Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:28 pm BST

PDB ID	:	5YK3
Title	:	human Ragulator complex
Authors	:	Wu, G.; Mu, Z.
Deposited on	:	2017-10-12
Resolution	:	3.01 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 following versions of software and data (see references ⓘ) were used in the production of this report:

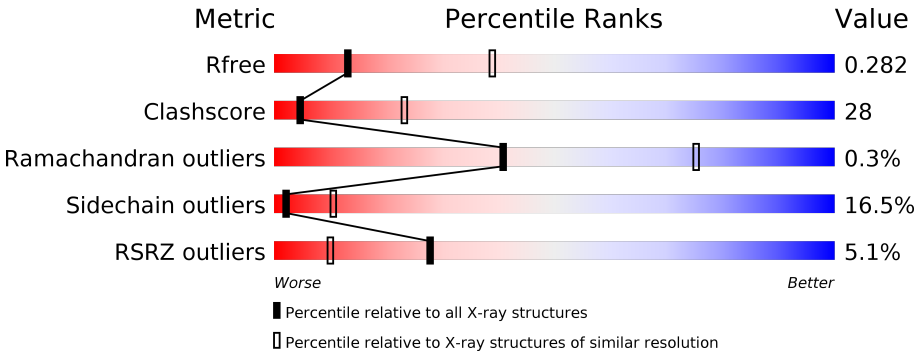
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.01 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.



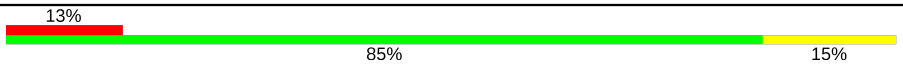
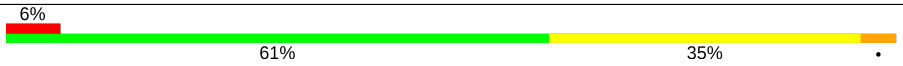
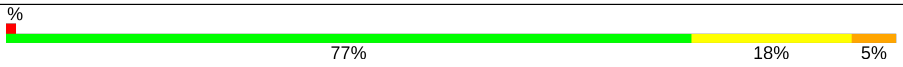
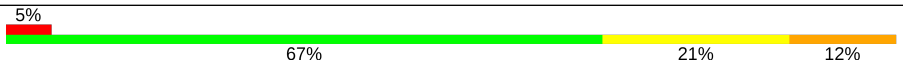
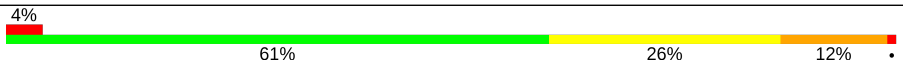
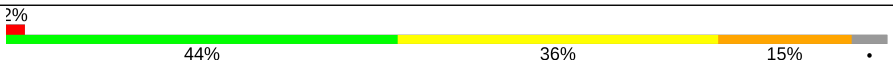
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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 on 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	H	124	2% 68% 26% 6%
1	m	124	2% 94% 6%
2	G	125	9% 58% 31% 9%
2	l	125	6% 84% 15%
3	o	90	2% 93% 7%
4	n	88	25% 77% 23%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	k	85	
6	C	123	
7	B	125	
8	E	91	
8	J	91	
9	D	96	
10	A	85	
10	F	85	
11	I	99	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 11608 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 Ragulator complex protein LAMTOR3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	m	124	Total	C	N	O	S	0	0	0
			941	606	154	180	1			
1	H	124	Total	C	N	O	S	0	0	0
			957	615	161	180	1			

- Molecule 2 is a protein called Ragulator complex protein LAMTOR2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	l	124	Total	C	N	O	S	0	0	0
			928	586	159	176	7			
2	G	123	Total	C	N	O	S	0	0	0
			903	567	152	178	6			

- Molecule 3 is a protein called Ragulator complex protein LAMTOR5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	o	90	Total	C	N	O	S	0	0	0
			657	402	114	134	7			

- Molecule 4 is a protein called Ragulator complex protein LAMTOR4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	n	88	Total	C	N	O	S	0	0	0
			630	395	114	119	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	5	ALA	-	expression tag	UNP Q0VGL1
n	7	ALA	GLN	engineered mutation	UNP Q0VGL1

- Molecule 5 is a protein called Ragulator complex protein LAMTOR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	k	85	Total	C	N	O	S	0	0	0
			658	420	113	124	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	77	ALA	-	expression tag	UNP Q6IAA8
k	78	ALA	-	expression tag	UNP Q6IAA8

- Molecule 6 is a protein called Ragulator complex protein LAMTOR3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	123	Total	C	N	O	S	0	0	0
			951	612	160	178	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	ALA	-	expression tag	UNP Q9UHA4

- Molecule 7 is a protein called Ragulator complex protein LAMTOR2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	B	125	Total	C	N	O	S	0	0	0
			916	574	157	179	6			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	ALA	-	expression tag	UNP Q9Y2Q5
B	2	ALA	-	expression tag	UNP Q9Y2Q5
B	3	ALA	-	expression tag	UNP Q9Y2Q5
B	122	ALA	VAL	engineered mutation	UNP Q9Y2Q5
B	125	ALA	SER	engineered mutation	UNP Q9Y2Q5

- Molecule 8 is a protein called Ragulator complex protein LAMTOR5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	E	91	Total	C	N	O	S	0	0	0
			666	406	115	138	7			
8	J	91	Total	C	N	O	S	0	0	0
			666	406	115	138	7			

- Molecule 9 is a protein called Ragulator complex protein LAMTOR4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	D	96	Total	C	N	O	S	0	0	0
			715	448	130	135	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	2	ALA	-	expression tag	UNP Q0VGL1
D	3	THR	-	expression tag	UNP Q0VGL1

- Molecule 10 is a protein called Ragulator complex protein LAMTOR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	A	85	Total	C	N	O	S	0	0	0
			665	423	117	124	1			
10	F	85	Total	C	N	O	S	0	0	0
			665	423	117	124	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	77	ALA	-	expression tag	UNP Q6IAA8
F	77	ALA	-	expression tag	UNP Q6IAA8

- Molecule 11 is a protein called Ragulator complex protein LAMTOR4.

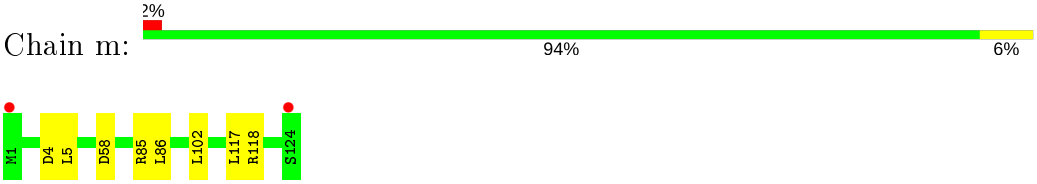
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	I	95	Total	C	N	O	S	0	0	0
			690	433	124	131	2			

3 Residue-property plots

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

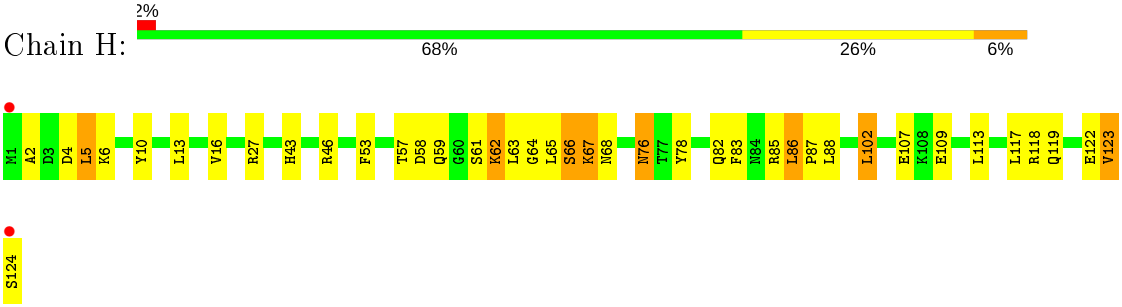
- Molecule 1: Ragulator complex protein LAMTOR3

Chain m:



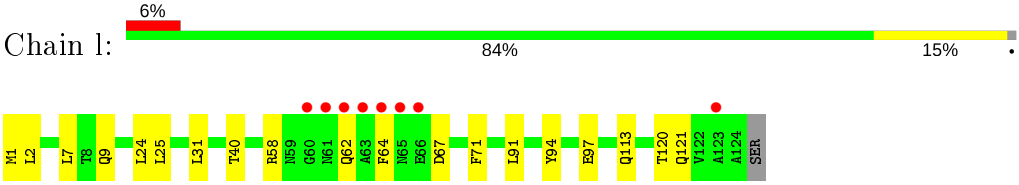
- Molecule 1: Ragulator complex protein LAMTOR3

