Full wwPDB X-ray Structure Validation Report (i)

Jan 14, 2024 – 03:47 am GMT

PDB ID	:	6S4S
Title	:	CBDP35 Native structure
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Deposited on	:	2019-06-28
Resolution	:	2.15 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:

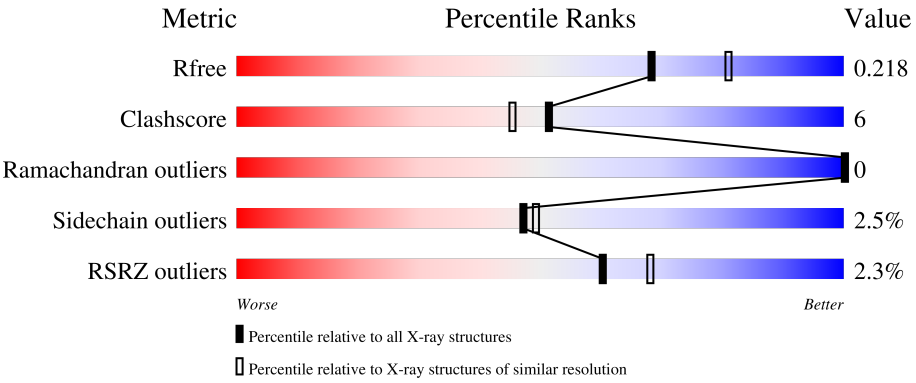
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	140	89% 11%
2	B	139	2% 88% 12%
2	D	139	89% 11%
2	E	139	90% 9%
2	F	139	89% 11%

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Mol	Chain	Length	Quality of chain
2	G	139	86% 11%
2	H	139	3% 86% 12%
2	I	139	6% 88% 12%
2	K	139	% 89% 11%
2	L	139	4% 91% 7%
3	C	140	4% 81% 18%
3	J	140	5% 82% 14%

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
4	MLI	C	301	-	-	X	-
4	MLI	G	302	-	-	X	-
4	MLI	G	303	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15077 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 PlyP35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	140	Total	C	N	O	S	0	0	0
			1140	734	204	197	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	HIS	-	expression tag	UNP A8ATR6
A	153	MET	-	expression tag	UNP A8ATR6
A	154	MET	-	expression tag	UNP A8ATR6
A	291	GLY	-	expression tag	UNP A8ATR6

- Molecule 2 is a protein called PlyP35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	139	Total	C	N	O	S	0	0	0
			1135	732	202	196	5			
2	D	139	Total	C	N	O	S	0	0	0
			1135	732	202	196	5			
2	E	139	Total	C	N	O	S	0	0	0
			1135	732	202	196	5			
2	F	139	Total	C	N	O	S	0	0	0
			1135	732	202	196	5			
2	G	139	Total	C	N	O	S	0	0	0
			1135	732	202	196	5			
2	H	139	Total	C	N	O	S	0	0	0
			1135	732	202	196	5			
2	I	139	Total	C	N	O	S	0	0	0
			1135	732	202	196	5			
2	L	139	Total	C	N	O	S	0	0	0
			1135	732	202	196	5			
2	K	139	Total	C	N	O	S	0	0	0
			1135	732	202	196	5			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	153	MET	-	initiating methionine	UNP A8ATR6
B	154	MET	-	expression tag	UNP A8ATR6
D	153	MET	-	initiating methionine	UNP A8ATR6
D	154	MET	-	expression tag	UNP A8ATR6
E	153	MET	-	initiating methionine	UNP A8ATR6
E	154	MET	-	expression tag	UNP A8ATR6
F	153	MET	-	initiating methionine	UNP A8ATR6
F	154	MET	-	expression tag	UNP A8ATR6
G	153	MET	-	initiating methionine	UNP A8ATR6
G	154	MET	-	expression tag	UNP A8ATR6
H	153	MET	-	initiating methionine	UNP A8ATR6
H	154	MET	-	expression tag	UNP A8ATR6
I	153	MET	-	initiating methionine	UNP A8ATR6
I	154	MET	-	expression tag	UNP A8ATR6
L	153	MET	-	initiating methionine	UNP A8ATR6
L	154	MET	-	expression tag	UNP A8ATR6
K	153	MET	-	initiating methionine	UNP A8ATR6
K	154	MET	-	expression tag	UNP A8ATR6

