Full wwPDB/EMDataBank EM Map/Model Validation Report (i)

Jan 10, 2019 – 09:27 AM EST

PDB ID	:	6IQW
EMDB ID:	:	EMD-9708
Title	:	Cryo-EM structure of Csm effector complex
Authors	:	Huo, Y.; Li, T.; Wang, N.; Dong, Q.; Wang, X.; Jiang, T.
Deposited on	:	2018-11-09
Resolution	:	3.35 Å(reported)

This is a Full wwPDB/EMDataBank EM Map/Model Validation Report for a publicly released PDB/EMDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

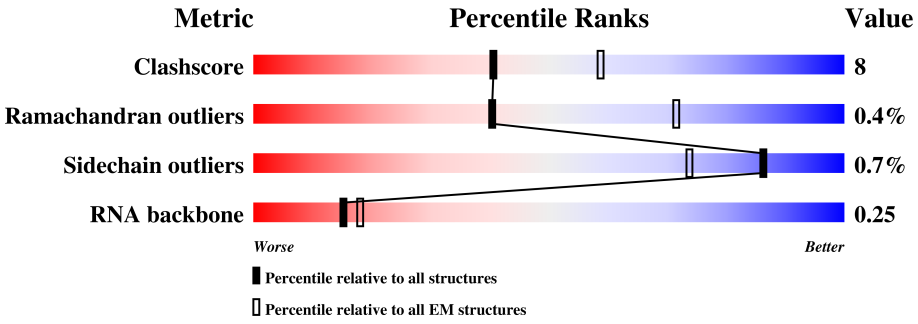
MolProbity	:	4.02b-467
Mogul	:	1.7.3 (157068), CSD as539be (2018)
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031633

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.35 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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%

Mol	Chain	Length	Quality of chain
1	A	777	85% 15% •
2	B	196	51% 17% • 32%
3	C	290	74% 20% 6%
3	D	290	70% 23% • 7%
4	E	289	69% 25% • •
5	F	397	71% 16% 13%
6	I	24	38% 42% 17% •

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 16935 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Csm1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	771	Total	C	N	O	S	0	0
			6131	3934	1071	1106	20		

- Molecule 2 is a protein called Csm2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	134	Total	C	N	O	S	0	0
			1094	706	187	197	4		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	MET	-	expression tag	UNP B6YWB9
B	-8	HIS	-	expression tag	UNP B6YWB9
B	-7	HIS	-	expression tag	UNP B6YWB9
B	-6	HIS	-	expression tag	UNP B6YWB9
B	-5	HIS	-	expression tag	UNP B6YWB9
B	-4	HIS	-	expression tag	UNP B6YWB9
B	-3	HIS	-	expression tag	UNP B6YWB9
B	-2	VAL	-	expression tag	UNP B6YWB9
B	-1	ILE	-	expression tag	UNP B6YWB9
B	0	PHE	-	expression tag	UNP B6YWB9
B	1	VAL	-	expression tag	UNP B6YWB9

- Molecule 3 is a protein called Csm3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	274	Total	C	N	O	S	0	0
			2113	1349	374	385	5		
3	D	271	Total	C	N	O	S	0	0
			2106	1345	374	381	6		

- Molecule 4 is a protein called Csm4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	277	Total	C	N	O	S	0	0
			2177	1421	364	388	4		

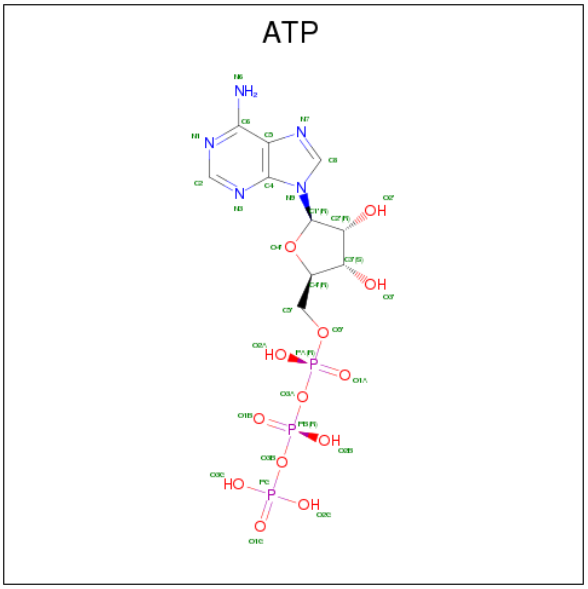
- Molecule 5 is a protein called Csm5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	346	Total	C	N	O	S	0	0
			2773	1772	478	512	11		

- Molecule 6 is a RNA chain called RNA (5'-R(*GP*UP*GP*GP*AP*AP*AP*GP*UP*GP*GP*CP*CP*CP*GP*AP*AP*AP*CP*CP*CP*UP*UP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
6	I	24	Total	C	N	O	P	0	0
			510	229	94	164	23		

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



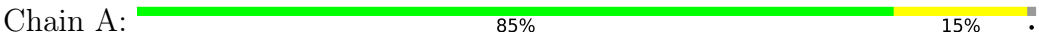
Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	N	O	P	0
			31	10	5	13	3	