Chain H:



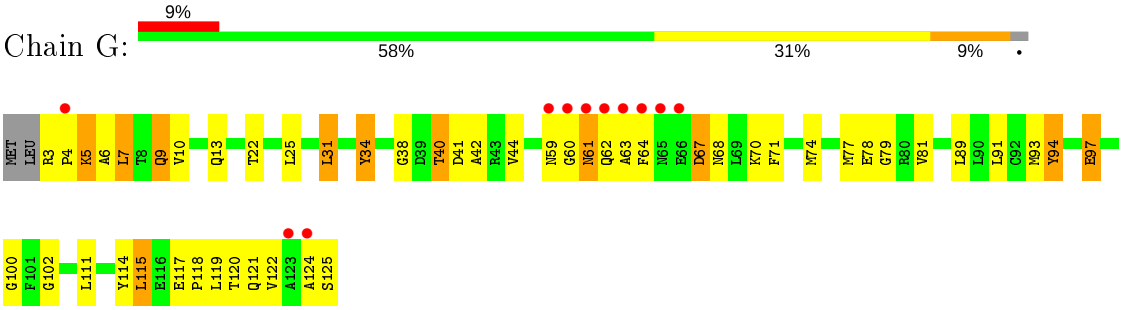
- Molecule 2: Ragulator complex protein LAMTOR2

Chain l:



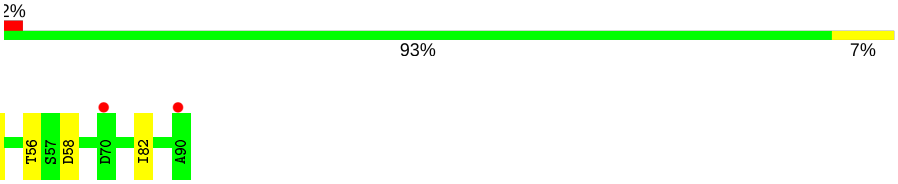
- Molecule 2: Ragulator complex protein LAMTOR2

Chain G:



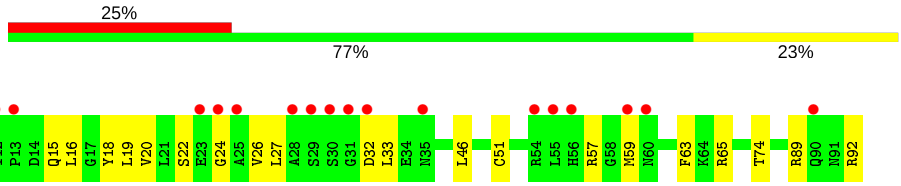
- Molecule 3: Ragulator complex protein LAMTOR5

Chain o:



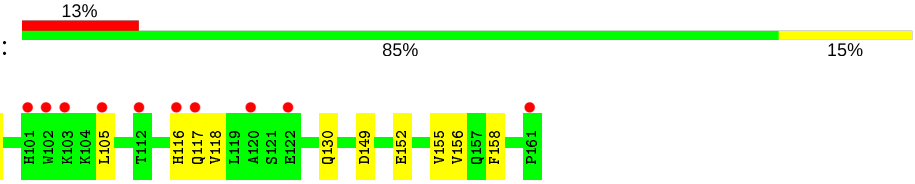
• Molecule 4: Ragulator complex protein LAMTOR4

Chain n:



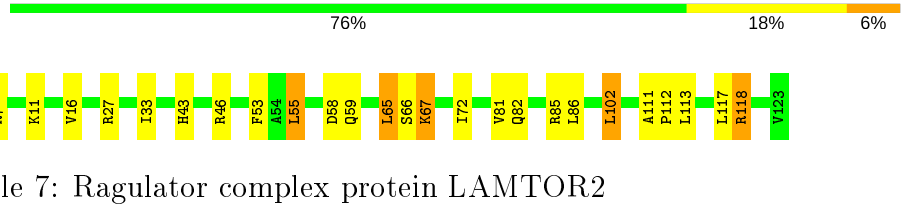
• Molecule 5: Ragulator complex protein LAMTOR1

Chain k:



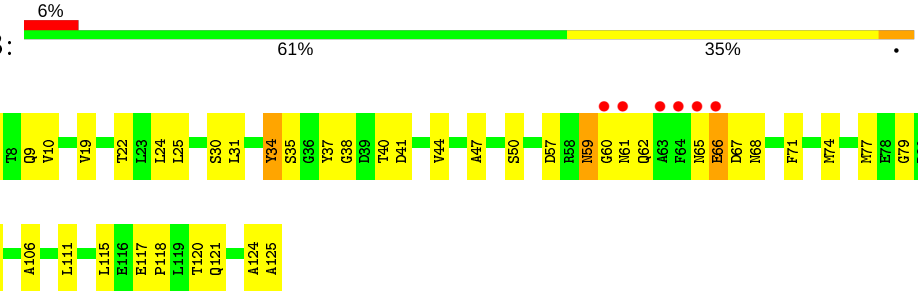
• Molecule 6: Ragulator complex protein LAMTOR3

Chain C:



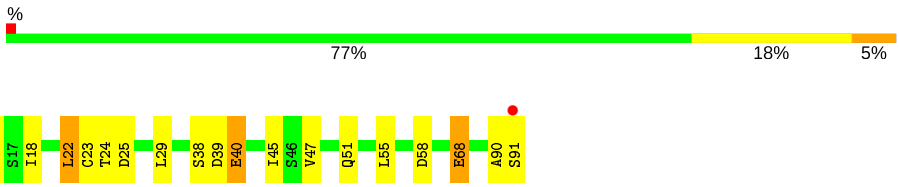
• Molecule 7: Ragulator complex protein LAMTOR2

Chain B:



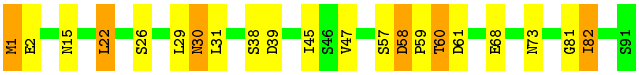
• Molecule 8: Ragulator complex protein LAMTOR5

Chain E:

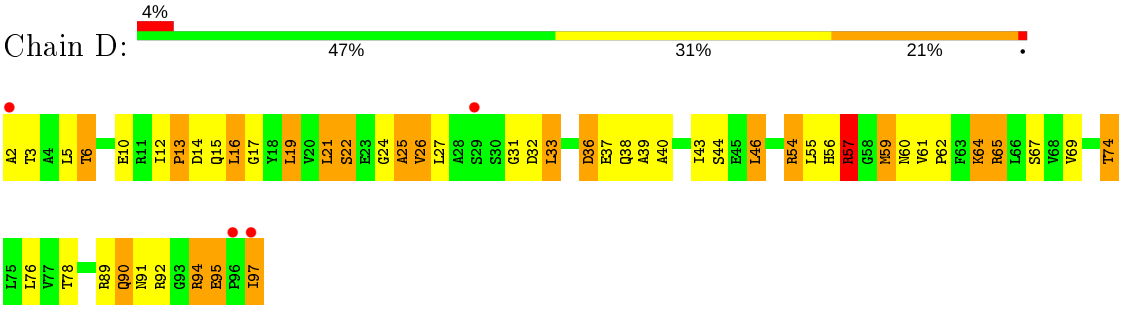


• Molecule 8: Ragulator complex protein LAMTOR5

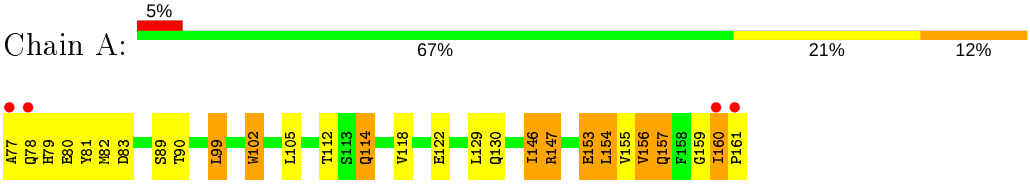
Chain J:



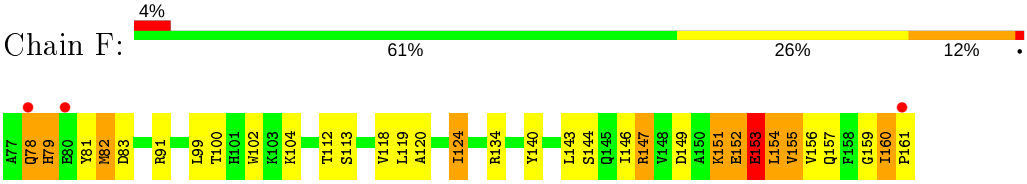
• Molecule 9: Ragulator complex protein LAMTOR4



