)

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.

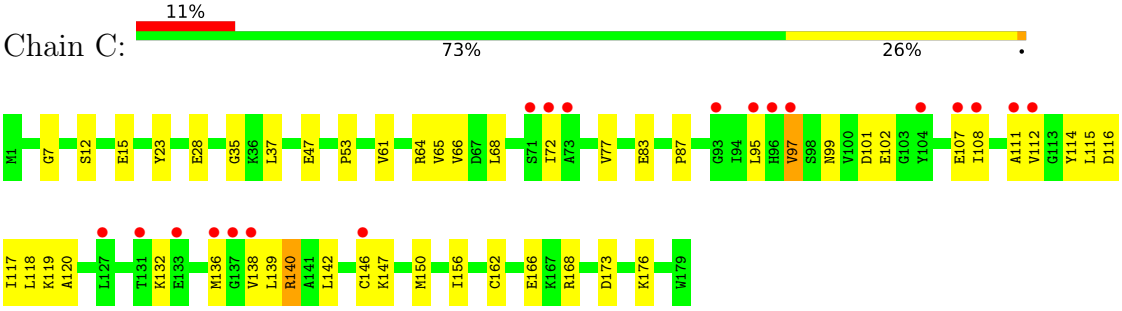
• Molecule 1: Putative uncharacterized protein AF_0206



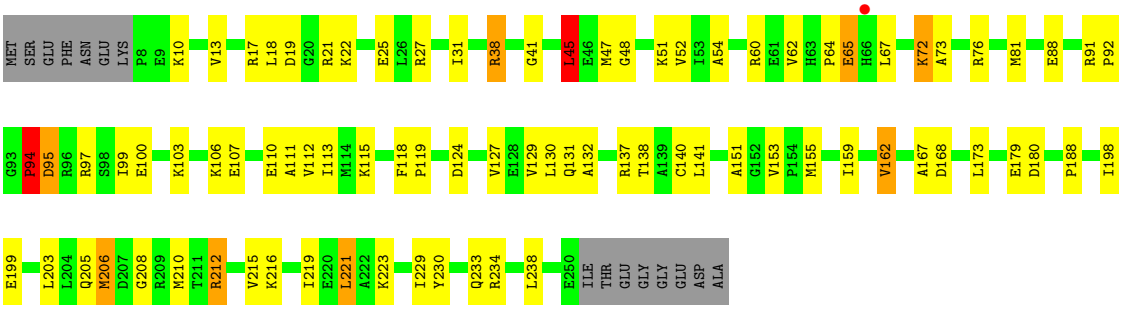
• Molecule 1: Putative uncharacterized protein AF_0206



• Molecule 1: Putative uncharacterized protein AF_0206

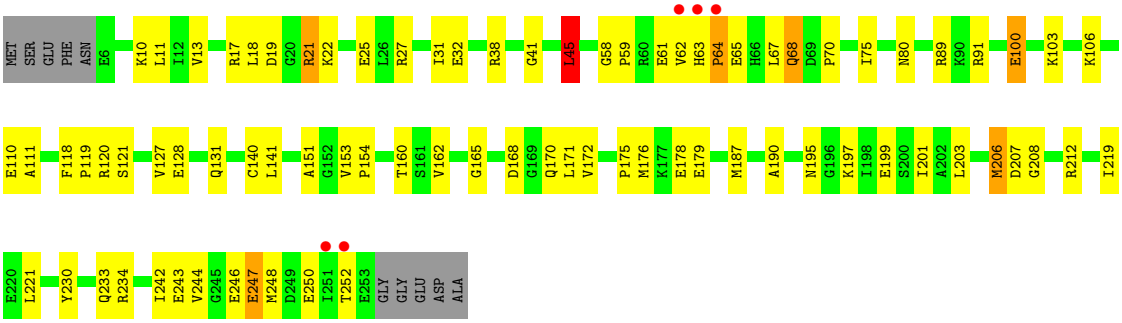


• Molecule 2: Probable exosome complex exonuclease 1



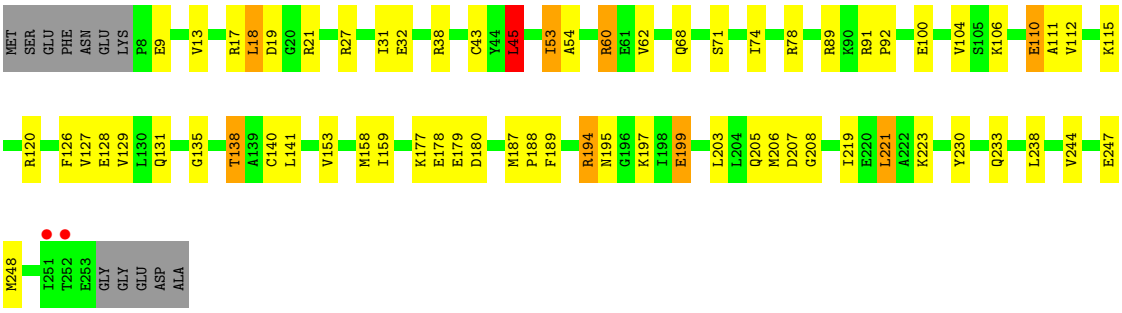
• Molecule 2: Probable exosome complex exonuclease 1

Chain E:



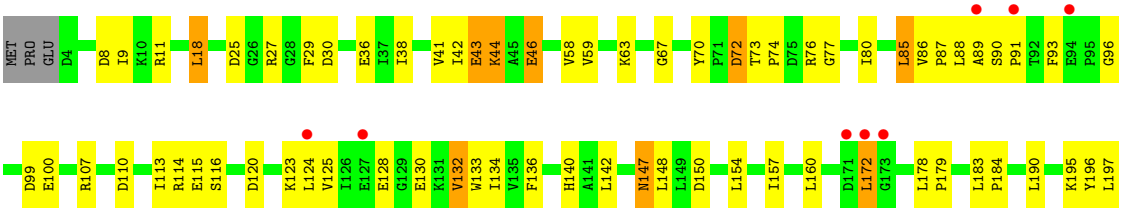
• Molecule 2: Probable exosome complex exonuclease 1

Chain F:

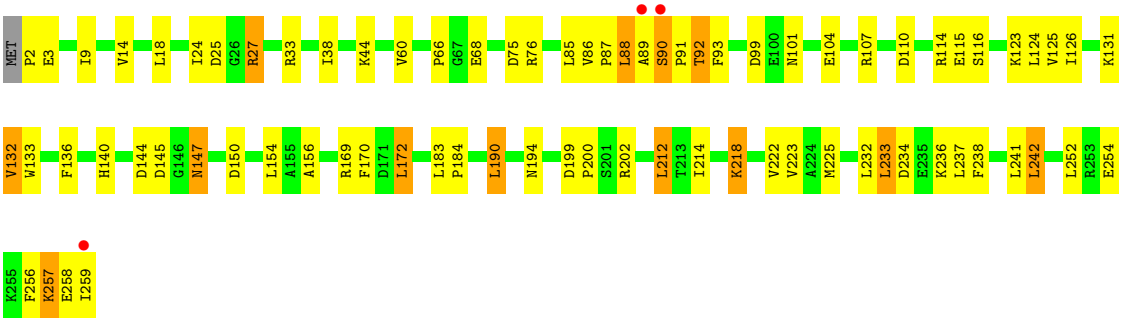


• Molecule 3: Probable exosome complex exonuclease 2

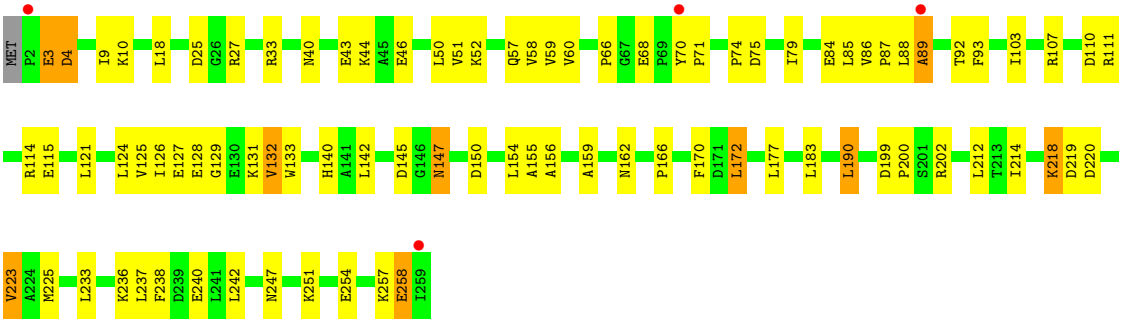
Chain G:



• Molecule 3: Probable exosome complex exonuclease 2

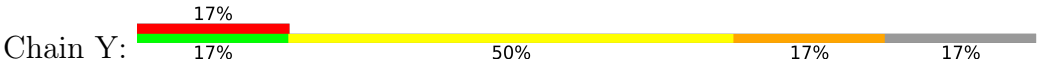


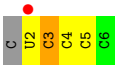
• Molecule 3: Probable exosome complex exonuclease 2



• Molecule 4: 5'-R(*C*UP*CP*CP*CP*C)-3'

• Molecule 4: 5'-R(*C*UP*CP*CP*CP*C)-3'





• Molecule 4: 5'-R(*C*UP*CP*CP*CP*C)-3'


C
U
C3
C6

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α, β, γ	138.27Å 138.27Å 262.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.06 – 2.40 48.89 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.06-2.40) 99.7 (48.89-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.88 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.4_129)	Depositor
R, R_{free}	0.197 , 0.256 0.187 , 0.245	Depositor DCC
R_{free} test set	5026 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	42.3	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 51.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16859	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.89% 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: ZN

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	0.31	0/1385	0.53	1/1855 (0.1%)
1	B	0.29	0/1385	0.48	0/1855
1	C	0.33	0/1385	0.52	0/1855
2	D	0.42	0/1929	0.61	1/2588 (0.0%)
2	E	0.45	0/1971	0.62	1/2645 (0.0%)
2	F	0.47	0/1953	0.63	1/2621 (0.0%)
3	G	0.39	0/1999	0.57	0/2713
3	H	0.46	0/2034	0.64	1/2759 (0.0%)
3	I	0.45	0/2034	0.62	0/2759
4	X	0.67	0/106	1.14	0/162
4	Y	0.67	0/109	1.20	0/166
4	Z	0.55	0/84	1.24	0/128
All	All	0.42	0/16374	0.61	5/22106 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	45	LEU	CA-CB-CG	8.24	134.26	115.30
2	F	45	LEU	CA-CB-CG	6.66	130.62	115.30
2	E	45	LEU	CA-CB-CG	6.38	129.97	115.30
1	A	118	LEU	CA-CB-CG	5.71	128.43	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	27	ARG	NE-CZ-NH1	-5.38	117.61	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	94	PRO	Peptide

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	1371	0	1409	35	0
1	B	1371	0	1410	43	0
1	C	1371	0	1409	32	0
2	D	1902	0	1948	69	0
2	E	1944	0	1990	83	0
2	F	1926	0	1972	65	0
3	G	1971	0	1994	90	0
3	H	2005	0	2025	73	0
3	I	2005	0	2025	79	0
4	X	97	0	56	2	0
4	Y	100	0	55	4	0
4	Z	77	0	46	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	A	30	0	0	0	0
6	B	7	0	0	0	0
6	C	38	0	0	1	0
6	D	63	0	0	0	0
6	E	99	0	0	6	0
6	F	136	0	0	8	0
6	G	66	0	0	2	0
6	H	126	0	0	1	0
6	I	136	0	0	1	0
6	X	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	Y	7	0	0	1	0
6	Z	3	0	0	0	0
All	All	16859	0	16339	500	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 16.