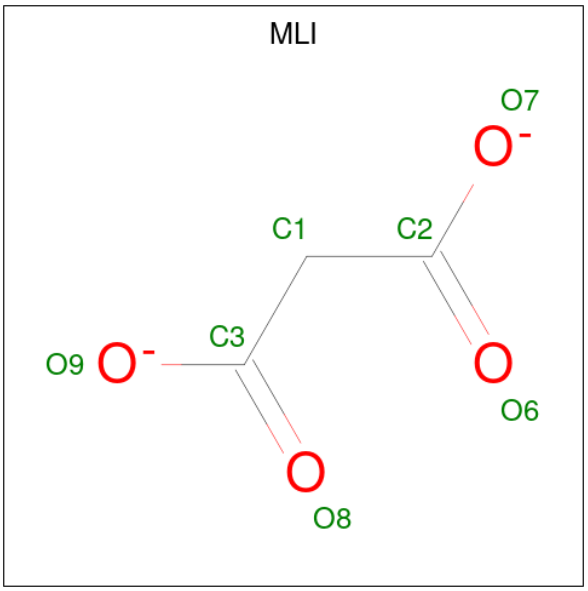
- Molecule 3 is a protein called PlyP35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	139	Total	C	N	O	S	0	0	0
			1136	732	203	196	5			
3	J	137	Total	C	N	O	S	0	0	0
			1118	721	199	194	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	152	HIS	-	expression tag	UNP A8ATR6
C	153	MET	-	expression tag	UNP A8ATR6
C	154	MET	-	expression tag	UNP A8ATR6
J	152	HIS	-	expression tag	UNP A8ATR6
J	153	MET	-	expression tag	UNP A8ATR6
J	154	MET	-	expression tag	UNP A8ATR6

- Molecule 4 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 7 3 4	0	0
4	C	1	Total C O 7 3 4	0	0
4	G	1	Total C O 7 3 4	0	0
4	G	1	Total C O 7 3 4	0	0
4	G	1	Total C O 7 3 4	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	132	Total O 132 132	0	0
5	B	116	Total O 116 116	0	0
5	C	105	Total O 105 105	0	0
5	D	158	Total O 158 158	0	0
5	E	105	Total O 105 105	0	0
5	F	98	Total O 98 98	0	0
5	G	141	Total O 141 141	0	0

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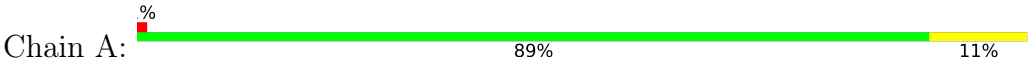
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	151	Total O 151 151	0	0
5	I	109	Total O 109 109	0	0
5	J	76	Total O 76 76	0	0
5	L	101	Total O 101 101	0	0
5	K	141	Total O 141 141	0	0

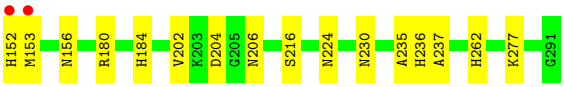
3 Residue-property plots (i)

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: PlyP35

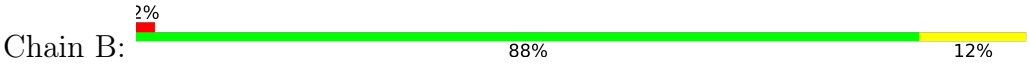
Chain A:

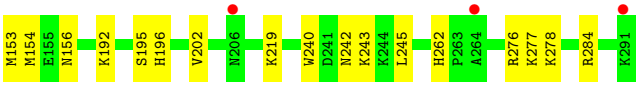




• Molecule 2: PlyP35

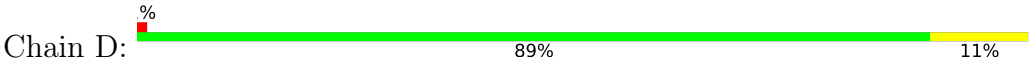
Chain B:





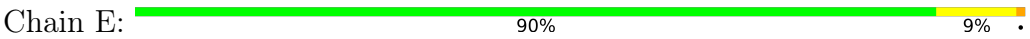
• Molecule 2: PlyP35

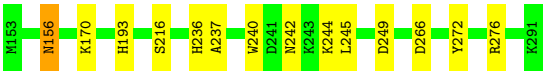
Chain D:



• Molecule 2: PlyP35

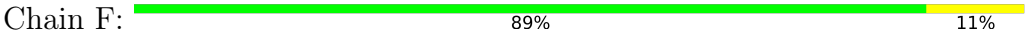
Chain E:





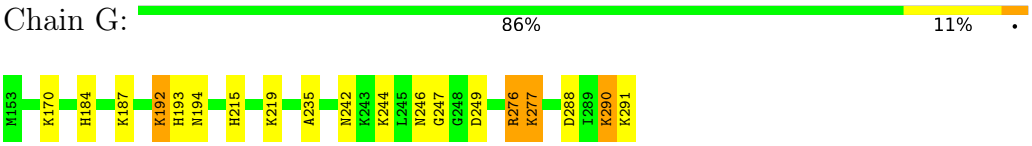
• Molecule 2: PlyP35

Chain F:



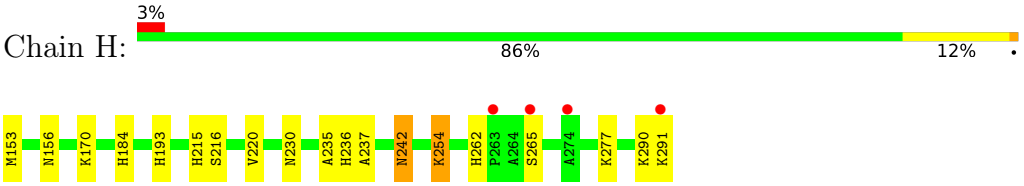
• Molecule 2: PlyP35

Chain G:



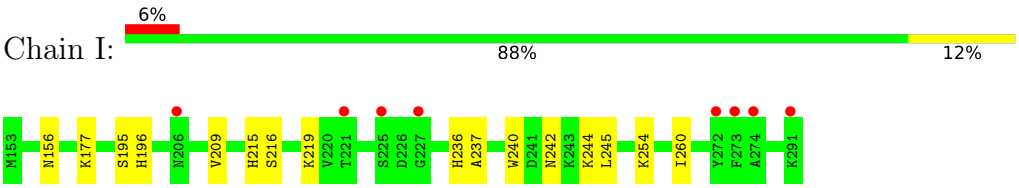
• Molecule 2: PlyP35

Chain H:



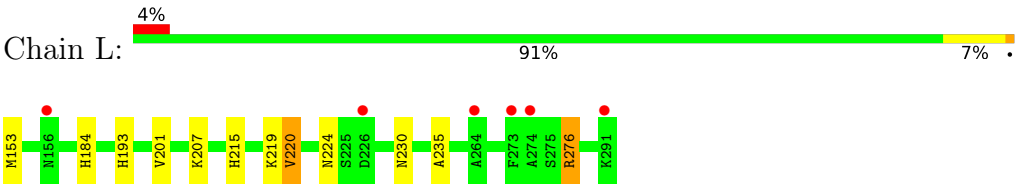
• Molecule 2: PlyP35

Chain I:



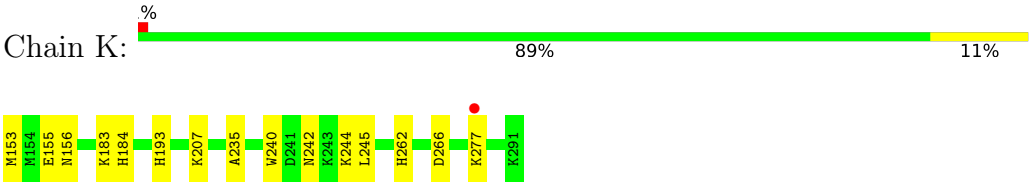
• Molecule 2: PlyP35

Chain L:



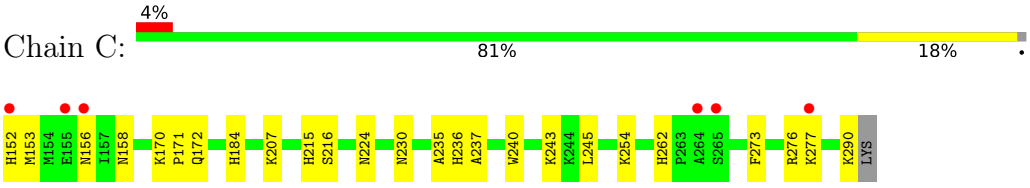
• Molecule 2: PlyP35

Chain K:



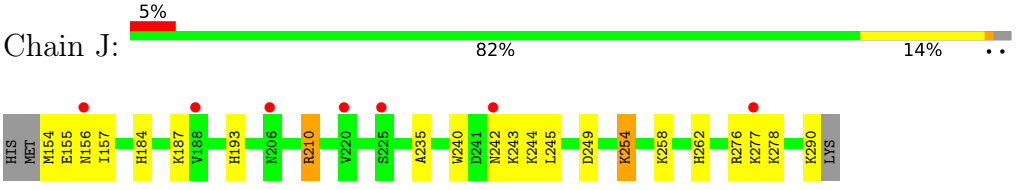
• Molecule 3: PlyP35

Chain C:



• Molecule 3: PlyP35

Chain J:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	333.32Å 95.12Å 83.85Å 90.00° 90.33° 90.00°	Depositor
Resolution (Å)	47.60 – 2.15 47.56 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.60-2.15) 99.9 (47.56-2.15)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.186 , 0.212 0.192 , 0.218	Depositor DCC
R_{free} test set	7164 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	32.0	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 49.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15077	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.20 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5806e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

Bond lengths and bond angles in the following residue types are not validated in this section: MLI