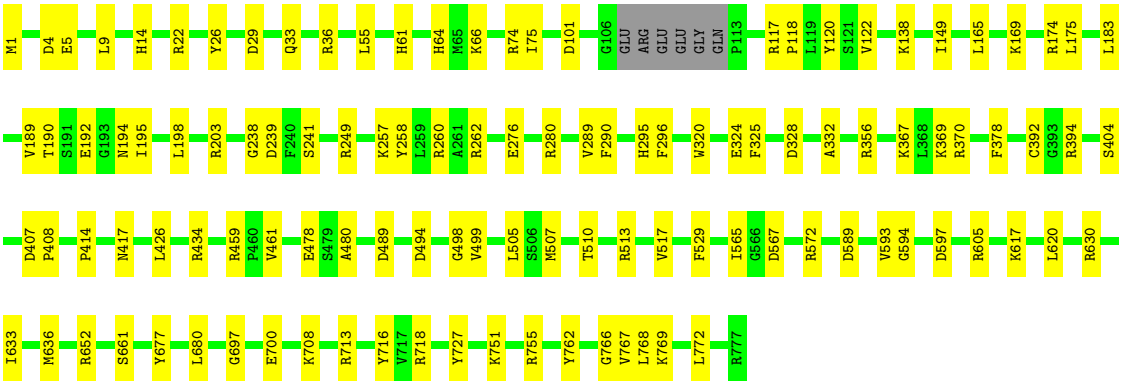
3 Residue-property plots (i)

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. 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. 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: Csm1

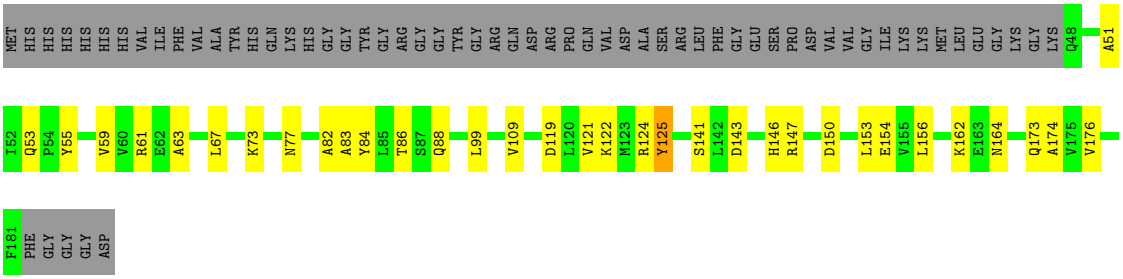
Chain A:





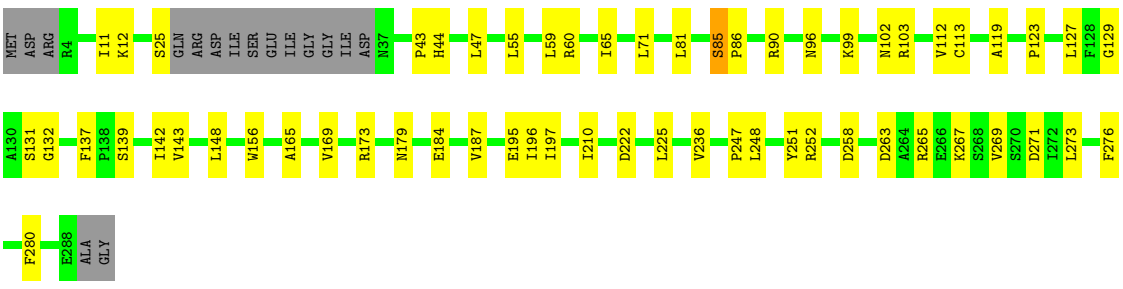
- Molecule 2: Csm2

Chain B:



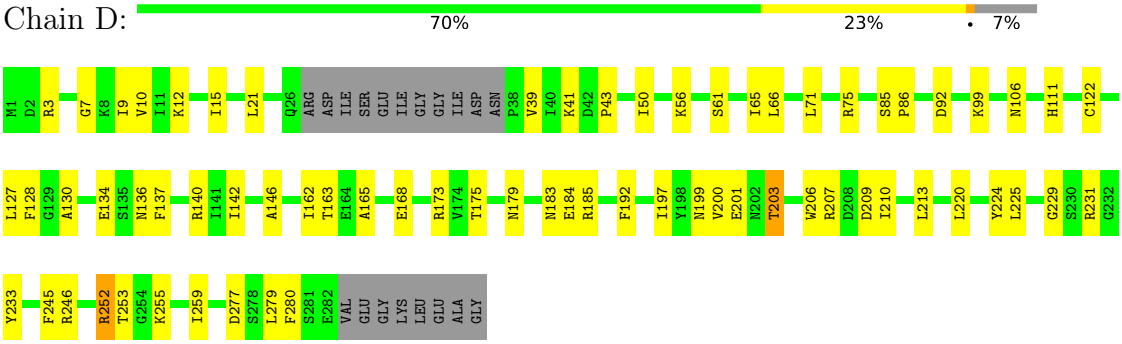
- Molecule 3: Csm3

Chain C:



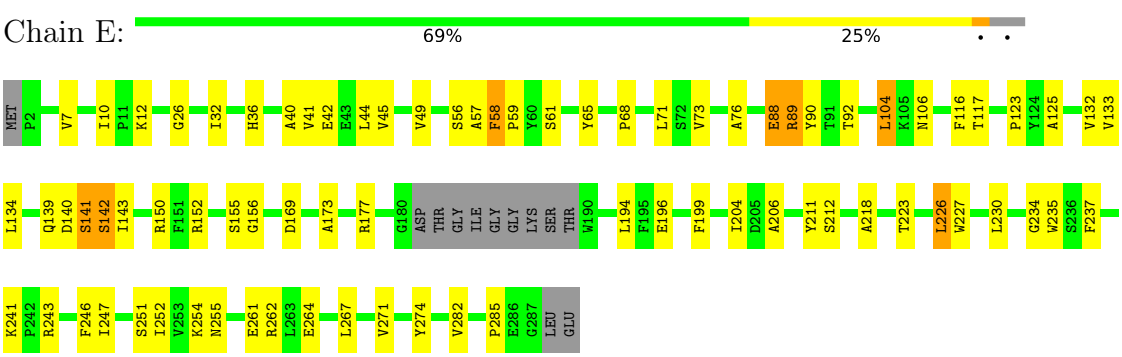
• Molecule 3: Csm3

Chain D:



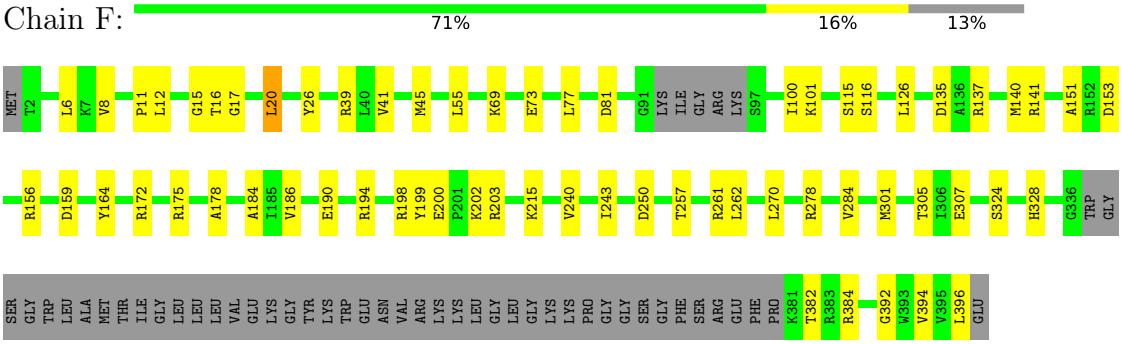
• Molecule 4: Csm4

Chain E:



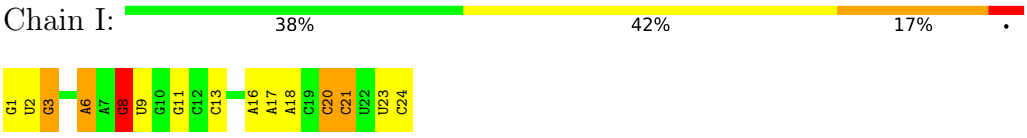
• Molecule 5: Csm5

Chain F:



• Molecule 6: RNA (5'-R(*GP*UP*GP*GP*AP*AP*AP*GP*UP*GP*GP*CP*CP*CP*GP*AP*AP*AP*CP*CP*CP*UP*UP*C)-3')

Chain I:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	61924	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.875	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	0.37	0/6273	0.51	1/8468 (0.0%)
2	B	0.30	0/1117	0.55	0/1505
3	C	0.39	0/2161	0.67	0/2922
3	D	0.38	0/2155	0.64	0/2911
4	E	0.43	0/2237	0.74	3/3034 (0.1%)
5	F	0.32	1/2833 (0.0%)	0.53	0/3836
6	I	0.64	0/570	0.99	2/887 (0.2%)
All	All	0.39	1/17346 (0.0%)	0.61	6/23563 (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	A	0	2
3	C	0	2
3	D	0	1
4	E	0	2
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	20	LEU	C-N	-5.61	1.21	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	226	LEU	CA-CB-CG	8.15	134.04	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	620	LEU	CA-CB-CG	5.54	128.03	115.30
6	I	8	G	C8-N9-C1'	-5.28	120.14	127.00
4	E	88	GLU	C-N-CA	-5.25	108.58	121.70
4	E	104	LEU	CA-CB-CG	5.04	126.90	115.30
6	I	8	G	C4-N9-C1'	5.02	133.03	126.50

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	325	PHE	Peptide
1	A	394	ARG	Peptide
3	C	85	SER	Peptide
3	C	99	LYS	Peptide
3	D	39	VAL	Peptide
4	E	141	SER	Peptide
4	E	58	PHE	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	6131	0	6132	69	0
2	B	1094	0	1109	26	0
3	C	2113	0	2057	42	0
3	D	2106	0	2059	49	0
4	E	2177	0	2172	68	0
5	F	2773	0	2765	39	0
6	I	510	0	262	14	0
7	A	31	0	12	1	0
All	All	16935	0	16568	274	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 8.