All (500) 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:E:61:GLU:HB3	2:E:63:HIS:HB3	1.34	1.06
2:E:62:VAL:H	2:E:63:HIS:HB2	1.25	0.99
2:E:19:ASP:OD2	2:E:21:ARG:HD3	1.63	0.98
3:G:43:GLU:O	3:G:44:LYS:HB2	1.65	0.96
3:G:214:ILE:HG12	3:G:225:MET:HE3	1.48	0.94
2:E:62:VAL:N	2:E:63:HIS:HB2	1.83	0.93
2:E:62:VAL:HG13	2:E:68:GLN:OE1	1.68	0.93
2:E:61:GLU:HB3	2:E:63:HIS:CB	1.97	0.92
2:D:38:ARG:HG3	3:I:202:ARG:HH11	1.31	0.91
2:E:206:MET:CE	3:H:222:VAL:HG12	2.00	0.91
1:B:123:ILE:HD13	1:B:130:SER:HB2	1.56	0.84
1:A:123:ILE:HG13	1:A:128:ARG:HG2	1.59	0.83
2:E:10:LYS:HG2	2:E:13:VAL:HG12	1.59	0.82
2:E:31:ILE:HG12	2:E:45:LEU:HD22	1.61	0.82
2:E:206:MET:HE2	3:H:222:VAL:HG12	1.61	0.82
3:I:115:GLU:HB2	3:I:223:VAL:HG13	1.59	0.82
3:I:114:ARG:HB2	3:I:114:ARG:HH21	1.44	0.82
2:D:100:GLU:HG2	3:G:107:ARG:NH2	1.95	0.82
1:A:99:ASN:HA	1:A:132:LYS:HE3	1.61	0.81
3:I:46:GLU:HG2	3:I:166:PRO:HG3	1.62	0.81
3:G:115:GLU:HB2	3:G:223:VAL:HG13	1.63	0.79
2:E:32:GLU:HG3	6:E:490:HOH:O	1.82	0.79
3:I:88:LEU:HD23	3:I:88:LEU:O	1.84	0.78
2:E:128:GLU:HG2	3:G:140:HIS:CE1	2.19	0.78
2:F:31:ILE:HG12	2:F:45:LEU:HD22	1.66	0.77
2:F:131:GLN:NE2	3:H:44:LYS:H	1.82	0.76
2:D:212:ARG:HH21	2:D:216:LYS:NZ	1.84	0.76
1:B:111:ALA:O	1:B:168:ARG:HB2	1.84	0.76
2:D:103:LYS:HD2	3:G:100:GLU:HG2	1.68	0.75
2:E:22:LYS:HD3	2:E:25:GLU:OE1	1.87	0.75
1:B:159:CYS:SG	1:B:162:CYS:HB3	2.27	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:125:VAL:HA	3:H:132:VAL:HG23	1.70	0.73
2:E:63:HIS:CG	2:E:64:PRO:HA	2.23	0.73
1:C:111:ALA:O	1:C:168:ARG:HB2	1.89	0.73
2:D:206:MET:HG2	3:G:225:MET:HG3	1.70	0.73
2:D:106:LYS:HE2	2:D:110:GLU:OE2	1.90	0.72
3:G:247:ASN:HD22	3:G:250:ARG:HH11	1.37	0.72
1:B:156:ILE:HD11	1:B:167:LYS:HB2	1.72	0.72
2:F:128:GLU:HG2	3:H:140:HIS:CE1	2.24	0.72
2:F:128:GLU:HG2	3:H:140:HIS:HE1	1.54	0.72
1:A:117:ILE:HD12	1:A:140:ARG:HD3	1.72	0.71
1:B:5:MET:HG3	2:E:234:ARG:HG3	1.72	0.71
3:I:114:ARG:HB2	3:I:114:ARG:NH2	2.05	0.71
2:D:206:MET:CG	3:G:225:MET:HG3	2.20	0.70
2:D:131:GLN:NE2	3:I:44:LYS:H	1.89	0.70
2:E:80:ASN:ND2	2:E:128:GLU:OE2	2.24	0.70
3:H:110:ASP:OD2	3:H:114:ARG:NH2	2.25	0.70
2:D:31:ILE:HG12	2:D:45:LEU:HD22	1.72	0.70
2:E:63:HIS:CD2	2:E:64:PRO:HA	2.27	0.69
3:H:86:VAL:HG23	3:H:88:LEU:HB3	1.75	0.69
1:C:119:LYS:HB2	1:C:139:LEU:HD11	1.75	0.68
2:D:230:TYR:HA	2:D:233:GLN:HE21	1.56	0.68
2:F:19:ASP:OD2	2:F:21:ARG:HD3	1.92	0.68
2:D:81:MET:SD	2:D:97:ARG:NH2	2.67	0.68
3:G:125:VAL:HA	3:G:132:VAL:HG23	1.75	0.68
3:G:247:ASN:ND2	3:G:250:ARG:NH1	2.43	0.67
2:E:19:ASP:OD1	2:E:21:ARG:HG2	1.95	0.67
3:I:59:VAL:HG23	3:I:142:LEU:HD11	1.76	0.67
2:E:206:MET:HE3	3:H:222:VAL:HG12	1.74	0.66
2:E:230:TYR:HA	2:E:233:GLN:HE21	1.61	0.65
3:I:59:VAL:HG23	3:I:142:LEU:CD1	2.26	0.65
3:I:110:ASP:OD2	3:I:114:ARG:NH2	2.29	0.65
1:B:16:TYR:CE2	1:B:39:ILE:HD13	2.33	0.64
3:G:247:ASN:ND2	3:G:250:ARG:HH11	1.95	0.64
1:B:53:PRO:HD3	1:B:85:ARG:HG2	1.79	0.64
3:G:18:LEU:HD22	3:G:195:LYS:HD3	1.79	0.64
3:G:116:SER:OG	3:G:184:PRO:HG3	1.98	0.64
1:B:159:CYS:SG	1:B:162:CYS:N	2.69	0.64
3:I:237:LEU:O	3:I:237:LEU:HD23	1.98	0.63
1:B:71:SER:HB2	1:B:96:HIS:CE1	2.32	0.63
3:G:87:PRO:HA	3:G:93:PHE:HB2	1.80	0.63
1:C:117:ILE:HG21	3:H:9:ILE:HD11	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:22:LYS:HG3	2:D:25:GLU:OE2	1.99	0.63
2:F:53:ILE:HG23	3:H:88:LEU:HD11	1.81	0.63
2:F:89:ARG:HD2	3:H:136:PHE:CG	2.34	0.63
1:A:99:ASN:HA	1:A:132:LYS:CE	2.29	0.62
2:F:127:VAL:HG11	2:F:140:CYS:HB3	1.81	0.62
1:A:119:LYS:HB2	1:A:139:LEU:HD11	1.81	0.62
1:B:53:PRO:HG2	1:B:85:ARG:O	1.99	0.62
3:G:220:ASP:OD2	3:G:250:ARG:NH2	2.30	0.62
2:D:212:ARG:HH21	2:D:216:LYS:HZ2	1.47	0.62
2:F:53:ILE:HD13	2:F:54:ALA:N	2.14	0.62
3:I:25:ASP:OD2	3:I:27:ARG:HD3	2.00	0.62
3:I:46:GLU:CG	3:I:166:PRO:HG3	2.28	0.62
1:B:85:ARG:NH2	2:E:151:ALA:O	2.29	0.61
2:F:13:VAL:O	2:F:13:VAL:HG23	1.99	0.61
3:G:247:ASN:HD22	3:G:250:ARG:NH1	1.98	0.61
3:G:38:ILE:N	3:G:38:ILE:HD12	2.15	0.61
3:G:25:ASP:OD2	3:G:27:ARG:HD3	2.00	0.61
3:G:110:ASP:OD2	3:G:114:ARG:NH2	2.34	0.61
3:G:120:ASP:HB3	3:G:123:LYS:HD2	1.82	0.61
2:F:112:VAL:HG21	2:F:159:ILE:HD11	1.82	0.60
2:F:138:THR:HG21	6:F:300:HOH:O	2.00	0.60
1:C:150:MET:HE1	1:C:166:GLU:HB2	1.83	0.60
2:D:212:ARG:HG2	3:G:242:LEU:HD13	1.83	0.60
2:D:95:ASP:O	2:D:99:ILE:HG12	2.02	0.60
3:I:59:VAL:CG2	3:I:142:LEU:HD11	2.32	0.60
2:D:127:VAL:HG11	2:D:140:CYS:SG	2.41	0.60
2:E:10:LYS:HG2	2:E:13:VAL:CG1	2.28	0.60
1:B:117:ILE:HG21	3:G:9:ILE:HD11	1.84	0.60
2:E:61:GLU:CB	2:E:63:HIS:HB3	2.22	0.60
1:B:114:TYR:CD2	1:B:115:LEU:HG	2.36	0.59
2:E:141:LEU:HD11	2:E:203:LEU:HD13	1.84	0.59
3:G:214:ILE:HG12	3:G:225:MET:CE	2.28	0.59
3:G:107:ARG:NH1	4:Y:5:C:OP1	2.35	0.59
2:D:60:ARG:HD3	2:D:124:ASP:OD1	2.02	0.59
2:D:38:ARG:HG3	3:I:202:ARG:NH1	2.10	0.59
3:H:169:ARG:HD2	3:H:170:PHE:CE2	2.37	0.58
3:I:107:ARG:NH1	4:X:5:C:OP2	2.36	0.58
1:C:118:LEU:HD21	1:C:120:ALA:HB2	1.85	0.58
1:B:173:ASP:HA	1:B:176:LYS:HD2	1.85	0.58
3:G:58:VAL:HG22	3:G:148:LEU:HD23	1.86	0.58
2:E:206:MET:HE1	3:H:223:VAL:C	2.23	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:VAL:HG21	1:C:168:ARG:HD3	1.86	0.58
2:E:64:PRO:HD2	2:E:67:LEU:HB2	1.85	0.57
3:I:218:LYS:HD3	6:I:282:HOH:O	2.04	0.57
3:G:242:LEU:O	3:G:246:ILE:HG13	2.04	0.57
3:H:256:PHE:C	3:H:258:GLU:H	2.08	0.57
1:B:118:LEU:HD21	1:B:120:ALA:HB2	1.86	0.57
2:F:230:TYR:HA	2:F:233:GLN:HE21	1.69	0.57
2:F:111:ALA:HA	6:F:516:HOH:O	2.05	0.57
1:A:147:LYS:HE3	2:F:71:SER:HA	1.87	0.56
1:A:157:LEU:HD12	1:A:168:ARG:HD2	1.86	0.56
2:E:61:GLU:HB3	2:E:63:HIS:HB2	1.86	0.56
2:E:89:ARG:HD2	3:G:136:PHE:CG	2.40	0.56
2:F:17:ARG:HD2	2:F:179:GLU:OE1	2.04	0.56