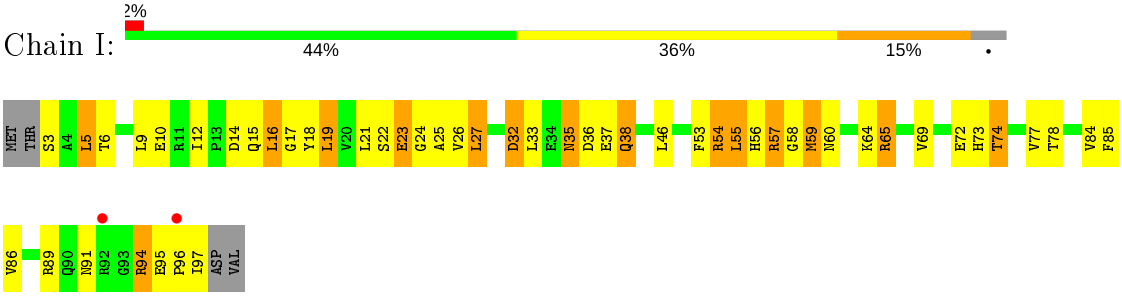
• Molecule 10: Ragulator complex protein LAMTOR1



• Molecule 10: Ragulator complex protein LAMTOR1



• Molecule 11: Ragulator complex protein LAMTOR4



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	126.64Å 126.64Å 614.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.01 48.34 – 3.01	Depositor EDS
% Data completeness (in resolution range)	86.7 (50.00-3.01) 86.8 (48.34-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.69 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.225 , 0.285 0.221 , 0.282	Depositor DCC
R_{free} test set	2569 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	40.2	Xtriage
Anisotropy	0.998	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 55.1	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	0.91	EDS
Total number of atoms	11608	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	H	0.35	0/974	0.55	0/1322
1	m	0.34	0/958	0.50	0/1304
2	G	0.37	0/913	0.60	0/1240
2	l	0.37	0/939	0.58	0/1272
3	o	0.40	0/663	0.55	0/899
4	n	0.41	0/638	0.69	1/866 (0.1%)
5	k	0.44	0/674	0.58	0/922
6	C	0.35	0/968	0.54	0/1314
7	B	0.39	0/926	0.62	0/1257
8	E	0.44	0/672	0.59	0/911
8	J	0.41	0/672	0.58	0/911
9	D	0.47	0/724	0.77	1/980 (0.1%)
10	A	0.46	1/681 (0.1%)	0.57	0/929
10	F	0.46	0/681	0.60	0/929
11	I	0.42	0/699	0.70	0/947
All	All	0.40	1/11782 (0.0%)	0.60	2/16003 (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
1	H	0	1
9	D	0	3
10	A	0	1
10	F	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	102	TRP	CD2-CE2	5.09	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	n	24	GLY	N-CA-C	-6.69	96.38	113.10
9	D	25	ALA	N-CA-C	-5.17	97.03	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	A	156	VAL	Peptide
9	D	33	LEU	Peptide
9	D	57	ARG	Peptide
9	D	94	ARG	Peptide
10	F	153	GLU	Peptide
1	H	122	GLU	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	H	957	0	982	46	0
1	m	941	0	949	0	0
2	G	903	0	893	65	0
2	l	928	0	938	0	0
3	o	657	0	659	0	0
4	n	630	0	607	0	0
5	k	658	0	648	0	0
6	C	951	0	980	30	0
7	B	916	0	916	41	0
8	E	666	0	666	21	0
8	J	666	0	666	35	0
9	D	715	0	720	70	0
10	A	665	0	665	51	0
10	F	665	0	665	49	0
11	I	690	0	672	88	0
All	All	11608	0	11626	439	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 28.