All (274) 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:B:51:ALA:O	2:B:55:TYR:CD2	1.76	1.39
2:B:51:ALA:O	2:B:55:TYR:HD2	0.95	1.25
4:E:89:ARG:HD3	4:E:90:TYR:CA	1.68	1.21
4:E:89:ARG:HD3	4:E:90:TYR:N	1.60	1.16
4:E:89:ARG:HD3	4:E:90:TYR:HA	1.31	1.11
2:B:51:ALA:HB1	2:B:55:TYR:HE2	1.18	1.06
4:E:89:ARG:CD	4:E:90:TYR:N	2.32	0.92
2:B:51:ALA:HB1	2:B:55:TYR:CE2	2.06	0.89
4:E:89:ARG:CD	4:E:90:TYR:CA	2.55	0.85
4:E:89:ARG:HH11	4:E:89:ARG:C	1.87	0.78
4:E:89:ARG:CD	4:E:90:TYR:HA	2.15	0.74
3:C:96:ASN:H	3:C:102:ASN:HD22	1.35	0.73
4:E:89:ARG:CG	4:E:90:TYR:N	2.51	0.72
4:E:89:ARG:HB2	4:E:89:ARG:NH1	2.07	0.70
4:E:89:ARG:HD3	4:E:89:ARG:C	2.13	0.69
3:D:130:ALA:HB3	3:D:137:PHE:H	1.58	0.68
4:E:59:PRO:HA	4:E:156:GLY:O	1.94	0.68
2:B:59:VAL:O	2:B:63:ALA:HB3	1.93	0.68
4:E:218:ALA:HB3	4:E:247:ILE:HB	1.77	0.66
4:E:88:GLU:O	4:E:89:ARG:C	2.28	0.65
3:D:203:THR:O	3:D:206:TRP:HB3	1.96	0.65
1:A:238:GLY:HA2	1:A:332:ALA:O	1.98	0.63
1:A:257:LYS:HG2	1:A:499:VAL:HB	1.81	0.63
2:B:51:ALA:C	2:B:55:TYR:HD2	1.95	0.62
3:C:173:ARG:HD2	3:D:61:SER:HB2	1.81	0.62
3:C:225:LEU:HD12	3:C:236:VAL:HG11	1.83	0.61
4:E:89:ARG:HD2	4:E:90:TYR:HB3	1.82	0.60
1:A:26:TYR:HB2	1:A:33:GLN:HG2	1.83	0.60
4:E:155:SER:OG	4:E:156:GLY:N	2.35	0.60
3:D:162:ILE:HG23	3:D:163:THR:HG23	1.84	0.60
3:D:85:SER:HB3	3:D:99:LYS:HG2	1.84	0.60
1:A:507:MET:HG2	1:A:513:ARG:HH12	1.67	0.59
6:I:16:A:H2'	6:I:17:A:H8	1.67	0.59
4:E:61:SER:OG	4:E:152:ARG:NH1	2.36	0.59
5:F:116:SER:HA	6:I:20:C:H1'	1.85	0.58
1:A:262:ARG:NH1	1:A:392:CYS:SG	2.75	0.58
3:D:252:ARG:HD3	3:D:253:THR:HG23	1.84	0.58
1:A:505:LEU:HD13	1:A:594:GLY:HA2	1.86	0.58
3:D:220:LEU:HD21	3:D:225:LEU:HD23	1.85	0.58
1:A:718:ARG:NH1	3:C:156:TRP:O	2.37	0.58
1:A:716:TYR:HE2	1:A:762:TYR:HB2	1.68	0.58
1:A:1:MET:HG3	1:A:5:GLU:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:7:GLY:HA3	3:D:200:VAL:HB	1.86	0.57
1:A:249:ARG:NH2	1:A:328:ASP:OD2	2.38	0.57
1:A:169:LYS:HB2	1:A:174:ARG:HG3	1.85	0.57
3:D:142:ILE:HB	3:D:197:ILE:HB	1.86	0.57
1:A:203:ARG:NH2	1:A:289:VAL:O	2.38	0.57
3:C:179:ASN:HD22	3:D:106:ASN:HB3	1.70	0.57
4:E:89:ARG:CA	4:E:89:ARG:HH11	2.17	0.57
4:E:89:ARG:NH1	4:E:92:THR:OG1	2.38	0.56
1:A:258:TYR:OH	1:A:262:ARG:NH1	2.38	0.56
3:D:165:ALA:HA	3:D:184:GLU:HA	1.87	0.56
5:F:198:ARG:NH2	5:F:200:GLU:OE1	2.36	0.56
2:B:73:LYS:O	2:B:77:ASN:ND2	2.39	0.56
3:D:9:ILE:HG22	3:D:245:PHE:HB2	1.86	0.56
3:D:173:ARG:HE	5:F:126:LEU:HD22	1.70	0.56
5:F:202:LYS:HG2	6:I:17:A:H1'	1.87	0.55
4:E:89:ARG:O	4:E:92:THR:N	2.37	0.54
2:B:153:LEU:HA	2:B:156:LEU:HB2	1.89	0.54
5:F:8:VAL:HA	5:F:394:VAL:HG12	1.89	0.54
2:B:51:ALA:CB	2:B:55:TYR:HE2	2.07	0.54
4:E:88:GLU:O	4:E:89:ARG:O	2.25	0.54
1:A:241:SER:OG	1:A:370:ARG:NH2	2.38	0.54
3:D:111:HIS:NE2	3:D:122:CYS:SG	2.80	0.54
1:A:414:PRO:HA	1:A:417:ASN:HB2	1.90	0.54
3:D:71:LEU:HD11	3:D:86:PRO:HG3	1.89	0.54
5:F:140:MET:HG2	5:F:151:ALA:HB1	1.88	0.54
5:F:137:ARG:O	5:F:141:ARG:NH2	2.39	0.54
1:A:276:GLU:OE1	1:A:434:ARG:NH2	2.41	0.53
4:E:251:SER:OG	4:E:252:ILE:N	2.37	0.53
1:A:55:LEU:HD13	1:A:75:ILE:HG12	1.90	0.53
5:F:159:ASP:OD1	5:F:159:ASP:N	2.42	0.53
4:E:89:ARG:CB	4:E:89:ARG:HH11	2.21	0.53
2:B:109:VAL:HG13	2:B:162:LYS:HB3	1.91	0.53
3:C:55:LEU:O	3:C:59:LEU:HB2	2.09	0.53
4:E:169:ASP:HA	4:E:173:ALA:HB3	1.89	0.53
1:A:276:GLU:OE2	1:A:280:ARG:NH2	2.42	0.52
3:D:168:GLU:OE2	3:D:183:ASN:ND2	2.42	0.52
4:E:89:ARG:HG3	4:E:90:TYR:H	1.75	0.52
3:C:103:ARG:HG3	3:C:112:VAL:HB	1.91	0.52
3:D:7:GLY:HA2	3:D:245:PHE:HE1	1.73	0.52
3:C:103:ARG:NH2	3:C:131:SER:O	2.43	0.52
5:F:45:MET:HG3	5:F:55:LEU:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:207:ARG:NH1	3:D:277:ASP:OD2	2.42	0.52
1:A:189:VAL:O	1:A:194:ASN:ND2	2.41	0.52
1:A:751:LYS:HE3	1:A:755:ARG:HH12	1.74	0.52
5:F:257:THR:O	5:F:261:ARG:HB2	2.10	0.52
5:F:384:ARG:NH1	6:I:23:U:OP2	2.43	0.52
5:F:190:GLU:OE1	5:F:203:ARG:NH2	2.42	0.51
4:E:211:TYR:HA	4:E:254:LYS:HB2	1.93	0.51
3:C:263:ASP:OD1	3:C:263:ASP:N	2.43	0.51
5:F:11:PRO:O	5:F:392:GLY:N	2.37	0.51