2:D:19:ASP:OD1	2:D:21:ARG:HG3	2.05	0.56
2:F:127:VAL:HG11	2:F:140:CYS:CB	2.34	0.56
3:G:72:ASP:O	3:G:74:PRO:HD3	2.05	0.56
3:H:91:PRO:HD2	3:H:202:ARG:HH12	1.69	0.56
2:E:17:ARG:HD3	2:E:179:GLU:OE1	2.05	0.56
3:I:214:ILE:HG12	3:I:225:MET:HE3	1.88	0.56
3:G:67:GLY:HA3	3:G:134:ILE:HD11	1.87	0.56
3:I:257:LYS:O	3:I:258:GLU:HB3	2.06	0.56
2:F:126:PHE:CE2	3:H:87:PRO:HB2	2.41	0.56
2:F:128:GLU:CG	3:H:140:HIS:CE1	2.88	0.56
3:G:147:ASN:ND2	3:G:150:ASP:H	2.04	0.56
3:H:214:ILE:HG12	3:H:225:MET:HE2	1.87	0.55
2:F:100:GLU:HG2	6:F:640:HOH:O	2.06	0.55
3:G:196:TYR:HD2	3:G:237:LEU:HD21	1.72	0.55
1:C:99:ASN:HA	1:C:132:LYS:HE3	1.87	0.55
2:D:100:GLU:HG2	3:G:107:ARG:HH22	1.72	0.55
1:B:142:LEU:HD23	1:B:149:GLU:HA	1.90	0.54
2:E:207:ASP:HB2	3:H:115:GLU:HG3	1.88	0.54
3:H:225:MET:HE1	3:H:238:PHE:CE1	2.42	0.54
2:E:10:LYS:O	2:E:11:LEU:HB2	2.07	0.54
3:I:124:LEU:HB3	3:I:133:TRP:HB2	1.89	0.54
1:C:68:LEU:HD22	1:C:108:ILE:HG23	1.90	0.54
2:F:188:PRO:HD2	2:F:205:GLN:O	2.08	0.54
3:H:190:LEU:HB2	3:H:200:PRO:HB3	1.90	0.54
2:E:62:VAL:N	2:E:63:HIS:CB	2.66	0.54
3:I:170:PHE:HB2	3:I:172:LEU:HD22	1.90	0.54
1:C:119:LYS:HG2	1:C:136:MET:SD	2.48	0.54
1:C:28:GLU:OE2	1:C:28:GLU:HA	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:127:VAL:CG1	2:D:140:CYS:SG	2.96	0.53
2:F:244:VAL:O	2:F:247:GLU:HG2	2.08	0.53
3:G:113:ILE:HD12	3:G:160:LEU:CD1	2.38	0.53
3:H:110:ASP:CG	3:H:114:ARG:HH22	2.10	0.53
2:D:22:LYS:HB2	2:D:25:GLU:HG3	1.91	0.53
2:F:78:ARG:HD2	6:F:336:HOH:O	2.07	0.53
2:E:62:VAL:HB	2:E:63:HIS:HA	1.89	0.53
2:E:62:VAL:HG11	2:E:65:GLU:HA	1.90	0.53
3:H:123:LYS:HD2	6:H:324:HOH:O	2.09	0.53
1:B:69:ARG:HB2	1:B:72:ILE:O	2.08	0.53
1:C:53:PRO:HG2	1:C:87:PRO:HA	1.91	0.53
2:D:110:GLU:HB3	2:D:115:LYS:HZ3	1.74	0.53
2:E:195:ASN:HA	6:E:272:HOH:O	2.08	0.53
2:F:128:GLU:CG	3:H:140:HIS:HE1	2.20	0.53
2:F:207:ASP:OD1	3:I:111:ARG:HG2	2.10	0.52
3:G:29:PHE:O	3:G:198:VAL:HG23	2.09	0.52
1:B:119:LYS:HB2	1:B:139:LEU:HD11	1.91	0.52
3:I:33:ARG:CD	3:I:199:ASP:OD1	2.57	0.52
2:F:199:GLU:CG	6:F:295:HOH:O	2.57	0.52
3:G:42:ILE:HG22	3:G:42:ILE:O	2.08	0.52
1:A:73:ALA:HB3	1:A:95:LEU:HB3	1.92	0.52
1:A:117:ILE:HG21	3:I:9:ILE:HD11	1.91	0.52
2:E:63:HIS:CE1	2:E:64:PRO:HA	2.45	0.52
3:I:87:PRO:HA	3:I:93:PHE:HB2	1.91	0.52
1:C:97:VAL:HG13	1:C:108:ILE:HB	1.91	0.52
3:I:237:LEU:HD23	3:I:237:LEU:C	2.31	0.52
1:A:69:ARG:HD2	1:A:69:ARG:N	2.22	0.52
2:F:131:GLN:HE21	3:H:44:LYS:H	1.56	0.52
2:D:141:LEU:HD11	2:D:203:LEU:HD13	1.92	0.52
2:E:131:GLN:HE21	3:G:42:ILE:HG23	1.74	0.52
3:H:116:SER:OG	3:H:184:PRO:HG3	2.10	0.51
2:E:75:ILE:O	2:E:106:LYS:HD2	2.11	0.51
2:F:197:LYS:HE2	6:F:784:HOH:O	2.10	0.51
3:G:244:VAL:O	3:G:247:ASN:HB2	2.10	0.51
3:I:88:LEU:O	3:I:89:ALA:HB2	2.11	0.51
1:B:111:ALA:HA	1:B:168:ARG:HA	1.92	0.51
2:E:38:ARG:HD2	6:G:887:HOH:O	2.10	0.51
3:I:92:THR:HG22	3:I:92:THR:O	2.11	0.51
3:I:125:VAL:HA	3:I:132:VAL:CG2	2.41	0.51
2:E:131:GLN:NE2	3:G:43:GLU:O	2.43	0.51
2:F:126:PHE:CD2	3:H:87:PRO:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:27:ARG:NH1	3:H:199:ASP:HB3	2.26	0.51
3:I:103:ILE:O	3:I:107:ARG:HG3	2.10	0.51
1:B:133:GLU:HB2	1:B:136:MET:HG2	1.92	0.50
1:A:61:VAL:HG13	1:A:77:VAL:HG13	1.94	0.50
1:B:141:ALA:HB1	1:B:168:ARG:HH11	1.77	0.50
3:I:52:LYS:HG2	3:I:57:GLN:HG2	1.94	0.50
2:D:132:ALA:O	3:I:44:LYS:HE3	2.12	0.50
3:G:196:TYR:C	3:G:197:LEU:HD12	2.31	0.50
3:H:257:LYS:C	3:H:259:ILE:H	2.14	0.50
3:I:114:ARG:HH21	3:I:114:ARG:CB	2.18	0.50
3:I:125:VAL:HA	3:I:132:VAL:HG23	1.94	0.50
1:C:65:VAL:HG21	1:C:112:VAL:HG12	1.92	0.50
2:D:131:GLN:HE21	3:I:44:LYS:H	1.58	0.50
3:G:115:GLU:CB	3:G:223:VAL:HG13	2.39	0.50
2:D:212:ARG:HH21	2:D:216:LYS:HZ1	1.55	0.50
3:G:8:ASP:O	3:G:11:ARG:HB3	2.12	0.50
3:H:33:ARG:HD3	3:H:199:ASP:OD1	2.12	0.50
3:H:75:ASP:C	3:H:76:ARG:HG2	2.32	0.50
2:E:63:HIS:CG	2:E:64:PRO:CA	2.94	0.50
2:E:127:VAL:HG11	2:E:140:CYS:HB3	1.93	0.49
3:G:251:LYS:O	3:G:254:GLU:HG2	2.12	0.49
2:F:187:MET:CE	2:F:189:PHE:CZ	2.95	0.49
3:H:110:ASP:CG	3:H:114:ARG:NH2	2.65	0.49
3:I:40:ASN:ND2	3:I:162:ASN:HD22	2.09	0.49
3:I:79:ILE:HD11	3:I:121:LEU:HD21	1.94	0.49
1:A:97:VAL:HG11	1:A:105:VAL:O	2.12	0.49
3:I:66:PRO:HD2	3:I:170:PHE:CE2	2.46	0.49
2:D:112:VAL:HG21	2:D:159:ILE:HD11	1.93	0.49
3:I:127:GLU:O	3:I:129:GLY:N	2.46	0.49
3:I:225:MET:HE2	3:I:238:PHE:CE1	2.48	0.49
1:A:5:MET:HG3	2:D:234:ARG:HG3	1.94	0.49
2:D:13:VAL:O	2:D:13:VAL:HG23	2.12	0.49
2:E:127:VAL:HG11	2:E:140:CYS:CB	2.42	0.49
2:F:208:GLY:H	3:I:115:GLU:HG3	1.77	0.49
1:C:65:VAL:HG21	1:C:112:VAL:CG1	2.43	0.49
1:C:146:CYS:O	1:C:147:LYS:HB2	2.12	0.49
2:D:51:LYS:HE3	3:I:43:GLU:OE1	2.13	0.49
2:D:127:VAL:HG11	2:D:140:CYS:CB	2.42	0.49
2:F:17:ARG:CD	2:F:179:GLU:OE1	2.61	0.49
1:C:173:ASP:HA	1:C:176:LYS:HD2	1.94	0.49
3:I:236:LYS:HE2	3:I:240:GLU:OE1	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:TYR:O	1:A:115:LEU:HB2	2.12	0.49
1:B:131:THR:C	1:B:133:GLU:H	2.15	0.49
3:H:126:ILE:HD13	3:H:172:LEU:HD21	1.95	0.49
2:E:206:MET:HE1	3:H:223:VAL:CA	2.43	0.48
3:G:67:GLY:HA3	3:G:134:ILE:CD1	2.43	0.48
3:H:234:ASP:OD1	3:H:236:LYS:HB3	2.13	0.48
1:A:123:ILE:HD13	1:A:130:SER:HB2	1.96	0.48
1:A:22:VAL:HG13	1:A:30:PHE:O	2.13	0.48
2:F:199:GLU:HG2	6:F:295:HOH:O	2.13	0.48
2:E:111:ALA:HB1	3:H:232:LEU:HG	1.96	0.48
3:H:2:PRO:HD2	3:H:3:GLU:OE1	2.13	0.48
2:E:247:GLU:HG2	2:E:247:GLU:O	2.12	0.48
3:G:197:LEU:HD12	3:G:197:LEU:N	2.28	0.48
3:H:33:ARG:CD	3:H:199:ASP:OD1	2.61	0.48
1:C:142:LEU:HD22	1:C:147:LYS:O	2.14	0.48
2:D:65:GLU:C	2:D:67:LEU:H	2.16	0.48
2:F:19:ASP:OD2	2:F:21:ARG:CD	2.62	0.48
3:G:11:ARG:HG3	3:G:207:VAL:HA	1.96	0.48
1:A:153:GLU:OE1	1:A:158:LYS:HD2	2.14	0.48