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	0.73	0/1173	0.89	0/1576
2	B	0.65	0/1167	0.90	2/1567 (0.1%)
2	D	0.70	0/1167	0.87	2/1567 (0.1%)
2	E	0.69	0/1167	0.92	2/1567 (0.1%)
2	F	0.70	0/1167	0.85	0/1567
2	G	0.70	0/1167	0.91	2/1567 (0.1%)
2	H	0.72	0/1167	0.89	0/1567
2	I	0.69	0/1167	0.88	0/1567
2	K	0.68	0/1167	0.84	0/1567
2	L	0.68	0/1167	0.89	1/1567 (0.1%)
3	C	0.66	0/1169	0.87	0/1571
3	J	0.65	0/1150	0.88	1/1546 (0.1%)
All	All	0.69	0/13995	0.88	10/18796 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	276	ARG	CG-CD-NE	-10.55	89.64	111.80
2	L	276	ARG	CG-CD-NE	-8.46	94.03	111.80
2	D	210	ARG	NE-CZ-NH2	-7.41	116.59	120.30
2	B	276	ARG	CG-CD-NE	-6.80	97.52	111.80
2	D	255	ARG	NE-CZ-NH2	-5.77	117.41	120.30
2	B	284	ARG	NE-CZ-NH2	-5.72	117.44	120.30
2	G	276	ARG	NE-CZ-NH2	-5.71	117.44	120.30
3	J	210	ARG	NE-CZ-NH2	-5.58	117.51	120.30
2	G	219	LYS	CB-CG-CD	5.22	125.18	111.60
2	E	276	ARG	NE-CZ-NH2	-5.04	117.78	120.30

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	1140	0	1127	16	0
2	B	1135	0	1130	12	0
2	D	1135	0	1130	11	0
2	E	1135	0	1130	13	0
2	F	1135	0	1130	12	0
2	G	1135	0	1130	18	0
2	H	1135	0	1130	25	0
2	I	1135	0	1130	12	0
2	K	1135	0	1130	14	0
2	L	1135	0	1130	7	0
3	C	1136	0	1124	22	0
3	J	1118	0	1108	19	0
4	B	7	0	2	1	0
4	C	7	0	2	2	0
4	G	21	0	6	6	0
5	A	132	0	0	3	0
5	B	116	0	0	4	0
5	C	105	0	0	2	0
5	D	158	0	0	2	0
5	E	105	0	0	3	0
5	F	98	0	0	2	0
5	G	141	0	0	5	0
5	H	151	0	0	6	0
5	I	109	0	0	3	0
5	J	76	0	0	4	0
5	K	141	0	0	3	0
5	L	101	0	0	2	0
All	All	15077	0	13539	151	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 6.