5:F:324:SER:O	5:F:328:HIS:NE2	2.43	0.51
5:F:215:LYS:HD2	5:F:250:ASP:HB2	1.91	0.51
4:E:12:LYS:HB2	4:E:194:LEU:HB3	1.91	0.51
1:A:510:THR:OG1	1:A:572:ARG:NH1	2.44	0.51
1:A:356:ARG:NH1	1:A:529:PHE:O	2.44	0.51
1:A:727:TYR:OH	2:B:173:GLN:O	2.25	0.51
1:A:61:HIS:O	1:A:64:HIS:NE2	2.43	0.51
1:A:118:PRO:HB3	1:A:149:ILE:HG12	1.92	0.50
4:E:243:ARG:NH1	6:I:3:G:O6	2.44	0.50
2:B:53:GLN:HB3	2:B:84:TYR:HB2	1.94	0.50
3:C:273:LEU:HA	3:C:276:PHE:HB3	1.93	0.50
1:A:630:ARG:HD2	4:E:143:ILE:HB	1.92	0.50
4:E:89:ARG:CB	4:E:89:ARG:NH1	2.72	0.50
3:D:15:ILE:HG13	3:D:192:PHE:HB2	1.94	0.50
1:A:14:HIS:NE2	1:A:101:ASP:OD1	2.37	0.50
1:A:183:LEU:HB3	1:A:198:LEU:HD23	1.94	0.49
4:E:65:TYR:HB2	4:E:104:LEU:HD11	1.92	0.49
5:F:153:ASP:OD1	5:F:156:ARG:NH1	2.45	0.49
5:F:39:ARG:NH2	5:F:81:ASP:OD2	2.45	0.49
3:C:129:GLY:HA2	3:C:137:PHE:HD2	1.77	0.49
3:C:142:ILE:HB	3:C:197:ILE:HB	1.93	0.49
1:A:4:ASP:N	1:A:4:ASP:OD1	2.43	0.49
1:A:239:ASP:OD2	1:A:367:LYS:NZ	2.41	0.49
1:A:36:ARG:NH1	1:A:36:ARG:O	2.43	0.49
2:B:67:LEU:HD11	2:B:164:ASN:HB3	1.94	0.49
3:C:131:SER:OG	3:C:132:GLY:N	2.40	0.49
3:C:276:PHE:O	3:C:280:PHE:N	2.43	0.49
3:D:50:ILE:HB	3:D:146:ALA:HB3	1.95	0.49
2:B:82:ALA:O	2:B:86:THR:N	2.45	0.48
3:D:277:ASP:HA	3:D:280:PHE:HB2	1.93	0.48
3:C:222:ASP:OD1	3:D:246:ARG:NH2	2.47	0.48
3:D:127:LEU:HD21	3:D:213:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:234:GLY:O	4:E:241:LYS:CB	2.61	0.48
5:F:135:ASP:OD1	5:F:135:ASP:N	2.46	0.48
2:B:124:ARG:HH22	2:B:154:GLU:HG3	1.79	0.48
3:C:65:ILE:HD13	3:D:3:ARG:HD2	1.94	0.48
3:D:185:ARG:HH11	3:D:233:TYR:HE1	1.62	0.48
4:E:7:VAL:HG12	4:E:199:PHE:HD1	1.79	0.48
5:F:278:ARG:HB2	5:F:284:VAL:HG21	1.95	0.48
1:A:260:ARG:NH2	1:A:489:ASP:O	2.47	0.48
1:A:589:ASP:N	1:A:589:ASP:OD1	2.41	0.48
2:B:51:ALA:O	2:B:55:TYR:CE2	2.55	0.48
4:E:32:ILE:HG22	4:E:41:VAL:HA	1.96	0.48
4:E:56:SER:OG	4:E:57:ALA:N	2.45	0.47
4:E:58:PHE:HE2	4:E:123:PRO:HD2	1.79	0.47
3:C:251:TYR:O	4:E:177:ARG:NH1	2.46	0.47
4:E:204:ILE:HG22	4:E:206:ALA:HB2	1.96	0.47
3:D:65:ILE:HG23	5:F:262:LEU:HD11	1.96	0.47
2:B:119:ASP:HA	2:B:122:LYS:HE3	1.96	0.47
4:E:140:ASP:OD2	4:E:142:SER:OG	2.30	0.47
3:D:231:ARG:HD3	5:F:115:SER:HB3	1.97	0.47
5:F:15:GLY:O	6:I:21:C:O2'	2.21	0.47
1:A:494:ASP:OD1	1:A:498:GLY:N	2.48	0.47
3:C:11:ILE:HB	3:C:196:ILE:HB	1.96	0.47
4:E:261:GLU:HG3	4:E:274:TYR:HA	1.97	0.47
5:F:26:TYR:CG	5:F:69:LYS:HD3	2.50	0.47
3:C:44:HIS:HD2	4:E:125:ALA:HB2	1.80	0.46
1:A:652:ARG:NH1	7:A:801:ATP:O2G	2.48	0.46
3:C:12:LYS:HG3	3:C:195:GLU:HG2	1.98	0.46
3:D:21:LEU:HD11	3:D:50:ILE:HD11	1.98	0.46
3:D:41:LYS:HE2	3:D:43:PRO:HB2	1.96	0.46
4:E:76:ALA:HB3	4:E:285:PRO:HG2	1.97	0.46
5:F:73:GLU:HG3	5:F:77:LEU:H	1.80	0.46
4:E:271:VAL:HG12	6:I:1:G:H3'	1.96	0.46
2:B:88:GLN:HB3	2:B:141:SER:HB3	1.97	0.46
4:E:227:TRP:HB2	4:E:247:ILE:HG23	1.98	0.46
5:F:186:VAL:O	5:F:270:LEU:N	2.48	0.46
2:B:143:ASP:HA	2:B:146:HIS:HB3	1.97	0.46
3:D:41:LYS:HD2	3:D:43:PRO:HD2	1.98	0.46
1:A:9:LEU:HD22	1:A:175:LEU:HD12	1.98	0.46
3:D:10:VAL:HG12	3:D:197:ILE:HG12	1.98	0.46
5:F:194:ARG:HA	5:F:194:ARG:HD3	1.74	0.46
4:E:89:ARG:CD	4:E:90:TYR:HB3	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:ARG:NH1	1:A:597:ASP:OD2	2.44	0.45
2:B:121:VAL:O	2:B:125:TYR:N	2.47	0.45
3:C:102:ASN:OD1	3:C:102:ASN:N	2.35	0.45
2:B:146:HIS:NE2	2:B:150:ASP:OD2	2.48	0.45
3:C:113:CYS:HB2	3:C:119:ALA:HB2	1.98	0.45
4:E:230:LEU:N	4:E:246:PHE:O	2.44	0.45
1:A:633:ILE:HA	1:A:636:MET:HB2	1.98	0.45
3:C:179:ASN:OD1	3:C:179:ASN:N	2.50	0.45
3:C:273:LEU:HD11	3:D:255:LYS:HG2	1.99	0.45
4:E:234:GLY:O	4:E:241:LYS:HB3	2.17	0.45
4:E:132:VAL:HG13	6:I:8:G:H5'	1.97	0.45
3:C:169:VAL:O	6:I:13:C:O2'	2.32	0.45
3:C:267:LYS:HG3	3:C:269:VAL:HG12	1.99	0.45
3:C:165:ALA:HA	3:C:184:GLU:HA	1.98	0.45
1:A:697:GLY:HA2	1:A:700:GLU:HG3	1.98	0.45
5:F:16:THR:OG1	5:F:17:GLY:N	2.50	0.45
1:A:661:SER:OG	1:A:713:ARG:NH1	2.50	0.45
4:E:45:VAL:HG12	4:E:49:VAL:HG23	1.98	0.45
3:D:9:ILE:HD12	3:D:210:ILE:HD12	1.99	0.44