All (439) 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)
10:F:154:LEU:CD1	10:F:157:GLN:H	1.31	1.40
10:F:154:LEU:CD1	10:F:157:GLN:N	1.90	1.24
10:A:160:ILE:HG23	10:A:161:PRO:CD	1.68	1.22
2:G:40:THR:HB	2:G:41:ASP:CA	1.68	1.21
10:A:160:ILE:HG23	10:A:161:PRO:HD2	1.18	1.16
11:I:54:ARG:HB2	11:I:59:MET:HA	1.26	1.16
10:F:154:LEU:HD11	10:F:157:GLN:N	1.57	1.15
11:I:54:ARG:CB	11:I:59:MET:HA	1.77	1.13
9:D:54:ARG:HD2	9:D:55:LEU:N	1.63	1.11
11:I:56:HIS:O	11:I:57:ARG:HD3	1.51	1.11
2:G:40:THR:CB	2:G:41:ASP:HA	1.80	1.11
11:I:23:GLU:C	11:I:25:ALA:HA	1.71	1.11
8:E:38:SER:OG	8:E:40:GLU:OE2	1.66	1.09
7:B:2:ALA:HB2	10:A:156:VAL:HA	1.35	1.09
11:I:95:GLU:OE1	11:I:96:PRO:HD2	1.52	1.08
2:G:5:LYS:HB3	2:G:5:LYS:HZ2	0.96	1.07
11:I:56:HIS:C	11:I:57:ARG:HD3	1.73	1.07
9:D:24:GLY:CA	9:D:26:VAL:HG12	1.85	1.06
9:D:17:GLY:HA2	9:D:32:ASP:HB2	1.36	1.06
11:I:22:SER:O	11:I:25:ALA:HB1	1.53	1.06
9:D:54:ARG:CD	9:D:55:LEU:N	2.19	1.05
10:A:160:ILE:CG2	10:A:161:PRO:HD2	1.85	1.05
10:F:154:LEU:HD13	10:F:157:GLN:H	0.94	1.04
2:G:5:LYS:HB3	2:G:5:LYS:NZ	1.60	1.02
1:H:66:SER:HB2	2:G:77:MET:HB2	1.42	1.02
11:I:5:LEU:H	11:I:5:LEU:HD12	1.25	1.02
9:D:24:GLY:HA3	9:D:26:VAL:CG1	1.89	1.02
6:C:118:ARG:HH11	6:C:118:ARG:HB3	1.20	1.00
9:D:60:ASN:O	9:D:62:PRO:HD3	1.62	1.00
9:D:24:GLY:HA3	9:D:26:VAL:HG12	1.03	0.99
2:G:117:GLU:HB3	2:G:118:PRO:HD3	1.45	0.98
11:I:59:MET:SD	11:I:59:MET:C	2.41	0.98
6:C:58:ASP:OD1	6:C:59:GLN:N	1.97	0.98
11:I:17:GLY:HA2	11:I:32:ASP:HB2	1.47	0.97
10:F:78:GLN:HA	10:F:82:MET:HG2	1.47	0.97
11:I:53:PHE:O	11:I:59:MET:O	1.83	0.96
1:H:86:LEU:HD22	1:H:87:PRO:N	1.80	0.96
7:B:60:GLY:HA2	7:B:61:ASN:C	1.88	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:23:GLU:O	11:I:25:ALA:HA	1.68	0.93
8:E:90:ALA:HA	8:E:91:SER:HB3	1.50	0.92
6:C:118:ARG:HH11	6:C:118:ARG:CB	1.83	0.92
8:J:29:LEU:HA	8:J:30:ASN:ND2	1.85	0.92
11:I:94:ARG:CG	11:I:94:ARG:HH11	1.82	0.92
11:I:16:LEU:O	11:I:33:LEU:CD1	2.17	0.91
11:I:22:SER:C	11:I:25:ALA:HB1	1.90	0.91
9:D:33:LEU:HD23	9:D:33:LEU:N	1.84	0.90
2:G:102:GLY:HA3	8:J:29:LEU:O	1.72	0.90
9:D:94:ARG:HD2	10:A:122:GLU:HG2	1.52	0.89
7:B:3:ALA:N	7:B:4:PRO:HA	1.86	0.89
6:C:4:ASP:OD2	6:C:7:ARG:NH1	2.04	0.89
2:G:4:PRO:O	10:F:155:VAL:CG1	2.20	0.88
8:J:30:ASN:HD22	8:J:30:ASN:N	1.72	0.87
9:D:54:ARG:CD	9:D:54:ARG:C	2.41	0.87
2:G:40:THR:HB	2:G:41:ASP:HA	0.90	0.87
7:B:2:ALA:HB2	10:A:156:VAL:CA	2.04	0.86
10:A:159:GLY:O	10:A:160:ILE:HD12	1.74	0.86
10:A:160:ILE:HG23	10:A:161:PRO:CG	2.06	0.86
9:D:54:ARG:HD3	9:D:54:ARG:C	1.96	0.86
11:I:5:LEU:H	11:I:5:LEU:CD1	1.88	0.85
11:I:94:ARG:HH11	11:I:94:ARG:HG3	1.41	0.85
11:I:22:SER:O	11:I:26:VAL:N	2.10	0.85
2:G:117:GLU:HB3	2:G:118:PRO:CD	2.06	0.85
8:J:1:MET:H3	8:J:1:MET:HE2	1.41	0.84
2:G:117:GLU:HA	2:G:117:GLU:OE2	1.75	0.84
7:B:3:ALA:H	7:B:4:PRO:HA	1.40	0.84
9:D:57:ARG:HA	9:D:59:MET:H	1.44	0.83
6:C:118:ARG:HB3	6:C:118:ARG:NH1	1.93	0.82
9:D:2:ALA:O	9:D:5:LEU:HG	1.79	0.82
2:G:78:GLU:HA	2:G:97:GLU:OE2	1.78	0.82
10:F:154:LEU:HD13	10:F:157:GLN:N	1.76	0.82
11:I:5:LEU:N	11:I:5:LEU:HD12	1.93	0.82
7:B:38:GLY:HA3	7:B:94:TYR:OH	1.79	0.82
9:D:54:ARG:CD	9:D:55:LEU:CA	2.57	0.82
10:F:155:VAL:O	10:F:155:VAL:HG12	1.78	0.82
9:D:54:ARG:CD	9:D:55:LEU:HA	2.10	0.81
1:H:123:VAL:O	1:H:123:VAL:HG13	1.77	0.81
11:I:22:SER:O	11:I:25:ALA:CB	2.27	0.81
11:I:16:LEU:O	11:I:33:LEU:HD12	1.81	0.81
1:H:86:LEU:HD13	1:H:86:LEU:O	1.79	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:D:54:ARG:HD3	9:D:55:LEU:N	1.96	0.81
10:F:154:LEU:HD13	10:F:156:VAL:H	1.47	0.80
1:H:65:LEU:HD13	2:G:79:GLY:HA3	1.63	0.80
1:H:64:GLY:C	1:H:65:LEU:HD23	2.01	0.80
11:I:74:THR:CG2	11:I:91:ASN:OD1	2.30	0.80
11:I:95:GLU:HG3	11:I:97:ILE:H	1.45	0.80
11:I:54:ARG:HA	11:I:59:MET:O	1.82	0.79
11:I:59:MET:SD	11:I:59:MET:O	2.41	0.79
1:H:86:LEU:C	1:H:86:LEU:HD22	2.02	0.79
10:A:112:THR:HG21	10:A:118:VAL:HG21	1.65	0.79
10:F:79:HIS:HB3	10:F:81:TYR:H	1.48	0.79
10:F:155:VAL:O	10:F:155:VAL:CG1	2.31	0.78
9:D:24:GLY:O	9:D:25:ALA:HB3	1.83	0.78
9:D:5:LEU:HD12	9:D:6:THR:N	1.97	0.78
2:G:5:LYS:NZ	2:G:5:LYS:CB	2.41	0.78
6:C:55:LEU:O	6:C:58:ASP:OD1	2.02	0.77
9:D:54:ARG:HD3	9:D:55:LEU:CA	2.13	0.77
10:A:160:ILE:CB	10:A:161:PRO:HD2	2.13	0.77
2:G:4:PRO:O	10:F:155:VAL:HG11	1.83	0.77
10:A:90:THR:HG22	10:F:91:ARG:HD3	1.67	0.76
10:A:160:ILE:CG2	10:A:161:PRO:CD	2.54	0.76
10:F:82:MET:SD	10:F:82:MET:N	2.57	0.76
10:F:99:LEU:HD21	10:F:102:TRP:HE3	1.51	0.76
9:D:14:ASP:HB2	9:D:92:ARG:NH2	2.00	0.76
11:I:23:GLU:HB2	11:I:26:VAL:HG23	1.68	0.76
8:J:29:LEU:C	8:J:30:ASN:ND2	2.39	0.75
10:F:112:THR:HG21	10:F:118:VAL:HG21	1.68	0.75
8:J:30:ASN:ND2	8:J:30:ASN:N	2.35	0.74
8:J:31:LEU:HD13	10:F:143:LEU:HD21	1.68	0.74
6:C:118:ARG:HH11	6:C:118:ARG:CG	2.00	0.74
2:G:5:LYS:H	10:F:155:VAL:HG21	1.52	0.74
10:A:153:GLU:OE2	10:A:154:LEU:N	2.21	0.74
7:B:34:TYR:CD1	7:B:34:TYR:C	2.61	0.74
7:B:62:GLN:CB	7:B:65:ASN:O	2.36	0.73
2:G:4:PRO:O	10:F:155:VAL:HG13	1.89	0.73
1:H:16:VAL:HG22	1:H:102:LEU:HD13	1.70	0.73
10:A:78:GLN:O	10:A:81:TYR:HB2	1.89	0.73
9:D:94:ARG:CG	9:D:95:GLU:O	2.37	0.72
2:G:102:GLY:CA	8:J:29:LEU:O	2.37	0.72
2:G:62:GLN:N	2:G:63:ALA:HA	2.04	0.72
1:H:65:LEU:HD11	2:G:94:TYR:CD1	2.24	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:64:GLY:O	1:H:65:LEU:HD23	1.89	0.72
7:B:60:GLY:CA	7:B:61:ASN:C	2.58	0.72
9:D:21:LEU:HD23	9:D:27:LEU:HD23	1.70	0.72
10:A:147:ARG:HG3	10:A:147:ARG:HH11	1.55	0.72
9:D:17:GLY:CA	9:D:32:ASP:HB2	2.16	0.71
1:H:2:ALA:O	1:H:6:LYS:HG3	1.91	0.71
10:A:147:ARG:CG	10:A:147:ARG:HH11	2.04	0.71
10:F:154:LEU:HD11	10:F:157:GLN:CB	2.10	0.71
10:F:151:LYS:HG2	10:F:152:GLU:N	2.05	0.71
6:C:66:SER:HB3	7:B:77:MET:HB2	1.73	0.70
9:D:94:ARG:HG3	9:D:95:GLU:O	1.91	0.70
11:I:54:ARG:O	11:I:54:ARG:HG2	1.89	0.70
8:J:29:LEU:CA	8:J:30:ASN:ND2	2.54	0.70
8:J:57:SER:O	8:J:59:PRO:HD3	1.91	0.70
10:F:159:GLY:O	10:F:161:PRO:HD3	1.92	0.70
1:H:65:LEU:N	1:H:65:LEU:HD23	2.04	0.70
11:I:74:THR:HG22	11:I:91:ASN:OD1	1.92	0.70
10:A:90:THR:CG2	10:F:91:ARG:HD3	2.22	0.69
11:I:54:ARG:HB3	11:I:59:MET:HA	1.69	0.69
9:D:54:ARG:HD3	9:D:55:LEU:HA	1.71	0.69
8:E:90:ALA:CA	8:E:91:SER:HB3	2.23	0.69
11:I:24:GLY:N	11:I:25:ALA:HA	2.04	0.68
8:E:2:GLU:HG2	8:E:2:GLU:O	1.94	0.68
9:D:24:GLY:O	9:D:25:ALA:CB	2.40	0.67
9:D:64:LYS:O	9:D:78:THR:HG22	1.93	0.67
9:D:17:GLY:HA2	9:D:32:ASP:CB	2.18	0.67
9:D:60:ASN:O	9:D:62:PRO:CD	2.42	0.67
11:I:56:HIS:C	11:I:57:ARG:CD	2.59	0.67
10:A:159:GLY:O	10:A:160:ILE:CD1	2.42	0.67
11:I:17:GLY:HA2	11:I:32:ASP:CB	2.24	0.67
11:I:27:LEU:HD11	11:I:37:GLU:HG3	1.77	0.67
10:F:160:ILE:HG22	10:F:160:ILE:O	1.94	0.66