3:I:225:MET:HE1	3:I:238:PHE:CZ	2.49	0.48
3:H:147:ASN:ND2	3:H:150:ASP:H	2.11	0.47
2:F:53:ILE:HD12	3:H:88:LEU:HD11	1.96	0.47
3:G:219:ASP:O	3:G:220:ASP:HB2	2.14	0.47
3:I:33:ARG:HD3	3:I:199:ASP:OD1	2.13	0.47
2:E:128:GLU:HG2	3:G:140:HIS:HE1	1.75	0.47
1:B:57:LYS:HE3	1:B:123:ILE:O	2.14	0.47
2:D:103:LYS:HD2	3:G:100:GLU:CG	2.40	0.47
2:D:188:PRO:HD2	2:D:205:GLN:O	2.14	0.47
2:E:128:GLU:CG	3:G:140:HIS:CE1	2.94	0.47
2:F:158:MET:HG3	2:F:230:TYR:HE1	1.80	0.47
3:G:178:LEU:HD12	3:G:179:PRO:HD2	1.97	0.47
1:A:102:GLU:HB2	1:A:132:LYS:HD3	1.97	0.47
1:A:119:LYS:HE2	1:A:135:GLU:HG2	1.95	0.47
2:D:173:LEU:HD13	2:D:221:LEU:HD22	1.96	0.47
2:F:247:GLU:CG	2:F:248:MET:N	2.77	0.47
3:G:77:GLY:HA2	3:G:132:VAL:CG1	2.45	0.47
1:C:72:ILE:C	1:C:108:ILE:HD13	2.35	0.47
2:F:106:LYS:HE3	2:F:110:GLU:OE2	2.15	0.47
3:I:126:ILE:HB	3:I:131:LYS:HB3	1.96	0.47
2:E:10:LYS:O	2:E:168:ASP:OD1	2.32	0.47
3:I:159:ALA:HA	3:I:162:ASN:OD1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:GLY:HA3	1:C:47:GLU:O	2.15	0.47
3:G:72:ASP:OD1	3:G:72:ASP:N	2.35	0.47
1:C:61:VAL:HG13	1:C:77:VAL:HG13	1.96	0.46
2:D:38:ARG:NH2	3:I:202:ARG:HG2	2.31	0.46
2:D:41:GLY:HA3	2:D:151:ALA:HB2	1.97	0.46
2:D:210:MET:CE	2:D:215:VAL:HA	2.45	0.46
3:I:86:VAL:HG21	3:I:140:HIS:CE1	2.50	0.46
2:E:13:VAL:HG23	2:E:13:VAL:O	2.14	0.46
2:E:17:ARG:CZ	2:E:172:VAL:HB	2.46	0.46
2:F:247:GLU:HG2	2:F:248:MET:N	2.31	0.46
1:A:4:VAL:O	1:A:34:ALA:HA	2.15	0.46
2:D:167:ALA:O	2:D:168:ASP:C	2.53	0.46
2:E:103:LYS:NZ	3:H:104:GLU:OE2	2.47	0.46
4:Y:4:C:H5	6:Y:449:HOH:O	1.97	0.46
1:A:119:LYS:HG2	1:A:136:MET:SD	2.56	0.46
3:G:85:LEU:O	3:G:93:PHE:HB3	2.16	0.46
2:D:38:ARG:HA	2:D:38:ARG:HD2	1.77	0.46
2:D:110:GLU:CB	2:D:115:LYS:HZ3	2.29	0.46
2:E:248:MET:C	2:E:250:GLU:H	2.18	0.46
3:I:219:ASP:O	3:I:220:ASP:HB2	2.15	0.46
2:D:206:MET:HG3	3:G:225:MET:HG3	1.95	0.46
2:F:126:PHE:CE2	3:H:87:PRO:CB	2.99	0.46
3:H:25:ASP:OD2	3:H:27:ARG:HD3	2.15	0.46
3:I:4:ASP:OD1	3:I:4:ASP:N	2.49	0.46
1:C:114:TYR:O	1:C:115:LEU:HB2	2.16	0.46
2:D:212:ARG:NH2	2:D:216:LYS:HZ2	2.13	0.46
3:H:194:ASN:O	3:H:237:LEU:HD13	2.16	0.46
3:I:225:MET:CE	3:I:238:PHE:CZ	2.99	0.46
2:E:243:GLU:O	2:E:247:GLU:HB3	2.16	0.45
1:A:119:LYS:NZ	1:A:135:GLU:HG2	2.31	0.45
2:E:62:VAL:CB	2:E:63:HIS:HA	2.45	0.45
3:G:77:GLY:HA2	3:G:132:VAL:HG13	1.98	0.45
1:B:168:ARG:O	1:B:170:ILE:HG13	2.17	0.45
1:C:53:PRO:HB3	1:C:83:GLU:CD	2.37	0.45
3:I:40:ASN:ND2	3:I:162:ASN:ND2	2.64	0.45
3:G:58:VAL:HG22	3:G:148:LEU:CD2	2.46	0.45
3:G:157:ILE:HG12	3:G:184:PRO:HD2	1.99	0.45
3:H:257:LYS:HB3	3:H:259:ILE:HG13	1.98	0.45
3:G:18:LEU:CD2	3:G:195:LYS:HD3	2.46	0.45
2:D:94:PRO:HB3	2:D:99:ILE:HD11	1.98	0.45
1:B:52:ILE:HA	1:B:53:PRO:HD3	1.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:65:GLU:C	2:D:67:LEU:N	2.69	0.45
2:E:153:VAL:HA	2:E:154:PRO:HD3	1.82	0.45
1:B:156:ILE:HG23	1:B:157:LEU:N	2.30	0.45
1:C:23:TYR:OH	2:F:194:ARG:HD3	2.17	0.45
2:F:187:MET:HG3	2:F:206:MET:HB2	1.99	0.45
3:I:3:GLU:HA	3:I:3:GLU:OE1	2.17	0.45
2:D:106:LYS:HE2	2:D:110:GLU:CD	2.37	0.45
1:C:138:VAL:HG12	1:C:140:ARG:H	1.81	0.44
2:D:72:LYS:O	2:D:119:PRO:HA	2.16	0.44
1:B:141:ALA:HB1	1:B:168:ARG:NH1	2.32	0.44
1:B:152:ARG:HA	1:B:157:LEU:HD23	1.99	0.44
3:G:172:LEU:HD12	3:G:172:LEU:HA	1.79	0.44
3:G:195:LYS:HD2	6:G:528:HOH:O	2.16	0.44
3:H:225:MET:HE1	3:H:238:PHE:HE1	1.81	0.44
2:D:73:ALA:HB2	2:D:118:PHE:O	2.17	0.44
2:D:208:GLY:H	3:G:115:GLU:HG3	1.81	0.44
2:E:17:ARG:CD	2:E:179:GLU:OE1	2.65	0.44
3:I:162:ASN:ND2	3:I:162:ASN:O	2.50	0.44
3:G:30:ASP:HA	3:G:198:VAL:CG2	2.48	0.44
3:H:124:LEU:HB3	3:H:133:TRP:HB2	1.98	0.44
3:I:84:GLU:HB3	3:I:86:VAL:HG13	1.98	0.44
1:B:61:VAL:CG1	1:B:77:VAL:HG13	2.47	0.44
2:D:137:ARG:NH1	2:D:205:GLN:OE1	2.49	0.44
2:D:198:ILE:HG21	2:D:223:LYS:CD	2.47	0.44
3:G:74:PRO:O	3:G:128:GLU:HG3	2.18	0.44
3:G:89:ALA:HB3	3:G:93:PHE:CE1	2.53	0.44
1:C:12:SER:HA	1:C:28:GLU:OE2	2.18	0.44
3:H:212:LEU:HD12	3:H:241:LEU:HD23	2.00	0.44
3:I:60:VAL:HG11	3:I:156:ALA:HA	1.99	0.44
3:H:60:VAL:HG11	3:H:156:ALA:HA	2.00	0.44
1:A:164:ARG:CG	1:A:165:VAL:N	2.81	0.43
1:B:61:VAL:HG22	1:B:79:SER:O	2.18	0.43
1:B:105:VAL:HG13	1:B:110:GLU:HB3	2.00	0.43
3:G:76:ARG:O	3:G:132:VAL:HG21	2.18	0.43
3:H:110:ASP:OD1	3:H:114:ARG:NH2	2.43	0.43
1:A:118:LEU:C	1:A:118:LEU:HD23	2.38	0.43
1:A:159:CYS:HA	1:A:160:PRO:HD3	1.87	0.43
2:E:165:GLY:HA3	2:E:175:PRO:HG3	2.00	0.43
3:G:41:VAL:O	3:G:41:VAL:HG12	2.17	0.43
2:D:162:VAL:HG22	2:D:229:ILE:HD12	2.00	0.43
1:A:111:ALA:O	1:A:168:ARG:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:135:GLY:O	2:F:138:THR:HG22	2.18	0.43
3:G:124:LEU:HB3	3:G:133:TRP:HB2	2.00	0.43
3:I:236:LYS:O	3:I:240:GLU:HG3	2.18	0.43
2:D:107:GLU:CD	3:G:229:GLY:H	2.21	0.43
2:D:212:ARG:C	2:D:212:ARG:HD2	2.39	0.43
1:B:56:VAL:HG23	1:B:57:LYS:N	2.33	0.43
2:F:208:GLY:O	3:I:223:VAL:HA	2.18	0.43
3:G:36:GLU:HG2	3:G:38:ILE:HD11	2.01	0.43
3:H:225:MET:CE	3:H:238:PHE:CE1	3.02	0.43
3:I:50:LEU:HD12	3:I:58:VAL:O	2.19	0.43
3:I:107:ARG:HH12	4:X:5:C:P	2.42	0.43
1:C:7:GLY:HA2	2:F:194:ARG:HG2	2.00	0.43
2:E:212:ARG:HG2	3:H:242:LEU:HD13	2.01	0.43
3:G:125:VAL:HA	3:G:132:VAL:CG2	2.46	0.43
3:H:33:ARG:NH1	3:H:145:ASP:O	2.52	0.43
3:I:74:PRO:O	3:I:75:ASP:HB3	2.18	0.43
3:I:147:ASN:ND2	3:I:150:ASP:H	2.16	0.43
1:B:119:LYS:HE2	1:B:135:GLU:O	2.19	0.43
1:B:173:ASP:OD2	1:B:176:LYS:HD2	2.19	0.43
3:H:125:VAL:HA	3:H:132:VAL:CG2	2.44	0.43
3:I:110:ASP:CG	3:I:114:ARG:HH22	2.21	0.43
1:B:33:VAL:HG21	1:B:48:SER:HB2	1.99	0.42
1:B:101:ASP:O	1:B:102:GLU:HB3	2.18	0.42
1:B:105:VAL:CG1	1:B:110:GLU:HB3	2.49	0.42
3:G:116:SER:HG	3:G:184:PRO:HG3	1.84	0.42