All (151) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:HIS:HE1	2:H:262:HIS:HE1	1.18	0.91
3:C:262:HIS:HE1	3:J:262:HIS:HE1	1.23	0.86
1:A:262:HIS:HE1	2:H:262:HIS:CE1	1.94	0.84
2:G:192:LYS:HE2	2:G:194:ASN:O	1.77	0.84
1:A:262:HIS:CE1	2:H:262:HIS:HE1	1.97	0.82
1:A:180:ARG:NH2	1:A:204:ASP:OD1	2.14	0.81
1:A:156:ASN:ND2	2:H:156:ASN:ND2	2.32	0.77
2:B:156:ASN:ND2	2:K:156:ASN:OD1	2.19	0.76
3:C:156:ASN:ND2	3:J:156:ASN:ND2	2.34	0.75
3:C:262:HIS:CE1	3:J:262:HIS:HE1	2.07	0.73
1:A:224:ASN:HD21	1:A:230:ASN:HD21	1.36	0.72
2:F:224:ASN:HD21	2:F:230:ASN:HD21	1.38	0.72
2:G:247:GLY:H	4:G:302:MLI:H11	1.56	0.71
2:D:224:ASN:HD21	2:D:230:ASN:HD21	1.40	0.70
1:A:262:HIS:CE1	2:H:262:HIS:CE1	2.76	0.68
3:J:193:HIS:HD2	5:J:371:HOH:O	1.76	0.68
3:C:158:ASN:HD22	3:C:290:LYS:HE3	1.61	0.66
2:G:193:HIS:NE2	2:H:193:HIS:HE1	1.93	0.66
3:C:184:HIS:HD2	3:C:235:ALA:H	1.45	0.65
2:I:242:ASN:HD21	2:I:244:LYS:HE2	1.61	0.65
2:G:246:ASN:HA	4:G:302:MLI:C1	2.27	0.64
2:D:220:VAL:O	2:K:183:LYS:HE2	1.97	0.64
2:L:220:VAL:HG13	5:L:346:HOH:O	1.97	0.64
2:G:249:ASP:OD2	2:G:276:ARG:NH2	2.30	0.64
3:C:262:HIS:HE1	3:J:262:HIS:CE1	2.11	0.63
2:K:184:HIS:HD2	2:K:235:ALA:H	1.46	0.63
2:H:184:HIS:HD2	2:H:235:ALA:H	1.46	0.63
2:L:184:HIS:HD2	2:L:235:ALA:H	1.47	0.62
2:I:156:ASN:OD1	2:I:260:ILE:CG2	2.47	0.62
2:G:184:HIS:HD2	2:G:235:ALA:H	1.47	0.61
3:J:249:ASP:OD2	3:J:276:ARG:NH2	2.33	0.61
3:J:184:HIS:HD2	3:J:235:ALA:H	1.48	0.61
3:J:276:ARG:HD3	5:J:310:HOH:O	2.00	0.61
1:A:184:HIS:HD2	1:A:235:ALA:H	1.48	0.60
2:H:156:ASN:HB3	5:H:330:HOH:O	2.01	0.60
3:C:224:ASN:HD21	3:C:230:ASN:HD21	1.50	0.59
1:A:224:ASN:ND2	1:A:230:ASN:HD21	2.00	0.59
1:A:156:ASN:HB3	5:H:330:HOH:O	2.02	0.58
5:F:394:HOH:O	2:G:187:LYS:HE3	2.02	0.58
2:G:193:HIS:NE2	2:H:193:HIS:CE1	2.71	0.58
2:F:224:ASN:ND2	2:F:230:ASN:HD21	2.01	0.58
2:E:242:ASN:ND2	2:E:244:LYS:HE2	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:154:MET:N	5:J:303:HOH:O	2.37	0.57
2:F:207:LYS:HE3	2:F:209:VAL:HG22	1.86	0.57
2:D:242:ASN:ND2	2:D:244:LYS:HE2	2.20	0.56
2:K:193:HIS:HD2	5:K:420:HOH:O	1.87	0.56
3:J:156:ASN:HB3	5:J:338:HOH:O	2.04	0.56
2:D:224:ASN:ND2	2:D:230:ASN:HD21	2.03	0.56
2:B:277:LYS:HE2	2:K:266:ASP:HB3	1.88	0.56
5:C:403:HOH:O	3:J:278:LYS:HA	2.06	0.55
2:E:156:ASN:OD1	2:F:156:ASN:ND2	2.39	0.55
2:H:184:HIS:HE1	5:H:420:HOH:O	1.90	0.55
2:D:216:SER:OG	2:D:236:HIS:HE1	1.91	0.54
2:G:288:ASP:HA	5:G:432:HOH:O	2.07	0.54
3:C:243:LYS:NZ	3:J:277:LYS:HB2	2.23	0.54
2:L:224:ASN:HD21	2:L:230:ASN:HD21	1.56	0.54
3:C:224:ASN:ND2	3:C:230:ASN:HD21	2.06	0.53
1:A:216:SER:OG	1:A:236:HIS:HE1	1.91	0.53
3:C:216:SER:OG	3:C:236:HIS:HE1	1.92	0.53
2:G:246:ASN:HA	4:G:302:MLI:H12	1.90	0.53
3:C:171:PRO:O	3:C:172:GLN:HG2	2.09	0.53
2:I:242:ASN:ND2	2:I:244:LYS:HE2	2.23	0.53
3:C:273:PHE:O	3:C:276:ARG:O	2.27	0.52
2:H:216:SER:OG	2:H:236:HIS:HE1	1.93	0.52
2:E:170:LYS:NZ	5:E:305:HOH:O	2.35	0.52
2:F:216:SER:OG	2:F:236:HIS:HE1	1.93	0.52
2:L:193:HIS:NE2	2:K:193:HIS:HE1	2.08	0.52
2:I:216:SER:OG	2:I:236:HIS:HE1	1.93	0.52
2:L:224:ASN:ND2	2:L:230:ASN:HD21	2.08	0.52
2:B:243:LYS:NZ	2:K:277:LYS:HB3	2.25	0.52
2:E:216:SER:OG	2:E:236:HIS:HE1	1.93	0.51
2:E:193:HIS:HD2	5:E:396:HOH:O	1.93	0.51
2:E:242:ASN:HD22	2:E:244:LYS:HE2	1.76	0.51
2:K:242:ASN:ND2	2:K:244:LYS:HE2	2.25	0.51
1:A:277:LYS:HE3	2:H:265:SER:OG	2.11	0.51
2:G:246:ASN:HA	4:G:302:MLI:H11	1.92	0.51
3:C:215:HIS:HD2	5:C:487:HOH:O	1.93	0.51
2:E:249:ASP:OD2	5:E:301:HOH:O	2.20	0.51
3:C:152:HIS:CD2	3:J:258:LYS:O	2.65	0.49
4:C:301:MLI:O7	4:C:301:MLI:O9	2.27	0.49
2:I:236:HIS:HD2	2:I:237:ALA:O	1.96	0.48
2:G:247:GLY:N	4:G:302:MLI:H11	2.27	0.48
2:D:242:ASN:HD21	2:D:244:LYS:HE2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:236:HIS:HD2	2:E:237:ALA:O	1.96	0.48
2:F:236:HIS:HD2	2:F:237:ALA:O	1.96	0.48
2:B:262:HIS:NE2	2:K:262:HIS:HE1	2.12	0.48
2:B:242:ASN:OD1	5:B:401:HOH:O	2.20	0.48
2:K:156:ASN:ND2	2:K:262:HIS:NE2	2.62	0.48
2:H:230:ASN:ND2	5:H:305:HOH:O	2.42	0.48
2:F:193:HIS:HD2	5:F:392:HOH:O	1.96	0.47