11:I:74:THR:HG23	11:I:91:ASN:OD1	1.95	0.66
1:H:86:LEU:HA	1:H:88:LEU:N	2.10	0.66
2:G:3:ARG:O	10:F:155:VAL:HG11	1.96	0.65
6:C:65:LEU:HG	7:B:79:GLY:HA3	1.76	0.65
9:D:22:SER:O	9:D:24:GLY:N	2.28	0.65
1:H:59:GLN:O	1:H:62:LYS:CG	2.45	0.65
9:D:59:MET:N	9:D:59:MET:SD	2.67	0.65
8:J:29:LEU:C	8:J:30:ASN:HD22	1.98	0.65
10:F:154:LEU:HD13	10:F:156:VAL:N	2.12	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:I:23:GLU:CD	11:I:23:GLU:N	2.49	0.65
7:B:59:ASN:N	7:B:59:ASN:OD1	2.29	0.64
7:B:3:ALA:N	7:B:4:PRO:CA	2.60	0.64
10:F:99:LEU:HD21	10:F:102:TRP:CE3	2.33	0.64
1:H:59:GLN:O	1:H:62:LYS:HG2	1.97	0.64
1:H:86:LEU:HD22	1:H:87:PRO:CA	2.27	0.64
8:J:1:MET:HB2	8:J:2:GLU:OE1	1.97	0.64
2:G:34:TYR:CD1	2:G:34:TYR:C	2.70	0.64
2:G:38:GLY:HA3	2:G:94:TYR:OH	1.97	0.64
7:B:60:GLY:HA2	7:B:61:ASN:O	1.97	0.64
2:G:61:ASN:OD1	2:G:68:ASN:OD1	2.16	0.64
8:J:59:PRO:O	8:J:60:THR:HG22	1.98	0.64
2:G:89:LEU:HD12	2:G:119:LEU:HD23	1.79	0.64
11:I:24:GLY:N	11:I:25:ALA:CA	2.60	0.63
8:J:58:ASP:OD2	8:J:61:ASP:N	2.32	0.63
2:G:74:MET:HB2	2:G:81:VAL:HB	1.78	0.63
11:I:94:ARG:H	11:I:94:ARG:HD3	1.63	0.63
11:I:35:ASN:O	11:I:36:ASP:C	2.37	0.63
8:J:26:SER:OG	8:J:81:GLY:O	2.15	0.63
11:I:17:GLY:CA	11:I:32:ASP:HB2	2.27	0.63
10:A:160:ILE:HG23	10:A:161:PRO:HG2	1.80	0.63
8:J:82:ILE:O	8:J:82:ILE:HG12	1.98	0.63
10:A:160:ILE:O	10:A:161:PRO:C	2.37	0.63
2:G:89:LEU:HD21	2:G:124:ALA:HB2	1.81	0.63
2:G:41:ASP:HB3	2:G:44:VAL:HG23	1.81	0.62
8:J:29:LEU:HA	8:J:30:ASN:HD22	1.64	0.62
10:A:153:GLU:OE2	10:A:153:GLU:CA	2.47	0.62
9:D:14:ASP:HB2	9:D:92:ARG:HH22	1.63	0.62
8:J:30:ASN:HB3	8:J:39:ASP:OD2	1.99	0.62
7:B:34:TYR:OH	7:B:37:TYR:OH	2.13	0.61
11:I:10:GLU:HG3	11:I:18:TYR:HE2	1.63	0.61
11:I:24:GLY:N	11:I:25:ALA:HB2	2.15	0.61
11:I:22:SER:O	11:I:25:ALA:CA	2.47	0.61
10:A:153:GLU:OE2	10:A:153:GLU:HA	2.00	0.61
9:D:36:ASP:O	9:D:38:GLN:N	2.32	0.61
6:C:58:ASP:OD1	6:C:59:GLN:HG2	2.00	0.61
9:D:97:ILE:HD12	9:D:97:ILE:C	2.20	0.60
9:D:67:SER:HB3	9:D:76:LEU:HD23	1.83	0.60
9:D:32:ASP:C	9:D:33:LEU:HD23	2.21	0.60
11:I:94:ARG:HH11	11:I:94:ARG:HG2	1.64	0.60
2:G:124:ALA:O	2:G:125:SER:C	2.39	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:30:ASN:CB	8:J:39:ASP:OD2	2.49	0.60
7:B:2:ALA:CB	10:A:156:VAL:HA	2.23	0.60
9:D:90:GLN:H	9:D:90:GLN:CD	2.05	0.60
11:I:72:GLU:C	11:I:91:ASN:ND2	2.55	0.60
2:G:115:LEU:O	2:G:119:LEU:HB2	2.02	0.59
2:G:41:ASP:OD2	2:G:42:ALA:N	2.35	0.59
2:G:10:VAL:HG11	2:G:115:LEU:HD21	1.85	0.59
8:J:1:MET:N	8:J:1:MET:HE2	2.14	0.59
7:B:7:LEU:HD23	10:A:154:LEU:HD11	1.85	0.59
8:J:29:LEU:HA	8:J:30:ASN:HD21	1.66	0.59
6:C:16:VAL:HG22	6:C:102:LEU:HD13	1.85	0.58
2:G:63:ALA:H	2:G:64:PHE:HA	1.68	0.58
11:I:36:ASP:O	11:I:36:ASP:CG	2.40	0.58
8:E:2:GLU:O	8:E:2:GLU:CG	2.51	0.58
7:B:22:THR:HG23	7:B:93:MET:HG2	1.86	0.58
9:D:19:LEU:HD12	9:D:21:LEU:HD21	1.84	0.58
10:A:89:SER:CB	1:H:124:SER:HA	2.34	0.58
11:I:56:HIS:HB3	11:I:57:ARG:HH11	1.69	0.58
11:I:3:SER:CB	11:I:6:THR:HG23	2.34	0.58
6:C:67:LYS:HB3	7:B:77:MET:HG3	1.86	0.58
11:I:73:HIS:N	11:I:91:ASN:ND2	2.52	0.58
11:I:94:ARG:NH1	11:I:94:ARG:HG3	2.15	0.58
9:D:54:ARG:HD2	9:D:55:LEU:CA	2.30	0.57
11:I:94:ARG:CG	11:I:94:ARG:NH1	2.53	0.57
9:D:69:VAL:HA	9:D:74:THR:HB	1.85	0.57
10:A:156:VAL:O	10:A:157:GLN:O	2.23	0.57
11:I:59:MET:SD	11:I:60:ASN:N	2.77	0.57
2:G:89:LEU:CD2	2:G:124:ALA:HB2	2.35	0.57
11:I:54:ARG:CA	11:I:59:MET:O	2.53	0.57
8:J:29:LEU:CA	8:J:30:ASN:HD22	2.15	0.57
1:H:86:LEU:CD2	1:H:87:PRO:HA	2.35	0.56
10:A:160:ILE:CG1	10:A:161:PRO:HD2	2.34	0.56
7:B:117:GLU:HB3	7:B:118:PRO:HD3	1.86	0.56
6:C:72:ILE:HG23	6:C:81:VAL:HG22	1.88	0.56
10:A:146:ILE:HG13	10:A:146:ILE:O	2.06	0.56
7:B:124:ALA:O	7:B:125:ALA:C	2.44	0.56
8:J:22:LEU:HD22	8:J:45:ILE:HD13	1.88	0.56
11:I:53:PHE:C	11:I:59:MET:O	2.44	0.56
11:I:95:GLU:OE1	11:I:96:PRO:CD	2.40	0.56
11:I:19:LEU:HD12	11:I:21:LEU:HD21	1.87	0.56
10:A:78:GLN:OE1	10:A:81:TYR:CE2	2.58	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:27:ARG:NH2	1:H:57:THR:HG21	2.21	0.56
10:A:78:GLN:O	10:A:81:TYR:N	2.37	0.55
11:I:56:HIS:O	11:I:57:ARG:CD	2.42	0.55
1:H:123:VAL:O	1:H:123:VAL:CG1	2.51	0.55
1:H:102:LEU:HG	8:J:47:VAL:HG21	1.88	0.55
11:I:16:LEU:O	11:I:33:LEU:HD13	2.05	0.55
11:I:35:ASN:N	11:I:35:ASN:OD1	2.36	0.55
2:G:122:VAL:CG1	10:F:156:VAL:HG11	2.37	0.55
6:C:43:HIS:HB2	6:C:46:ARG:HH21	1.71	0.55
2:G:9:GLN:NE2	2:G:9:GLN:C	2.60	0.55
1:H:61:SER:HB3	1:H:67:LYS:HD2	1.89	0.55
2:G:9:GLN:C	2:G:9:GLN:HE21	2.09	0.55
11:I:24:GLY:N	11:I:25:ALA:CB	2.70	0.55
1:H:27:ARG:HH22	1:H:57:THR:CG2	2.19	0.55
1:H:85:ARG:NH1	1:H:107:GLU:OE2	2.40	0.55
11:I:59:MET:SD	11:I:60:ASN:CB	2.95	0.54
11:I:9:LEU:HD23	11:I:9:LEU:N	2.22	0.54
11:I:33:LEU:HD12	11:I:33:LEU:H	1.71	0.54
6:C:102:LEU:HD12	8:E:47:VAL:HG21	1.90	0.54
11:I:3:SER:CB	11:I:6:THR:CG2	2.86	0.54
7:B:62:GLN:H	7:B:66:GLU:HG3	1.72	0.54
9:D:54:ARG:O	9:D:55:LEU:C	2.45	0.54
11:I:14:ASP:N	11:I:14:ASP:OD2	2.41	0.54
8:E:68:GLU:HG3	9:D:65:ARG:O	2.09	0.53
2:G:9:GLN:HE21	2:G:10:VAL:N	2.06	0.53
10:F:153:GLU:HB2	10:F:154:LEU:HB2	1.89	0.53
9:D:54:ARG:HD2	9:D:55:LEU:H	1.65	0.53
10:A:78:GLN:CD	10:A:81:TYR:CE2	2.82	0.53
11:I:32:ASP:OD2	11:I:32:ASP:N	2.42	0.52
10:F:160:ILE:O	10:F:160:ILE:CG2	2.57	0.52
2:G:5:LYS:N	10:F:155:VAL:HG21	2.21	0.52
11:I:12:ILE:HG12	10:F:120:ALA:HB2	1.92	0.52
1:H:86:LEU:C	1:H:86:LEU:HD13	2.29	0.52
7:B:41:ASP:HB3	7:B:44:VAL:HG23	1.92	0.52
1:H:63:LEU:HD13	2:G:81:VAL:HG21	1.92	0.52
1:H:5:LEU:HD11	1:H:113:LEU:HD11	1.92	0.51
11:I:23:GLU:C	11:I:25:ALA:CA	2.62	0.51
2:G:6:ALA:O	2:G:7:LEU:C	2.46	0.51
11:I:85:PHE:HB3	10:F:119:LEU:HD11	1.92	0.51
10:A:147:ARG:NH1	10:A:147:ARG:CG	2.68	0.51
8:J:68:GLU:HG2	10:F:124:ILE:HD11	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4:PRO:C	10:F:155:VAL:HG11	2.30	0.51
7:B:10:VAL:HG11	7:B:115:LEU:HD21	1.92	0.51
1:H:43:HIS:HB2	1:H:46:ARG:HH21	1.75	0.51
1:H:86:LEU:HD23	1:H:87:PRO:HA	1.92	0.51
6:C:118:ARG:NH1	6:C:118:ARG:CG	2.67	0.51
2:G:115:LEU:HD23	2:G:115:LEU:N	2.27	0.50
6:C:111:ALA:N	6:C:112:PRO:HD2	2.26	0.50
9:D:54:ARG:NE	9:D:55:LEU:HA	2.26	0.50
2:G:22:THR:HG23	2:G:93:MET:HG2	1.93	0.50
10:A:99:LEU:HD21	10:A:102:TRP:CZ3	2.47	0.50
7:B:74:MET:HB2	7:B:81:VAL:HB	1.93	0.50
9:D:36:ASP:HB3	9:D:39:ALA:HB3	1.93	0.50
6:C:118:ARG:HH11	6:C:118:ARG:HG2	1.75	0.50
2:G:122:VAL:CG1	10:F:156:VAL:CG1	2.89	0.50
7:B:2:ALA:HB1	7:B:3:ALA:HB2	1.94	0.50
9:D:16:LEU:O	9:D:33:LEU:HG	2.12	0.50
8:J:82:ILE:HG21	10:F:143:LEU:CD1	2.41	0.50
10:A:78:GLN:HB3	10:A:81:TYR:CD2	2.47	0.49
7:B:19:VAL:HG11	7:B:93:MET:CE	2.42	0.49
8:E:22:LEU:HD22	8:E:45:ILE:HD13	1.93	0.49