4:E:89:ARG:HG3	4:E:90:TYR:N	2.27	0.44
5:F:69:LYS:O	5:F:73:GLU:N	2.39	0.44
1:A:369:LYS:HG2	4:E:226:LEU:H	1.81	0.44
1:A:29:ASP:O	1:A:33:GLN:NE2	2.50	0.44
3:D:12:LYS:HA	3:D:12:LYS:HD2	1.72	0.44
5:F:184:ALA:HB2	5:F:199:TYR:HB2	2.00	0.44
1:A:320:TRP:CE2	1:A:324:GLU:HG3	2.53	0.44
1:A:169:LYS:HD2	1:A:478:GLU:HB3	2.00	0.44
1:A:567:ASP:OD1	1:A:567:ASP:N	2.42	0.44
3:C:258:ASP:N	3:C:258:ASP:OD1	2.51	0.44
1:A:378:PHE:O	4:E:262:ARG:NH2	2.51	0.44
3:C:47:LEU:HD12	3:C:148:LEU:HG	1.99	0.44
3:D:259:ILE:HG23	3:D:279:LEU:HD12	1.99	0.44
3:D:179:ASN:N	3:D:179:ASN:OD1	2.48	0.44
3:D:209:ASP:O	3:D:213:LEU:N	2.51	0.44
4:E:40:ALA:HA	4:E:44:LEU:HD13	2.00	0.43
3:C:71:LEU:HD11	3:C:86:PRO:HD3	2.00	0.43
3:D:175:THR:OG1	5:F:175:ARG:NH2	2.41	0.43
3:D:142:ILE:N	3:D:197:ILE:O	2.40	0.43
5:F:41:VAL:HG13	5:F:55:LEU:HD13	2.00	0.43
3:C:81:LEU:HD13	3:C:123:PRO:HD2	2.00	0.43
4:E:89:ARG:HB2	4:E:89:ARG:CZ	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:ILE:HG21	1:A:605:ARG:HG2	1.99	0.43
3:D:140:ARG:NH2	3:D:201:GLU:OE1	2.52	0.43
3:C:252:ARG:HE	4:E:36:HIS:CE1	2.37	0.43
4:E:26:GLY:O	6:I:1:G:O2'	2.36	0.43
5:F:101:LYS:HD2	5:F:240:VAL:HG12	2.00	0.43
1:A:120:TYR:HE2	1:A:192:GLU:HA	1.83	0.43
1:A:617:LYS:HA	1:A:617:LYS:HD2	1.83	0.43
1:A:677:TYR:OH	1:A:766:GLY:O	2.28	0.43
3:C:55:LEU:HB3	3:C:143:VAL:HG11	2.01	0.42
4:E:106:ASN:ND2	4:E:117:THR:OG1	2.52	0.42
1:A:138:LYS:HA	1:A:138:LYS:HD3	1.82	0.42
3:C:12:LYS:NZ	3:C:195:GLU:OE2	2.43	0.42
3:C:25:SER:OG	3:C:25:SER:O	2.36	0.42
3:D:85:SER:H	3:D:99:LYS:HA	1.84	0.42
2:B:61:ARG:HD2	2:B:147:ARG:HB3	2.01	0.42
1:A:290:PHE:O	1:A:296:PHE:HA	2.19	0.42
1:A:517:VAL:HG22	1:A:593:VAL:HG12	2.00	0.42
1:A:768:LEU:HD23	1:A:768:LEU:HA	1.90	0.42
1:A:727:TYR:CZ	2:B:174:ALA:HA	2.55	0.42
3:C:60:ARG:HD3	3:C:60:ARG:HA	1.80	0.42
5:F:301:MET:O	5:F:305:THR:OG1	2.35	0.42
1:A:66:LYS:HE3	1:A:66:LYS:HB3	1.89	0.42
3:D:10:VAL:HG11	3:D:246:ARG:NH2	2.34	0.42
4:E:73:VAL:HG21	4:E:116:PHE:HE1	1.84	0.42
4:E:89:ARG:CD	4:E:90:TYR:CB	2.98	0.42
5:F:307:GLU:OE2	5:F:382:THR:OG1	2.37	0.42
4:E:125:ALA:HB3	4:E:150:ARG:HB3	2.02	0.41
1:A:407:ASP:HA	1:A:408:PRO:HD3	1.92	0.41
3:D:224:TYR:CD1	3:D:229:GLY:HA3	2.55	0.41
4:E:10:ILE:N	4:E:196:GLU:O	2.49	0.41
4:E:264:GLU:HB2	4:E:271:VAL:HG23	2.01	0.41
4:E:235:TRP:HZ3	6:I:3:G:H1'	1.85	0.41
2:B:99:LEU:HD21	2:B:176:VAL:HG21	2.02	0.41
3:C:187:VAL:HG13	3:D:43:PRO:HB3	2.03	0.41
4:E:139:GLN:HE22	4:E:141:SER:HB3	1.84	0.41
1:A:117:ARG:NH1	1:A:120:TYR:OH	2.53	0.41
3:D:136:ASN:ND2	6:I:11:G:N3	2.68	0.41
2:B:51:ALA:C	2:B:55:TYR:CD2	2.77	0.41
3:D:140:ARG:O	3:D:199:ASN:N	2.48	0.41
5:F:6:LEU:HD13	5:F:396:LEU:HD13	2.03	0.41
1:A:122:VAL:HG23	1:A:195:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:708:LYS:HE3	1:A:708:LYS:HB3	1.89	0.41
3:C:103:ARG:HD3	3:C:103:ARG:HA	1.92	0.41
3:D:56:LYS:HE2	3:D:128:PHE:HD1	1.86	0.41
3:C:139:SER:N	6:I:6:A:OP1	2.47	0.41
1:A:117:ARG:HB3	1:A:190:THR:HB	2.02	0.41
4:E:212:SER:HA	4:E:282:VAL:HB	2.03	0.41
4:E:71:LEU:HD13	4:E:251:SER:HB2	2.03	0.41
1:A:404:SER:OG	1:A:417:ASN:OD1	2.38	0.41
4:E:133:VAL:HG11	4:E:143:ILE:HD13	2.03	0.41
5:F:116:SER:OG	6:I:21:C:OP1	2.35	0.41
1:A:505:LEU:HA	1:A:505:LEU:HD23	1.86	0.41
3:C:11:ILE:HD11	3:C:210:ILE:HD11	2.03	0.41
3:C:267:LYS:O	3:C:271:ASP:N	2.49	0.41
2:B:83:ALA:HA	2:B:86:THR:HG22	2.03	0.41
3:C:90:ARG:NH1	3:D:134:GLU:OE1	2.53	0.41
1:A:165:LEU:HD23	1:A:165:LEU:HA	1.87	0.41
3:D:92:ASP:OD1	3:D:92:ASP:N	2.49	0.41
5:F:12:LEU:HD23	5:F:243:ILE:HD12	2.02	0.41
1:A:461:VAL:HG23	1:A:480:ALA:HB2	2.02	0.40
5:F:164:TYR:OH	5:F:178:ALA:O	2.38	0.40
1:A:238:GLY:O	1:A:295:HIS:HA	2.21	0.40
1:A:769:LYS:HA	1:A:772:LEU:HB2	2.03	0.40
4:E:237:PHE:HB2	4:E:267:LEU:HD11	2.03	0.40
5:F:20:LEU:HB2	5:F:100:ILE:HB	2.03	0.40
1:A:426:LEU:HD23	1:A:426:LEU:HA	1.95	0.40
1:A:680:LEU:HB3	1:A:767:VAL:HG21	2.04	0.40
4:E:223:THR:HG21	4:E:255:ASN:HB2	2.02	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 PDB entries followed by that with respect to all EM entries.