3:G:183:LEU:HD13	3:G:253:ARG:HG2	2.01	0.42
3:I:51:VAL:CG2	3:I:155:ALA:HB2	2.49	0.42
3:I:225:MET:HE1	3:I:238:PHE:HZ	1.83	0.42
1:A:123:ILE:CG1	1:A:128:ARG:HG2	2.40	0.42
2:D:27:ARG:HD2	2:D:48:GLY:HA3	2.01	0.42
2:E:63:HIS:ND1	2:E:64:PRO:HA	2.34	0.42
3:H:218:LYS:HB2	3:H:218:LYS:HE3	1.65	0.42
3:I:110:ASP:CG	3:I:114:ARG:NH2	2.72	0.42
1:A:36:LYS:HD2	1:A:38:ILE:HD11	2.00	0.42
1:B:156:ILE:HD13	1:B:156:ILE:HA	1.85	0.42
1:C:101:ASP:O	1:C:102:GLU:HB3	2.19	0.42
2:D:19:ASP:CG	2:D:21:ARG:HG3	2.40	0.42
2:E:38:ARG:HH22	3:G:202:ARG:NH2	2.17	0.42
2:E:175:PRO:HD2	6:E:265:HOH:O	2.18	0.42
3:H:66:PRO:HD2	3:H:170:PHE:CE1	2.55	0.42
3:I:172:LEU:HD12	3:I:172:LEU:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:76:ARG:NE	2:D:124:ASP:OD2	2.51	0.42
2:D:91:ARG:HA	2:D:92:PRO:HD3	1.85	0.42
2:D:210:MET:HE1	2:D:215:VAL:HA	2.01	0.42
3:G:120:ASP:OD1	3:G:123:LYS:HE2	2.19	0.42
3:H:85:LEU:O	3:H:93:PHE:HB3	2.19	0.42
3:H:252:LEU:HD23	3:H:252:LEU:HA	1.88	0.42
1:C:118:LEU:HD23	1:C:119:LYS:N	2.35	0.42
2:E:106:LYS:O	2:E:110:GLU:HG3	2.20	0.42
2:E:244:VAL:O	2:E:248:MET:HG3	2.20	0.42
1:C:12:SER:OG	1:C:15:GLU:HG3	2.20	0.42
2:E:41:GLY:HA3	2:E:151:ALA:HB2	2.02	0.42
2:E:242:ILE:O	2:E:246:GLU:HG2	2.20	0.42
2:F:21:ARG:CZ	2:F:27:ARG:HG3	2.49	0.42
2:F:141:LEU:HD11	2:F:203:LEU:HD13	2.01	0.42
2:F:178:GLU:OE1	2:F:178:GLU:N	2.53	0.42
3:G:86:VAL:HG21	3:G:140:HIS:CE1	2.55	0.42
3:H:90:SER:OG	3:H:92:THR:HB	2.20	0.42
1:B:61:VAL:HG13	1:B:62:LEU:N	2.34	0.42
1:B:102:GLU:HA	1:B:102:GLU:OE1	2.20	0.42
2:E:58:GLY:HA2	2:E:59:PRO:C	2.40	0.42
2:F:38:ARG:HG3	3:H:144:ASP:O	2.20	0.42
2:F:126:PHE:CZ	3:H:87:PRO:CB	3.02	0.42
3:G:59:VAL:HG23	3:G:142:LEU:HD11	2.02	0.42
3:G:86:VAL:C	3:G:88:LEU:H	2.22	0.42
2:F:60:ARG:H	2:F:60:ARG:HG3	1.77	0.42
2:F:91:ARG:HA	2:F:92:PRO:HD3	1.84	0.42
2:F:128:GLU:HB2	3:H:88:LEU:HD13	2.01	0.42
2:E:197:LYS:HB2	6:E:279:HOH:O	2.20	0.42
1:A:56:VAL:HG22	1:A:59:ASP:OD1	2.20	0.41
2:D:208:GLY:N	3:G:115:GLU:HG3	2.35	0.41
2:E:62:VAL:O	2:E:120:ARG:O	2.37	0.41
2:F:32:GLU:O	2:F:43:CYS:HA	2.20	0.41
3:I:115:GLU:CB	3:I:223:VAL:HG13	2.41	0.41
2:D:54:ALA:HB2	2:D:127:VAL:HG22	2.01	0.41
2:F:219:ILE:O	2:F:223:LYS:HG3	2.20	0.41
3:G:46:GLU:HG2	3:G:63:LYS:HA	2.02	0.41
3:G:70:TYR:CZ	4:Y:3:C:C6	3.08	0.41
3:H:126:ILE:HB	3:H:131:LYS:HB3	2.02	0.41
3:I:237:LEU:C	3:I:237:LEU:CD2	2.89	0.41
1:A:16:TYR:CE2	1:A:39:ILE:HD13	2.55	0.41
2:E:176:MET:HG2	2:E:179:GLU:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:196:TYR:CD2	3:G:237:LEU:HD21	2.53	0.41
3:I:251:LYS:O	3:I:254:GLU:HB2	2.20	0.41
1:A:119:LYS:CE	1:A:135:GLU:HG2	2.50	0.41
2:E:21:ARG:CZ	2:E:27:ARG:HG3	2.50	0.41
2:E:219:ILE:HD11	3:H:238:PHE:CE2	2.56	0.41
2:F:89:ARG:HD2	3:H:136:PHE:CD2	2.55	0.41
3:G:43:GLU:O	3:G:44:LYS:CB	2.45	0.41
3:H:14:VAL:HG22	3:H:24:ILE:HD11	2.02	0.41
3:I:10:LYS:HA	3:I:10:LYS:HD3	1.93	0.41
1:C:64:ARG:HA	1:C:116:ASP:O	2.21	0.41
2:D:113:ILE:HA	2:D:155:MET:HG2	2.02	0.41
2:E:187:MET:HG3	2:E:206:MET:HB3	2.01	0.41
1:A:156:ILE:HA	1:A:156:ILE:HD13	1.80	0.41
1:C:87:PRO:HG3	6:C:182:HOH:O	2.21	0.41
2:D:38:ARG:NH1	3:I:145:ASP:OD2	2.54	0.41
2:E:22:LYS:NZ	6:E:435:HOH:O	2.48	0.41
2:E:208:GLY:O	3:H:223:VAL:HA	2.20	0.41
2:F:53:ILE:HD13	2:F:53:ILE:C	2.41	0.41
1:A:111:ALA:O	1:A:168:ARG:CB	2.68	0.41
2:D:38:ARG:HE	3:I:202:ARG:NH1	2.18	0.41
2:D:215:VAL:O	2:D:219:ILE:HG13	2.20	0.41
2:E:70:PRO:O	2:E:119:PRO:HB3	2.21	0.41
2:E:160:THR:O	2:E:190:ALA:HA	2.21	0.41
2:F:159:ILE:HD13	2:F:159:ILE:HA	1.93	0.41
1:B:84:ASN:N	1:B:84:ASN:HD22	2.17	0.41
2:E:64:PRO:O	2:E:65:GLU:HG2	2.21	0.41
3:H:89:ALA:O	3:H:93:PHE:CD1	2.74	0.41
2:D:111:ALA:HB1	3:G:232:LEU:HG	2.03	0.41
2:E:61:GLU:CB	2:E:63:HIS:CB	2.85	0.41
2:F:68:GLN:OE1	2:F:120:ARG:HD3	2.21	0.41
2:F:126:PHE:CZ	3:H:87:PRO:HB3	2.56	0.41
2:F:195:ASN:HA	6:F:302:HOH:O	2.21	0.41
2:F:221:LEU:HD23	2:F:221:LEU:HA	1.87	0.41
3:G:72:ASP:HB2	3:G:73:THR:HG23	2.02	0.41
3:G:86:VAL:C	3:G:88:LEU:N	2.75	0.41
3:I:33:ARG:HD2	3:I:199:ASP:OD1	2.19	0.41
1:A:61:VAL:CG1	1:A:77:VAL:HG13	2.51	0.41
3:G:90:SER:HB2	3:G:91:PRO:HD2	2.03	0.41
3:I:68:GLU:O	3:I:68:GLU:CG	2.67	0.41
3:I:190:LEU:HB2	3:I:200:PRO:HB3	2.03	0.41
2:D:45:LEU:HD11	2:D:47:MET:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:100:GLU:OE1	3:H:107:ARG:NH2	2.54	0.40
3:G:80:ILE:CD1	4:Y:2:U:H2'	2.51	0.40
3:H:99:ASP:OD1	3:H:101:ASN:HB2	2.22	0.40
3:I:70:TYR:HA	3:I:71:PRO:HD3	1.95	0.40
1:A:146:CYS:O	1:A:147:LYS:HB2	2.21	0.40
3:G:30:ASP:HA	3:G:198:VAL:HG21	2.03	0.40
1:B:142:LEU:HD22	1:B:147:LYS:O	2.21	0.40
1:C:68:LEU:HD23	1:C:68:LEU:HA	1.89	0.40
2:E:106:LYS:NZ	6:E:332:HOH:O	2.52	0.40
2:E:201:ILE:HB	3:H:233:LEU:HB3	2.03	0.40
2:F:74:ILE:O	2:F:74:ILE:HG13	2.21	0.40
2:F:177:LYS:HB3	2:F:178:GLU:OE1	2.20	0.40
1:B:177:GLY:O	1:B:178:GLU:HG3	2.21	0.40
2:D:17:ARG:HD2	2:D:179:GLU:OE1	2.21	0.40
2:E:118:PHE:O	2:E:121:SER:HB2	2.21	0.40
2:F:18:LEU:HD12	2:F:18:LEU:HA	1.89	0.40
3:G:58:VAL:CG2	3:G:148:LEU:HD23	2.49	0.40
3:I:33:ARG:NH1	3:I:145:ASP:O	2.54	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	177/179 (99%)	167 (94%)	9 (5%)	1 (1%)	25 36
1	B	177/179 (99%)	151 (85%)	24 (14%)	2 (1%)	14 20
1	C	177/179 (99%)	163 (92%)	14 (8%)	0	100 100
2	D	241/258 (93%)	224 (93%)	13 (5%)	4 (2%)	9 11
2	E	246/258 (95%)	230 (94%)	15 (6%)	1 (0%)	34 48
2	F	244/258 (95%)	239 (98%)	4 (2%)	1 (0%)	34 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	G	252/259 (97%)	236 (94%)	13 (5%)	3 (1%)	13 19
3	H	256/259 (99%)	239 (93%)	15 (6%)	2 (1%)	19 29
3	I	256/259 (99%)	244 (95%)	9 (4%)	3 (1%)	13 19
All	All	2026/2088 (97%)	1893 (93%)	116 (6%)	17 (1%)	19 29