11:I:64:LYS:HG3	10:F:112:THR:HG22	1.94	0.49
9:D:94:ARG:HG2	9:D:95:GLU:O	2.13	0.49
11:I:36:ASP:OD2	11:I:38:GLN:HG3	2.12	0.49
7:B:47:ALA:O	7:B:50:SER:OG	2.27	0.49
11:I:94:ARG:HD3	11:I:94:ARG:N	2.27	0.49
1:H:86:LEU:CD2	1:H:87:PRO:CA	2.91	0.49
11:I:19:LEU:HG	11:I:86:VAL:HB	1.95	0.49
11:I:21:LEU:HB2	11:I:84:VAL:HB	1.95	0.49
7:B:117:GLU:HB3	7:B:118:PRO:CD	2.43	0.49
2:G:62:GLN:N	2:G:63:ALA:CA	2.76	0.48
9:D:90:GLN:HG2	9:D:92:ARG:HE	1.79	0.48
8:E:47:VAL:O	8:E:51:GLN:HG3	2.13	0.48
10:F:144:SER:O	10:F:147:ARG:HD3	2.12	0.48
9:D:37:GLU:HA	9:D:40:ALA:HB3	1.96	0.48
10:A:153:GLU:C	10:A:153:GLU:OE2	2.52	0.48
9:D:5:LEU:C	9:D:5:LEU:HD12	2.33	0.48
8:E:22:LEU:HG	8:E:23:CYS:N	2.28	0.48
1:H:27:ARG:HH22	1:H:57:THR:HG21	1.78	0.48
10:A:99:LEU:HD21	10:A:102:TRP:HZ3	1.78	0.48
7:B:2:ALA:CB	10:A:156:VAL:CA	2.86	0.47
9:D:69:VAL:HG11	10:A:129:LEU:HD11	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:58:ASP:OD1	6:C:58:ASP:C	2.50	0.47
9:D:22:SER:O	9:D:26:VAL:HG13	2.14	0.47
1:H:102:LEU:HD23	1:H:102:LEU:HA	1.76	0.47
11:I:95:GLU:CD	11:I:96:PRO:HD2	2.31	0.47
8:E:51:GLN:HB2	9:D:46:LEU:HD23	1.96	0.47
1:H:53:PHE:HB2	1:H:82:GLN:OE1	2.15	0.47
11:I:55:LEU:N	11:I:55:LEU:HD13	2.29	0.47
2:G:59:ASN:OD1	2:G:59:ASN:O	2.33	0.47
1:H:87:PRO:HD2	1:H:118:ARG:HD3	1.96	0.47
2:G:40:THR:CB	2:G:41:ASP:CA	2.56	0.47
9:D:31:GLY:C	9:D:32:ASP:OD2	2.53	0.47
9:D:56:HIS:HB3	9:D:57:ARG:HH21	1.80	0.47
11:I:56:HIS:O	11:I:58:GLY:N	2.48	0.47
9:D:65:ARG:NH2	9:D:76:LEU:HD22	2.30	0.47
2:G:3:ARG:CB	2:G:4:PRO:CD	2.93	0.47
8:E:90:ALA:CA	8:E:91:SER:CB	2.91	0.46
2:G:62:GLN:CB	2:G:63:ALA:HA	2.41	0.46
11:I:10:GLU:HG3	11:I:18:TYR:CE2	2.47	0.46
7:B:2:ALA:HA	7:B:3:ALA:HA	1.79	0.46
9:D:22:SER:O	9:D:22:SER:OG	2.32	0.46
2:G:122:VAL:HG12	10:F:156:VAL:HG11	1.96	0.46
8:J:82:ILE:HG21	10:F:143:LEU:HD12	1.97	0.46
8:E:22:LEU:HD21	8:E:24:THR:HG23	1.98	0.46
7:B:34:TYR:CD1	7:B:35:SER:N	2.84	0.46
9:D:24:GLY:CA	9:D:26:VAL:CG1	2.70	0.46
10:A:160:ILE:HG13	10:A:161:PRO:HD2	1.98	0.46
9:D:12:ILE:HG23	9:D:13:PRO:HD2	1.98	0.46
2:G:89:LEU:CD2	2:G:124:ALA:CB	2.94	0.46
8:E:58:ASP:C	8:E:58:ASP:OD2	2.54	0.46
10:A:78:GLN:O	10:A:81:TYR:CB	2.62	0.46
8:J:1:MET:HE3	8:J:1:MET:C	2.37	0.46
7:B:2:ALA:CB	10:A:156:VAL:N	2.78	0.45
7:B:62:GLN:H	7:B:66:GLU:HA	1.81	0.45
10:F:151:LYS:HG2	10:F:152:GLU:HG2	1.98	0.45
1:H:76:ASN:HA	2:G:70:LYS:HE2	1.98	0.45
7:B:57:ASP:O	7:B:60:GLY:O	2.34	0.45
2:G:102:GLY:N	8:J:29:LEU:O	2.48	0.45
2:G:40:THR:HB	2:G:41:ASP:C	2.33	0.45
1:H:59:GLN:O	1:H:62:LYS:HG3	2.16	0.45
10:F:79:HIS:HB3	10:F:81:TYR:N	2.23	0.45
10:A:77:ALA:HA	10:A:78:GLN:HA	1.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:90:ALA:HA	8:E:91:SER:CB	2.23	0.45
10:F:146:ILE:O	10:F:146:ILE:HG22	2.16	0.45
1:H:10:TYR:CD2	1:H:13:LEU:HD12	2.51	0.45
6:C:102:LEU:CD1	8:E:47:VAL:HG21	2.47	0.45
9:D:56:HIS:C	9:D:57:ARG:HD3	2.37	0.45
9:D:57:ARG:CA	9:D:59:MET:H	2.23	0.45
11:I:69:VAL:HG13	11:I:74:THR:HG22	1.99	0.45
8:J:1:MET:HB2	8:J:2:GLU:H	1.67	0.45
7:B:34:TYR:HD1	7:B:35:SER:N	2.15	0.45
2:G:31:LEU:HD21	2:G:34:TYR:HB3	1.98	0.45
8:J:60:THR:HG23	8:J:60:THR:O	2.16	0.45
2:G:122:VAL:HG11	10:F:156:VAL:HG13	2.00	0.44
11:I:22:SER:C	11:I:25:ALA:CB	2.74	0.44
10:F:140:TYR:O	10:F:143:LEU:HB2	2.17	0.44
8:J:57:SER:O	8:J:59:PRO:CD	2.64	0.44
1:H:85:ARG:O	1:H:86:LEU:C	2.55	0.44
6:C:4:ASP:O	6:C:7:ARG:HB2	2.18	0.44
2:G:114:TYR:HD2	2:G:115:LEU:CD2	2.31	0.44
2:G:60:GLY:HA2	2:G:67:ASP:O	2.18	0.44
6:C:11:LYS:HB3	10:A:105:LEU:HD11	2.00	0.43
6:C:2:ALA:O	6:C:6:LYS:HG3	2.18	0.43
9:D:94:ARG:HG3	9:D:97:ILE:O	2.18	0.43
11:I:95:GLU:CG	11:I:97:ILE:H	2.24	0.43
7:B:60:GLY:HA2	7:B:62:GLN:N	2.29	0.43
9:D:61:VAL:HA	9:D:62:PRO:HD2	1.81	0.43
11:I:73:HIS:N	11:I:91:ASN:HD21	2.14	0.43
8:E:15:ASN:HA	8:E:16:PRO:HD3	1.87	0.43
10:A:155:VAL:O	10:A:155:VAL:HG13	2.18	0.43
6:C:118:ARG:NH1	6:C:118:ARG:HG2	2.34	0.43
6:C:53:PHE:HB2	6:C:82:GLN:OE1	2.18	0.43
10:F:152:GLU:HG2	10:F:152:GLU:H	1.50	0.43
2:G:13:GLN:NE2	10:F:149:ASP:O	2.51	0.43
2:G:9:GLN:HE22	2:G:13:GLN:HE21	1.67	0.43
1:H:83:PHE:CD2	1:H:107:GLU:HG3	2.53	0.43
10:A:114:GLN:O	10:A:118:VAL:HG23	2.18	0.42
8:J:22:LEU:HD22	8:J:45:ILE:CD1	2.49	0.42
9:D:74:THR:HG22	9:D:91:ASN:OD1	2.19	0.42
11:I:54:ARG:CB	11:I:59:MET:CA	2.72	0.42
8:E:25:ASP:OD1	8:E:25:ASP:C	2.58	0.42
7:B:34:TYR:OH	7:B:37:TYR:CZ	2.47	0.42
1:H:57:THR:OG1	1:H:68:ASN:HB3	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:114:GLN:HB3	10:A:114:GLN:HE21	1.65	0.42
11:I:22:SER:O	11:I:25:ALA:C	2.56	0.42
6:C:67:LYS:CB	7:B:77:MET:HG3	2.48	0.42
6:C:55:LEU:O	6:C:59:GLN:HG2	2.20	0.42
1:H:102:LEU:HD21	11:I:53:PHE:CE2	2.55	0.42
6:C:5:LEU:HD11	6:C:113:LEU:HD11	2.01	0.42
6:C:6:LYS:HE3	6:C:33:ILE:HG13	2.02	0.42
11:I:69:VAL:HA	11:I:74:THR:HB	2.02	0.42
2:G:89:LEU:HD21	2:G:124:ALA:CB	2.50	0.41
9:D:3:THR:HA	9:D:6:THR:HG23	2.02	0.41
9:D:89:ARG:HD3	9:D:90:GLN:NE2	2.35	0.41
1:H:123:VAL:O	1:H:124:SER:CB	2.68	0.41
10:A:146:ILE:CG1	10:A:146:ILE:O	2.69	0.41
7:B:61:ASN:CA	7:B:68:ASN:OD1	2.68	0.41
9:D:14:ASP:O	9:D:16:LEU:HD23	2.21	0.41
1:H:119:GLN:O	10:F:91:ARG:NH2	2.53	0.41
8:E:15:ASN:HB3	8:E:18:ILE:HB	2.03	0.41
1:H:86:LEU:HA	1:H:87:PRO:C	2.40	0.41
2:G:100:GLY:HA3	8:J:30:ASN:O	2.20	0.41
11:I:65:ARG:HA	11:I:78:THR:HG22	2.03	0.41
8:J:30:ASN:HB2	8:J:39:ASP:OD2	2.20	0.41
8:E:55:LEU:HD21	9:D:43:ILE:HG13	2.03	0.41
6:C:102:LEU:HG	8:E:47:VAL:HG21	2.03	0.41
1:H:65:LEU:HD11	2:G:94:TYR:HD1	1.82	0.41
11:I:77:VAL:HA	11:I:85:PHE:O	2.22	0.40
7:B:106:ALA:O	10:A:146:ILE:HD11	2.20	0.40
10:A:78:GLN:HB3	10:A:81:TYR:CG	2.57	0.40
10:A:89:SER:HB2	1:H:124:SER:HA	2.03	0.40
9:D:69:VAL:HG11	10:A:129:LEU:CD1	2.50	0.40
9:D:24:GLY:C	9:D:26:VAL:H	2.10	0.40
2:G:117:GLU:CB	2:G:118:PRO:CD	2.82	0.40
11:I:54:ARG:HA	11:I:59:MET:C	2.41	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	H	122/124 (98%)	119 (98%)	3 (2%)	0	100	100
1	m	122/124 (98%)	117 (96%)	5 (4%)	0	100	100
2	G	121/125 (97%)	108 (89%)	13 (11%)	0	100	100
2	l	122/125 (98%)	119 (98%)	3 (2%)	0	100	100
3	o	88/90 (98%)	83 (94%)	5 (6%)	0	100	100
4	n	86/88 (98%)	82 (95%)	4 (5%)	0	100	100
5	k	83/85 (98%)	75 (90%)	8 (10%)	0	100	100
6	C	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
7	B	123/125 (98%)	118 (96%)	4 (3%)	1 (1%)	19	55
8	E	89/91 (98%)	85 (96%)	4 (4%)	0	100	100
8	J	89/91 (98%)	85 (96%)	4 (4%)	0	100	100
9	D	94/96 (98%)	81 (86%)	12 (13%)	1 (1%)	14	48
10	A	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	13	46
10	F	83/85 (98%)	77 (93%)	5 (6%)	1 (1%)	13	46
11	I	93/99 (94%)	84 (90%)	9 (10%)	0	100	100
All	All	1519/1556 (98%)	1428 (94%)	87 (6%)	4 (0%)	41	75