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	767/777 (99%)	718 (94%)	49 (6%)	0	100	100
2	B	132/196 (67%)	126 (96%)	6 (4%)	0	100	100
3	C	270/290 (93%)	209 (77%)	58 (22%)	3 (1%)	16	52
3	D	267/290 (92%)	205 (77%)	60 (22%)	2 (1%)	24	61
4	E	273/289 (94%)	200 (73%)	70 (26%)	3 (1%)	16	52
5	F	340/397 (86%)	306 (90%)	34 (10%)	0	100	100
All	All	2049/2239 (92%)	1764 (86%)	277 (14%)	8 (0%)	40	72

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	68	PRO
4	E	142	SER
3	C	43	PRO
3	C	247	PRO
3	D	75	ARG
3	D	203	THR
4	E	42	GLU
3	C	85	SER

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	639/652 (98%)	636 (100%)	3 (0%)	90	95
2	B	116/163 (71%)	115 (99%)	1 (1%)	81	91
3	C	217/247 (88%)	214 (99%)	3 (1%)	69	86
3	D	217/247 (88%)	215 (99%)	2 (1%)	81	91
4	E	225/240 (94%)	223 (99%)	2 (1%)	81	91
5	F	298/340 (88%)	297 (100%)	1 (0%)	93	97
All	All	1712/1889 (91%)	1700 (99%)	12 (1%)	86	93