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	64	PRO
3	I	89	ALA
3	I	128	GLU
1	A	106	LYS
1	B	169	LYS
2	F	9	GLU
3	G	44	LYS
1	B	132	LYS
2	D	94	PRO
3	G	96	GLY
3	I	258	GLU
2	D	65	GLU
2	D	95	ASP
2	E	64	PRO
3	H	90	SER
3	G	205	MET
3	H	257	LYS

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	149/149 (100%)	133 (89%)	16 (11%)	6 9
1	B	149/149 (100%)	141 (95%)	8 (5%)	22 36
1	C	149/149 (100%)	141 (95%)	8 (5%)	22 36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	202/214 (94%)	183 (91%)	19 (9%)	8 13
2	E	207/214 (97%)	192 (93%)	15 (7%)	14 23
2	F	205/214 (96%)	189 (92%)	16 (8%)	12 19
3	G	222/227 (98%)	202 (91%)	20 (9%)	9 14
3	H	226/227 (100%)	210 (93%)	16 (7%)	14 23
3	I	226/227 (100%)	209 (92%)	17 (8%)	13 21
All	All	1735/1770 (98%)	1600 (92%)	135 (8%)	12 19

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	61	VAL
1	A	69	ARG
1	A	72	ILE
1	A	74	LEU
1	A	79	SER
1	A	95	LEU
1	A	98	SER
1	A	104	TYR
1	A	112	VAL
1	A	118	LEU
1	A	134	GLU
1	A	156	ILE
1	A	162	CYS
1	A	168	ARG
1	A	169	LYS
1	B	37	LEU
1	B	50	SER
1	B	54	GLU
1	B	56	VAL
1	B	95	LEU
1	B	104	TYR
1	B	107	GLU
1	B	156	ILE
1	C	37	LEU
1	C	66	VAL
1	C	95	LEU
1	C	97	VAL
1	C	107	GLU