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	A	157	GLN
10	F	155	VAL
7	B	3	ALA
9	D	13	PRO

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	H	107/108 (99%)	94 (88%)	13 (12%)	5 20
1	m	104/108 (96%)	96 (92%)	8 (8%)	13 41
2	G	91/98 (93%)	74 (81%)	17 (19%)	1 8
2	l	94/98 (96%)	75 (80%)	19 (20%)	1 6
3	o	75/76 (99%)	69 (92%)	6 (8%)	12 39
4	n	63/72 (88%)	44 (70%)	19 (30%)	0 1
5	k	71/74 (96%)	58 (82%)	13 (18%)	1 8
6	C	106/106 (100%)	95 (90%)	11 (10%)	7 26
7	B	90/93 (97%)	72 (80%)	18 (20%)	1 6
8	E	77/77 (100%)	69 (90%)	8 (10%)	7 26
8	J	77/77 (100%)	68 (88%)	9 (12%)	5 21
9	D	76/79 (96%)	56 (74%)	20 (26%)	0 2
10	A	73/75 (97%)	61 (84%)	12 (16%)	2 11
10	F	73/75 (97%)	58 (80%)	15 (20%)	1 5
11	I	70/83 (84%)	52 (74%)	18 (26%)	0 2
All	All	1247/1299 (96%)	1041 (84%)	206 (16%)	2 10