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ARG
1	A	74	ARG
1	A	459	ARG
2	B	125	TYR
3	C	127	LEU
3	C	248	LEU
3	C	265	ARG
3	D	66	LEU
3	D	252	ARG
4	E	89	ARG
4	E	134	LEU
5	F	172	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
3	C	22	HIS
3	C	44	HIS
3	C	96	ASN
3	C	136	ASN
4	E	36	HIS
4	E	106	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	I	23/24 (95%)	8 (34%)	1 (4%)

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	I	2	U
6	I	3	G
6	I	6	A
6	I	9	U
6	I	18	A
6	I	20	C
6	I	21	C

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Mol	Chain	Res	Type
6	I	24	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	I	8	G

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
7	ATP	A	801	-	27,33,33	0.96	2 (7%)	27,52,52	1.83	4 (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
7	ATP	A	801	-	-	0/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	801	ATP	C8-N9	-2.21	1.34	1.36
7	A	801	ATP	C5-C4	2.61	1.46	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	801	ATP	N3-C2-N1	-5.79	123.91	128.86
7	A	801	ATP	PA-O3A-PB	-3.85	119.70	132.63
7	A	801	ATP	PB-O3B-PG	-3.51	120.83	132.63
7	A	801	ATP	C4-C5-N7	-2.76	106.75	109.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	801	ATP	1	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.