2:H:254:LYS:HB2	2:H:254:LYS:HE2	1.36	0.47
2:L:215:HIS:HE1	5:L:301:HOH:O	1.95	0.47
5:A:301:HOH:O	2:H:277:LYS:HG2	2.14	0.47
5:A:301:HOH:O	2:H:277:LYS:CG	2.62	0.47
2:D:183:LYS:HE2	2:H:220:VAL:HB	1.97	0.47
2:H:215:HIS:HD2	5:H:405:HOH:O	1.97	0.47
2:I:209:VAL:HG12	5:I:339:HOH:O	2.14	0.47
2:I:215:HIS:HE1	5:I:317:HOH:O	1.97	0.46
3:C:236:HIS:HD2	3:C:237:ALA:O	1.98	0.46
2:I:195:SER:OG	2:I:196:HIS:HD2	1.98	0.46
2:D:236:HIS:HD2	2:D:237:ALA:O	1.99	0.46
2:G:215:HIS:HD2	5:G:507:HOH:O	1.98	0.46
1:A:216:SER:OG	1:A:236:HIS:CE1	2.68	0.45
3:C:170:LYS:HG2	2:D:170:LYS:HG2	1.98	0.45
3:C:262:HIS:CE1	3:J:262:HIS:CE1	2.93	0.45
2:H:236:HIS:HD2	2:H:237:ALA:O	1.99	0.45
2:H:242:ASN:ND2	5:H:307:HOH:O	2.43	0.45
3:J:254:LYS:H	3:J:254:LYS:CD	2.28	0.45
1:A:156:ASN:HD22	2:H:156:ASN:ND2	2.12	0.45
2:D:216:SER:OG	2:D:236:HIS:CE1	2.68	0.45
4:G:303:MLI:O7	5:G:401:HOH:O	2.20	0.45
3:C:216:SER:OG	3:C:236:HIS:CE1	2.70	0.45
3:J:242:ASN:HD21	3:J:244:LYS:HE3	1.82	0.45
2:E:272:TYR:CD1	2:F:270:PRO:HG3	2.52	0.44
2:H:216:SER:OG	2:H:236:HIS:CE1	2.70	0.44
2:G:170:LYS:HG2	2:H:170:LYS:HG2	2.00	0.44
2:B:192:LYS:NZ	5:B:408:HOH:O	2.48	0.44
1:A:236:HIS:HD2	1:A:237:ALA:O	1.99	0.44
5:A:389:HOH:O	2:H:262:HIS:CD2	2.71	0.44
2:E:272:TYR:CG	2:F:270:PRO:HG3	2.53	0.44
2:B:195:SER:OG	2:B:196:HIS:HD2	2.01	0.44
2:I:216:SER:OG	2:I:236:HIS:CE1	2.70	0.44
2:E:216:SER:OG	2:E:236:HIS:CE1	2.70	0.43
2:F:216:SER:OG	2:F:236:HIS:CE1	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:277:LYS:HB3	3:J:243:LYS:NZ	2.33	0.43
2:B:153:MET:HA	5:K:368:HOH:O	2.17	0.43
2:G:290:LYS:HD3	2:G:290:LYS:C	2.39	0.43
3:C:243:LYS:HZ2	3:J:277:LYS:HB2	1.83	0.43
2:K:240:TRP:CE3	2:K:245:LEU:HD22	2.54	0.43
2:B:154:MET:HE2	5:B:427:HOH:O	2.18	0.42
2:F:240:TRP:CE3	2:F:245:LEU:HD22	2.54	0.42
2:I:254:LYS:HA	5:I:327:HOH:O	2.19	0.42
2:B:202:VAL:HG12	4:B:301:MLI:H11	2.01	0.42
2:E:266:ASP:HB3	2:F:277:LYS:HE2	2.01	0.42
2:G:215:HIS:HE1	5:G:402:HOH:O	2.01	0.42
2:G:277:LYS:HD2	5:G:508:HOH:O	2.19	0.42
2:K:184:HIS:HE1	5:K:417:HOH:O	2.02	0.41
1:A:277:LYS:CE	2:H:265:SER:OG	2.67	0.41
2:G:242:ASN:ND2	2:G:244:LYS:HE2	2.35	0.41
2:I:240:TRP:CE3	2:I:245:LEU:HD22	2.56	0.41
2:K:155:GLU:O	2:K:262:HIS:HD2	2.04	0.41
2:D:223:LYS:NZ	5:D:307:HOH:O	2.52	0.41
2:B:240:TRP:CE3	2:B:245:LEU:HD22	2.56	0.41
4:C:301:MLI:H11	5:D:344:HOH:O	2.20	0.41
2:E:240:TRP:CE3	2:E:245:LEU:HD22	2.55	0.41
3:J:240:TRP:CE3	3:J:245:LEU:HD22	2.56	0.41
3:C:240:TRP:CE3	3:C:245:LEU:HD22	2.56	0.41
2:I:156:ASN:OD1	2:I:260:ILE:HG22	2.17	0.41
2:B:219:LYS:HE3	5:B:504:HOH:O	2.20	0.40
3:C:207:LYS:HA	3:C:207:LYS:HD3	1.95	0.40
2:L:193:HIS:NE2	2:K:193:HIS:CE1	2.87	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	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
2	B	137/139 (99%)	136 (99%)	1 (1%)	0	100	100
2	D	137/139 (99%)	136 (99%)	1 (1%)	0	100	100
2	E	137/139 (99%)	136 (99%)	1 (1%)	0	100	100
2	F	137/139 (99%)	136 (99%)	1 (1%)	0	100	100
2	G	137/139 (99%)	136 (99%)	1 (1%)	0	100	100
2	H	137/139 (99%)	135 (98%)	2 (2%)	0	100	100
2	I	137/139 (99%)	136 (99%)	1 (1%)	0	100	100
2	K	137/139 (99%)	136 (99%)	1 (1%)	0	100	100
2	L	137/139 (99%)	136 (99%)	1 (1%)	0	100	100
3	C	137/140 (98%)	136 (99%)	1 (1%)	0	100	100
3	J	135/140 (96%)	134 (99%)	1 (1%)	0	100	100
All	All	1643/1671 (98%)	1628 (99%)	15 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	122/122 (100%)	118 (97%)	4 (3%)	38	37
2	B	122/122 (100%)	121 (99%)	1 (1%)	81	86
2	D	122/122 (100%)	120 (98%)	2 (2%)	62	67
2	E	122/122 (100%)	121 (99%)	1 (1%)	81	86
2	F	122/122 (100%)	120 (98%)	2 (2%)	62	67
2	G	122/122 (100%)	118 (97%)	4 (3%)	38	37
2	H	122/122 (100%)	117 (96%)	5 (4%)	30	29
2	I	122/122 (100%)	120 (98%)	2 (2%)	62	67
2	K	122/122 (100%)	120 (98%)	2 (2%)	62	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	L	122/122 (100%)	116 (95%)	6 (5%)	25 21
3	C	122/123 (99%)	120 (98%)	2 (2%)	62 67
3	J	120/123 (98%)	114 (95%)	6 (5%)	24 21
All	All	1462/1466 (100%)	1425 (98%)	37 (2%)	47 49