All (206) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	m	4	ASP
1	m	5	LEU
1	m	58	ASP
1	m	85	ARG
1	m	86	LEU
1	m	102	LEU
1	m	117	LEU
1	m	118	ARG
2	l	1	MET
2	l	2	LEU
2	l	7	LEU
2	l	9	GLN
2	l	24	LEU
2	l	25	LEU
2	l	31	LEU
2	l	40	THR
2	l	58	ARG
2	l	62	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	l	64	PHE
2	l	67	ASP
2	l	71	PHE
2	l	91	LEU
2	l	94	TYR
2	l	97	GLU
2	l	113	GLN
2	l	120	THR
2	l	121	GLN
3	o	23	CYS
3	o	29	LEU
3	o	39	ASP
3	o	56	THR
3	o	58	ASP
3	o	82	ILE
4	n	15	GLN
4	n	16	LEU
4	n	18	TYR
4	n	19	LEU
4	n	20	VAL
4	n	22	SER
4	n	26	VAL
4	n	27	LEU
4	n	32	ASP
4	n	33	LEU
4	n	46	LEU
4	n	51	CYS
4	n	57	ARG
4	n	59	MET
4	n	63	PHE
4	n	65	ARG
4	n	74	THR
4	n	89	ARG
4	n	92	ARG
5	k	79	HIS
5	k	80	GLU
5	k	98	SER
5	k	105	LEU
5	k	116	HIS
5	k	117	GLN
5	k	118	VAL
5	k	130	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	k	149	ASP
5	k	152	GLU
5	k	155	VAL
5	k	156	VAL
5	k	158	PHE
6	C	4	ASP
6	C	5	LEU
6	C	27	ARG
6	C	55	LEU
6	C	65	LEU
6	C	67	LYS
6	C	85	ARG
6	C	86	LEU
6	C	102	LEU
6	C	117	LEU
6	C	118	ARG
7	B	9	GLN
7	B	24	LEU
7	B	25	LEU
7	B	30	SER
7	B	31	LEU
7	B	34	TYR
7	B	40	THR
7	B	59	ASN
7	B	66	GLU
7	B	67	ASP
7	B	71	PHE
7	B	88	ASN
7	B	91	LEU
7	B	94	TYR
7	B	97	GLU
7	B	111	LEU
7	B	120	THR
7	B	121	GLN
8	E	2	GLU
8	E	5	LEU
8	E	15	ASN
8	E	22	LEU
8	E	29	LEU
8	E	39	ASP
8	E	40	GLU
8	E	68	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	D	6	THR
9	D	10	GLU
9	D	15	GLN
9	D	16	LEU
9	D	19	LEU
9	D	21	LEU
9	D	22	SER
9	D	26	VAL
9	D	36	ASP
9	D	44	SER
9	D	46	LEU
9	D	54	ARG
9	D	57	ARG
9	D	59	MET
9	D	64	LYS
9	D	65	ARG
9	D	74	THR
9	D	90	GLN
9	D	95	GLU
9	D	97	ILE
10	A	79	HIS
10	A	80	GLU
10	A	82	MET
10	A	83	ASP
10	A	99	LEU
10	A	114	GLN
10	A	130	GLN
10	A	146	ILE
10	A	147	ARG
10	A	153	GLU
10	A	154	LEU
10	A	160	ILE
1	H	4	ASP
1	H	5	LEU
1	H	58	ASP
1	H	62	LYS
1	H	66	SER
1	H	67	LYS
1	H	76	ASN
1	H	78	TYR
1	H	86	LEU
1	H	102	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	109	GLU
1	H	117	LEU
1	H	123	VAL
2	G	5	LYS
2	G	7	LEU
2	G	9	GLN
2	G	25	LEU
2	G	31	LEU
2	G	34	TYR
2	G	40	THR
2	G	61	ASN
2	G	67	ASP
2	G	71	PHE
2	G	91	LEU
2	G	94	TYR
2	G	97	GLU
2	G	111	LEU
2	G	115	LEU
2	G	120	THR
2	G	121	GLN
8	J	1	MET
8	J	15	ASN
8	J	22	LEU
8	J	30	ASN
8	J	38	SER
8	J	58	ASP
8	J	60	THR
8	J	73	ASN
8	J	82	ILE
11	I	5	LEU
11	I	15	GLN
11	I	16	LEU
11	I	19	LEU
11	I	23	GLU
11	I	27	LEU
11	I	32	ASP
11	I	35	ASN
11	I	38	GLN
11	I	46	LEU
11	I	54	ARG
11	I	55	LEU
11	I	57	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	I	59	MET
11	I	65	ARG
11	I	74	THR
11	I	89	ARG
11	I	94	ARG
10	F	78	GLN
10	F	79	HIS
10	F	82	MET
10	F	83	ASP
10	F	100	THR
10	F	104	LYS
10	F	113	SER
10	F	124	ILE
10	F	134	ARG
10	F	147	ARG
10	F	151	LYS
10	F	152	GLU
10	F	153	GLU
10	F	154	LEU
10	F	160	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
2	l	9	GLN
2	l	113	GLN
2	l	121	GLN
4	n	15	GLN
4	n	90	GLN
5	k	79	HIS
5	k	117	GLN
5	k	145	GLN
5	k	157	GLN
7	B	121	GLN
9	D	82	GLN
10	A	78	GLN
10	A	114	GLN
2	G	9	GLN
2	G	59	ASN
2	G	121	GLN
8	J	30	ASN
11	I	56	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	F	114	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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	H	124/124 (100%)	-0.27	2 (1%) 72 43	37, 53, 81, 99	0
1	m	124/124 (100%)	-0.34	2 (1%) 72 43	28, 54, 74, 115	0
2	G	123/125 (98%)	0.17	11 (8%) 9 3	39, 57, 103, 143	0
2	l	124/125 (99%)	-0.11	8 (6%) 18 5	25, 42, 91, 148	0
3	o	90/90 (100%)	-0.20	2 (2%) 62 32	37, 59, 97, 108	0
4	n	88/88 (100%)	1.15	22 (25%) 0 0	65, 109, 134, 154	0
5	k	85/85 (100%)	0.46	11 (12%) 3 1	38, 69, 115, 124	0
6	C	123/123 (100%)	-0.41	0 100 100	21, 46, 66, 102	0
7	B	125/125 (100%)	-0.00	7 (5%) 24 8	21, 49, 87, 138	0
8	E	91/91 (100%)	-0.28	1 (1%) 80 55	25, 35, 55, 65	0
8	J	91/91 (100%)	-0.31	0 100 100	30, 47, 78, 99	0
9	D	96/96 (100%)	0.05	4 (4%) 36 14	23, 47, 75, 86	0
10	A	85/85 (100%)	-0.08	4 (4%) 31 11	32, 49, 74, 88	0
10	F	85/85 (100%)	0.05	3 (3%) 44 18	37, 58, 79, 96	0
11	I	95/99 (95%)	0.10	2 (2%) 63 34	41, 68, 101, 107	0
All	All	1549/1556 (99%)	-0.03	79 (5%) 28 10	21, 53, 108, 154	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	B	63	ALA	6.5
2	G	64	PHE	6.5
7	B	64	PHE	6.2
2	l	61	ASN	5.5
2	G	65	ASN	5.1
2	l	63	ALA	5.0
1	H	124	SER	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	n	6	THR	4.4
5	k	120	ALA	4.3
2	l	62	GLN	4.3
2	l	64	PHE	4.2
8	E	91	SER	4.1
9	D	2	ALA	4.1
2	G	62	GLN	4.1
4	n	7	ALA	4.1
10	A	161	PRO	4.0
1	m	124	SER	3.9
1	m	1	MET	3.8
2	G	66	GLU	3.8
9	D	29	SER	3.8
2	l	66	GLU	3.7
1	H	1	MET	3.7
2	G	61	ASN	3.7
5	k	117	GLN	3.7
7	B	61	ASN	3.7
2	G	60	GLY	3.6
4	n	29	SER	3.6
9	D	96	PRO	3.5
2	l	123	ALA	3.5
10	F	78	GLN	3.5
4	n	90	GLN	3.4
4	n	55	LEU	3.4
5	k	122	GLU	3.3
2	G	63	ALA	3.2
10	A	77	ALA	3.2
2	l	65	ASN	3.2
5	k	112	THR	3.1
7	B	65	ASN	3.1
5	k	101	HIS	3.0
2	G	4	PRO	3.0
4	n	5	ALA	2.9
4	n	25	ALA	2.9
2	G	59	ASN	2.9
4	n	9	LEU	2.9
3	o	70	ASP	2.8
2	l	60	GLY	2.8
2	G	123	ALA	2.8
4	n	54	ARG	2.7
10	F	80	GLU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	G	124	ALA	2.6
4	n	31	GLY	2.6
10	A	78	GLN	2.6
10	F	161	PRO	2.5
11	I	96	PRO	2.5
4	n	60	ASN	2.5
4	n	24	GLY	2.5
5	k	105	LEU	2.5
4	n	30	SER	2.5
5	k	103	LYS	2.4
4	n	8	GLY	2.4
4	n	23	GLU	2.4
5	k	102	TRP	2.4
4	n	32	ASP	2.4
5	k	78	ALA	2.3
4	n	59	MET	2.2
4	n	12	ILE	2.2
9	D	97	ILE	2.2
10	A	160	ILE	2.2
11	I	92	ARG	2.2
4	n	35	ASN	2.2
5	k	116	HIS	2.1
3	o	90	ALA	2.1
7	B	60	GLY	2.1
7	B	66	GLU	2.1
4	n	28	ALA	2.1
5	k	161	PRO	2.1
4	n	13	PRO	2.0
7	B	1	ALA	2.0
4	n	56	HIS	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 carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.