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Mol	Chain	Res	Type
1	C	140	ARG
1	C	156	ILE
1	C	162	CYS
2	D	10	LYS
2	D	18	LEU
2	D	38	ARG
2	D	45	LEU
2	D	52	VAL
2	D	62	VAL
2	D	72	LYS
2	D	88	GLU
2	D	129	VAL
2	D	130	LEU
2	D	138	THR
2	D	153	VAL
2	D	162	VAL
2	D	180	ASP
2	D	199	GLU
2	D	206	MET
2	D	212	ARG
2	D	221	LEU
2	D	238	LEU
2	E	18	LEU
2	E	21	ARG
2	E	45	LEU
2	E	68	GLN
2	E	91	ARG
2	E	100	GLU
2	E	162	VAL
2	E	170	GLN
2	E	171	LEU
2	E	178	GLU
2	E	199	GLU
2	E	206	MET
2	E	221	LEU
2	E	247	GLU
2	E	252	THR
2	F	18	LEU
2	F	45	LEU
2	F	53	ILE
2	F	60	ARG
2	F	62	VAL

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Mol	Chain	Res	Type
2	F	104	VAL
2	F	110	GLU
2	F	115	LYS
2	F	129	VAL
2	F	138	THR
2	F	153	VAL
2	F	180	ASP
2	F	194	ARG
2	F	199	GLU
2	F	221	LEU
2	F	238	LEU
3	G	18	LEU
3	G	43	GLU
3	G	46	GLU
3	G	72	ASP
3	G	85	LEU
3	G	99	ASP
3	G	130	GLU
3	G	132	VAL
3	G	147	ASN
3	G	154	LEU
3	G	172	LEU
3	G	190	LEU
3	G	212	LEU
3	G	223	VAL
3	G	233	LEU
3	G	237	LEU
3	G	241	LEU
3	G	242	LEU
3	G	250	ARG
3	G	257	LYS
3	H	18	LEU
3	H	38	ILE
3	H	68	GLU
3	H	88	LEU
3	H	92	THR
3	H	132	VAL
3	H	147	ASN
3	H	154	LEU
3	H	172	LEU
3	H	183	LEU
3	H	190	LEU

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Mol	Chain	Res	Type
3	H	212	LEU
3	H	218	LYS
3	H	233	LEU
3	H	242	LEU
3	H	254	GLU
3	I	3	GLU
3	I	4	ASP
3	I	18	LEU
3	I	85	LEU
3	I	132	VAL
3	I	147	ASN
3	I	154	LEU
3	I	172	LEU
3	I	177	LEU
3	I	183	LEU
3	I	190	LEU
3	I	212	LEU
3	I	218	LYS
3	I	223	VAL
3	I	233	LEU
3	I	242	LEU
3	I	247	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	B	70	ASN
1	B	84	ASN
1	C	70	ASN
1	C	84	ASN
2	D	66	HIS
2	D	131	GLN
2	D	170	GLN
2	D	228	GLN
2	D	233	GLN
2	E	131	GLN
2	E	195	ASN
2	E	228	GLN
2	E	233	GLN
2	F	131	GLN
2	F	228	GLN

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Mol	Chain	Res	Type
2	F	233	GLN
3	G	140	HIS
3	G	147	ASN
3	G	247	ASN
3	H	40	ASN
3	H	140	HIS
3	H	147	ASN
3	H	221	ASN
3	I	40	ASN
3	I	147	ASN
3	I	162	ASN
3	I	247	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	X	4/6 (66%)	0	0
4	Y	4/6 (66%)	1 (25%)	0
4	Z	3/6 (50%)	0	0
All	All	11/18 (61%)	1 (9%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	Y	3	C

There are no RNA pucker outliers to report.

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 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	179/179 (100%)	0.28	8 (4%) 33 31	40, 62, 86, 120	9 (5%)
1	B	179/179 (100%)	0.86	29 (16%) 1 1	36, 83, 118, 135	12 (6%)
1	C	179/179 (100%)	0.50	19 (10%) 6 5	27, 57, 92, 117	8 (4%)
2	D	243/258 (94%)	-0.10	1 (0%) 92 91	28, 41, 69, 92	6 (2%)
2	E	248/258 (96%)	-0.07	5 (2%) 65 63	25, 37, 77, 109	2 (0%)
2	F	246/258 (95%)	-0.20	2 (0%) 86 84	22, 32, 70, 99	4 (1%)
3	G	254/259 (98%)	0.01	8 (3%) 49 47	32, 48, 76, 88	2 (0%)
3	H	258/259 (99%)	-0.06	3 (1%) 79 77	22, 33, 74, 86	5 (1%)
3	I	258/259 (99%)	-0.09	4 (1%) 72 70	22, 34, 73, 103	3 (1%)
4	X	5/6 (83%)	1.08	1 (20%) 1 0	53, 55, 73, 104	0
4	Y	5/6 (83%)	1.52	1 (20%) 1 0	59, 65, 83, 112	0
4	Z	4/6 (66%)	0.27	0 100 100	60, 60, 60, 65	0
All	All	2058/2106 (97%)	0.09	81 (3%) 39 38	22, 43, 92, 135	51 (2%)

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Y	2	U	7.1
1	B	104	TYR	5.8
3	I	259	ILE	5.7
1	A	104	TYR	5.3
1	A	106	LYS	5.1
3	G	89	ALA	4.9
4	X	2	U	4.9
3	H	259	ILE	4.9
3	H	89	ALA	4.8
1	B	167	LYS	4.6
1	B	100	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	123	ILE	4.5
1	C	108	ILE	4.5
1	B	97	VAL	4.4
1	C	96	HIS	4.3
2	E	64	PRO	4.2
1	B	153	GLU	4.0
2	E	252	THR	3.9
1	B	170	ILE	3.6
1	B	131	THR	3.6
1	B	130	SER	3.6
1	B	105	VAL	3.5
2	E	251	ILE	3.4
1	C	104	TYR	3.4
1	A	105	VAL	3.3
1	A	95	LEU	3.3
1	B	120	ALA	3.3
1	C	131	THR	3.2
1	B	127	LEU	3.2
1	A	112	VAL	3.1
1	C	111	ALA	3.1
2	E	63	HIS	3.1
1	B	101	ASP	3.0
1	B	129	LEU	3.0
3	I	89	ALA	3.0
1	B	155	ASP	2.9
1	B	151	VAL	2.9
1	B	73	ALA	2.9
3	G	94	GLU	2.8
1	B	164	ARG	2.8
1	A	96	HIS	2.8
3	H	90	SER	2.7
3	G	124	LEU	2.7
1	B	126	ASN	2.7
1	B	71	SER	2.7
3	G	172	LEU	2.6
1	B	128	ARG	2.6
1	B	107	GLU	2.6
1	C	136	MET	2.6
2	E	62	VAL	2.6
3	G	173	GLY	2.5
1	C	93	GLY	2.5
1	C	107	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	152	ARG	2.4
1	C	146	CYS	2.4
1	C	72	ILE	2.4
2	F	252	THR	2.4
2	F	251	ILE	2.4
1	B	119	LYS	2.4
1	B	176	LYS	2.3
1	B	165	VAL	2.3
1	C	127	LEU	2.3
1	B	96	HIS	2.3
1	A	75	ILE	2.3
3	I	2	PRO	2.3
1	B	99	ASN	2.3
1	C	73	ALA	2.3
1	C	97	VAL	2.2
2	D	66	HIS	2.2
1	C	95	LEU	2.2
3	G	171	ASP	2.2
3	I	70	TYR	2.1
1	A	128	ARG	2.1
1	C	138	VAL	2.1
1	C	71	SER	2.1
3	G	91	PRO	2.0
1	B	93	GLY	2.0
3	G	127	GLU	2.0
1	C	112	VAL	2.0
1	C	137	GLY	2.0
1	C	133	GLU	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, 95^{th} 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
5	ZN	B	180	1/1	0.86	0.07	96,96,96,96	0
5	ZN	C	180	1/1	0.96	0.05	71,71,71,71	0
5	ZN	A	180	1/1	0.97	0.08	59,59,59,59	0

6.5 Other polymers (i)

There are no such residues in this entry.