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	HIS
1	A	153	MET
1	A	202	VAL
1	A	206	ASN
2	B	278	LYS
3	C	153	MET
3	C	254	LYS
2	D	245	LEU
2	D	254	LYS
2	E	156	ASN
2	F	153	MET
2	F	278	LYS
2	G	192	LYS
2	G	277	LYS
2	G	290	LYS
2	G	291	LYS
2	H	153	MET
2	H	242	ASN
2	H	254	LYS
2	H	290	LYS
2	H	291	LYS
2	I	177	LYS
2	I	219	LYS
3	J	155	GLU
3	J	157	ILE
3	J	187	LYS
3	J	210	ARG
3	J	254	LYS
3	J	290	LYS
2	L	153	MET
2	L	201	VAL
2	L	207	LYS
2	L	219	LYS

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Mol	Chain	Res	Type
2	L	220	VAL
2	L	276	ARG
2	K	153	MET
2	K	207	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	ASN
1	A	184	HIS
1	A	215	HIS
1	A	224	ASN
1	A	236	HIS
1	A	262	HIS
2	B	156	ASN
2	B	196	HIS
2	B	224	ASN
2	B	230	ASN
3	C	156	ASN
3	C	158	ASN
3	C	184	HIS
3	C	215	HIS
3	C	224	ASN
3	C	236	HIS
3	C	262	HIS
2	D	224	ASN
2	D	236	HIS
2	D	242	ASN
2	E	236	HIS
2	E	242	ASN
2	F	175	ASN
2	F	224	ASN
2	F	236	HIS
2	F	262	HIS
2	G	184	HIS
2	G	215	HIS
2	G	224	ASN
2	G	230	ASN
2	G	242	ASN
2	G	262	HIS
2	H	156	ASN
2	H	175	ASN

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Mol	Chain	Res	Type
2	H	184	HIS
2	H	193	HIS
2	H	215	HIS
2	H	224	ASN
2	H	230	ASN
2	H	236	HIS
2	H	262	HIS
2	I	196	HIS
2	I	236	HIS
2	I	242	ASN
3	J	156	ASN
3	J	175	ASN
3	J	184	HIS
3	J	193	HIS
3	J	224	ASN
3	J	230	ASN
3	J	242	ASN
3	J	262	HIS
2	L	184	HIS
2	L	224	ASN
2	L	234	ASN
2	K	156	ASN
2	K	175	ASN
2	K	184	HIS
2	K	193	HIS
2	K	224	ASN
2	K	230	ASN
2	K	242	ASN
2	K	262	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

5 ligands are modelled in this entry.

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	MLI	G	301	-	6,6,6	1.23	1 (16%)	7,7,7	1.31	1 (14%)
4	MLI	G	303	-	6,6,6	1.88	2 (33%)	7,7,7	1.24	1 (14%)
4	MLI	C	301	-	6,6,6	2.25	5 (83%)	7,7,7	0.58	0
4	MLI	B	301	-	6,6,6	1.22	0	7,7,7	1.12	0
4	MLI	G	302	-	6,6,6	2.20	1 (16%)	7,7,7	1.73	1 (14%)

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	MLI	G	301	-	-	0/4/4/4	-
4	MLI	G	303	-	-	4/4/4/4	-
4	MLI	C	301	-	-	0/4/4/4	-
4	MLI	B	301	-	-	2/4/4/4	-
4	MLI	G	302	-	-	3/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	302	MLI	O7-C2	-4.70	1.14	1.30
4	G	303	MLI	O8-C3	3.37	1.33	1.22
4	C	301	MLI	O8-C3	3.17	1.32	1.22
4	C	301	MLI	O7-C2	-2.42	1.22	1.30
4	C	301	MLI	O9-C3	-2.21	1.23	1.30
4	C	301	MLI	C1-C3	2.20	1.54	1.51
4	G	303	MLI	C1-C3	2.16	1.54	1.51
4	G	301	MLI	C1-C2	2.13	1.54	1.51
4	C	301	MLI	C1-C2	2.05	1.54	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	302	MLI	C3-C1-C2	4.12	127.29	112.87
4	G	303	MLI	O6-C2-C1	-2.16	115.78	122.08
4	G	301	MLI	O8-C3-C1	-2.10	115.93	122.08

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	302	MLI	C2-C1-C3-O8
4	G	302	MLI	C2-C1-C3-O9
4	G	303	MLI	C2-C1-C3-O9
4	B	301	MLI	C2-C1-C3-O9
4	G	302	MLI	C3-C1-C2-O6
4	G	303	MLI	C3-C1-C2-O7
4	B	301	MLI	C2-C1-C3-O8
4	G	303	MLI	C3-C1-C2-O6
4	G	303	MLI	C2-C1-C3-O8

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	303	MLI	1	0
4	C	301	MLI	2	0
4	B	301	MLI	1	0
4	G	302	MLI	5	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	140/140 (100%)	0.19	2 (1%) 75 80	20, 32, 58, 113	1 (0%)
2	B	139/139 (100%)	0.14	3 (2%) 62 69	21, 35, 61, 76	1 (0%)
2	D	139/139 (100%)	0.18	1 (0%) 87 91	20, 29, 61, 80	1 (0%)
2	E	139/139 (100%)	0.17	0 100 100	26, 37, 65, 80	1 (0%)
2	F	139/139 (100%)	0.09	0 100 100	24, 38, 63, 80	1 (0%)
2	G	139/139 (100%)	0.17	0 100 100	19, 31, 61, 79	1 (0%)
2	H	139/139 (100%)	0.21	4 (2%) 51 61	19, 29, 62, 81	1 (0%)
2	I	139/139 (100%)	0.42	8 (5%) 23 31	25, 44, 78, 90	1 (0%)
2	K	139/139 (100%)	0.21	1 (0%) 87 91	23, 34, 62, 91	1 (0%)
2	L	139/139 (100%)	0.43	6 (4%) 35 45	28, 42, 74, 91	1 (0%)
3	C	139/140 (99%)	0.30	6 (4%) 35 45	22, 39, 69, 112	1 (0%)
3	J	137/140 (97%)	0.40	7 (5%) 28 36	31, 48, 79, 95	0
All	All	1667/1671 (99%)	0.24	38 (2%) 60 68	19, 37, 70, 113	11 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	152	HIS	6.2
3	C	152	HIS	5.4
2	L	291	LYS	5.1
2	L	264	ALA	4.2
2	I	274	ALA	4.0
3	C	264	ALA	3.8
2	I	221	THR	3.7
2	I	272	TYR	3.5
2	B	206	ASN	3.2
3	J	277	LYS	3.1
2	H	291	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
2	I	291	LYS	2.9
2	I	227	GLY	2.8
2	I	206	ASN	2.8
2	L	156	ASN	2.6
3	C	155	GLU	2.6
1	A	153	MET	2.5
2	I	225	SER	2.5
3	C	265	SER	2.4
3	J	225	SER	2.4
2	H	274	ALA	2.3
3	J	206	ASN	2.3
3	J	220	VAL	2.3
2	L	226	ASP	2.3
2	H	263	PRO	2.2
3	J	242	ASN	2.2
2	L	273	PHE	2.2
3	C	156	ASN	2.2
2	B	264	ALA	2.2
2	D	264	ALA	2.1
3	C	277	LYS	2.1
2	L	274	ALA	2.1
3	J	156	ASN	2.0
2	H	265	SER	2.0
2	I	273	PHE	2.0
2	B	291	LYS	2.0
2	K	277	LYS	2.0
3	J	188	VAL	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
4	MLI	G	303	7/7	0.80	0.18	35,61,66,69	0
4	MLI	G	301	7/7	0.82	0.26	63,63,70,80	0
4	MLI	G	302	7/7	0.84	0.27	37,42,56,67	0
4	MLI	C	301	7/7	0.89	0.19	38,58,64,69	0
4	MLI	B	301	7/7	0.90	0.20	46,55,61,71	0

6.5 Other polymers (i)

There are no such residues in this entry.