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

Jul 31, 2018 – 10:33 AM EDT

PDB ID	:	6D83
EMDB ID:	:	EMD-7453
Title	:	Structure of the cargo bound AP-1:Arf1:tetherin-Nef (L164A, L165A) dileucine mutant dimer monomeric subunit
Authors	:	Buffalo, C.Z.; Morris, K.L.; Hurley, J.H.
Deposited on	:	2018-04-25
Resolution	:	4.27 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.

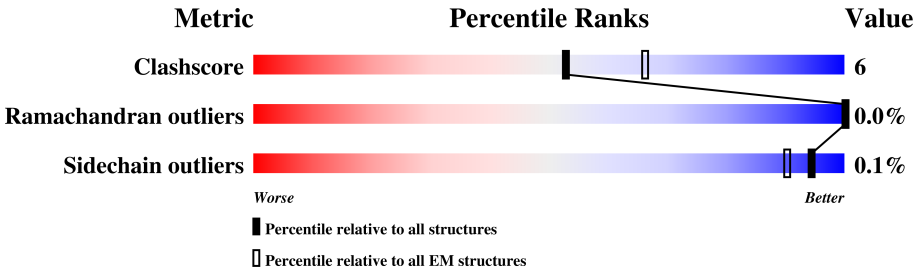
MolProbity	:	4.02b-467
Mogul	:	1.7.3 (157068), CSD as539be (2018)
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20031172

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 4.27 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

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	L	264	96%
1	T	264	5% 95%
2	B	586	82% 15%
3	C	193	68% 17% 15%
3	H	193	68% 16% 16%
4	G	601	82% 15%
5	M	423	79% 19%
6	S	154	80% 12% 8%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 16588 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 Bone marrow stromal antigen 2,Protein Nef.

Mol	Chain	Residues	Atoms	AltConf	Trace
1	T	13	Total C N O S 105 64 16 23 2	0	0
1	L	10	Total C N O 70 41 14 15	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	-26	MET	-	expression tag	UNP Q10589
T	-25	SER	-	expression tag	UNP Q10589
T	-24	TYR	-	expression tag	UNP Q10589
T	-23	TYR	-	expression tag	UNP Q10589
T	-22	HIS	-	expression tag	UNP Q10589
T	-21	HIS	-	expression tag	UNP Q10589
T	-20	HIS	-	expression tag	UNP Q10589
T	-19	HIS	-	expression tag	UNP Q10589
T	-18	HIS	-	expression tag	UNP Q10589
T	-17	HIS	-	expression tag	UNP Q10589
T	-16	ASP	-	expression tag	UNP Q10589
T	-15	TYR	-	expression tag	UNP Q10589
T	-14	ASP	-	expression tag	UNP Q10589
T	-13	ILE	-	expression tag	UNP Q10589
T	-12	PRO	-	expression tag	UNP Q10589
T	-11	THR	-	expression tag	UNP Q10589
T	-10	THR	-	expression tag	UNP Q10589
T	-9	GLU	-	expression tag	UNP Q10589
T	-8	ASN	-	expression tag	UNP Q10589
T	-7	LEU	-	expression tag	UNP Q10589
T	-6	TYR	-	expression tag	UNP Q10589
T	-5	PHE	-	expression tag	UNP Q10589
T	-4	GLN	-	expression tag	UNP Q10589
T	-3	GLY	-	expression tag	UNP Q10589
T	-2	ALA	-	expression tag	UNP Q10589
T	-1	MET	-	expression tag	UNP Q10589

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Chain	Residue	Modelled	Actual	Comment	Reference
T	0	GLY	-	expression tag	UNP Q10589
T	1	SER	-	expression tag	UNP Q10589
T	22	GLY	-	linker	UNP Q10589
T	23	SER	-	linker	UNP Q10589
T	24	ASP	-	linker	UNP Q10589
T	25	GLU	-	linker	UNP Q10589
T	26	ALA	-	linker	UNP Q10589
T	27	SER	-	linker	UNP Q10589
T	28	GLU	-	linker	UNP Q10589
T	29	GLY	-	linker	UNP Q10589
T	30	SER	-	linker	UNP Q10589
T	31	GLY	-	linker	UNP Q10589
T	195	ALA	LEU	engineered mutation	UNP Q90VU7
T	196	ALA	LEU	engineered mutation	UNP Q90VU7
L	3	MET	-	expression tag	UNP Q10589
L	4	SER	-	expression tag	UNP Q10589
L	5	TYR	-	expression tag	UNP Q10589
L	6	TYR	-	expression tag	UNP Q10589
L	7	HIS	-	expression tag	UNP Q10589
L	8	HIS	-	expression tag	UNP Q10589
L	9	HIS	-	expression tag	UNP Q10589
L	10	HIS	-	expression tag	UNP Q10589
L	11	HIS	-	expression tag	UNP Q10589
L	12	HIS	-	expression tag	UNP Q10589
L	13	ASP	-	expression tag	UNP Q10589
L	14	TYR	-	expression tag	UNP Q10589
L	15	ASP	-	expression tag	UNP Q10589
L	16	ILE	-	expression tag	UNP Q10589
L	17	PRO	-	expression tag	UNP Q10589
L	18	THR	-	expression tag	UNP Q10589
L	19	THR	-	expression tag	UNP Q10589
L	20	GLU	-	expression tag	UNP Q10589
L	21	ASN	-	expression tag	UNP Q10589
L	22	LEU	-	expression tag	UNP Q10589
L	23	TYR	-	expression tag	UNP Q10589
L	24	PHE	-	expression tag	UNP Q10589
L	25	GLN	-	expression tag	UNP Q10589
L	26	GLY	-	expression tag	UNP Q10589
L	27	ALA	-	expression tag	UNP Q10589
L	28	MET	-	expression tag	UNP Q10589
L	29	GLY	-	expression tag	UNP Q10589
L	30	SER	-	expression tag	UNP Q10589

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Chain	Residue	Modelled	Actual	Comment	Reference
L	51	GLY	-	linker	UNP Q10589
L	52	SER	-	linker	UNP Q10589
L	53	ASP	-	linker	UNP Q10589
L	54	GLU	-	linker	UNP Q10589
L	55	ALA	-	linker	UNP Q10589
L	56	SER	-	linker	UNP Q10589
L	57	GLU	-	linker	UNP Q10589
L	58	GLY	-	linker	UNP Q10589
L	59	SER	-	linker	UNP Q10589
L	60	GLY	-	linker	UNP Q10589
L	224	ALA	LEU	engineered mutation	UNP Q90VU7
L	225	ALA	LEU	engineered mutation	UNP Q90VU7

- Molecule 2 is a protein called AP-1 complex subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	570	Total	C	N	O	S	0	0
			4513	2883	741	862	27		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP Q10567
B	0	SER	-	expression tag	UNP Q10567
B	359	ARG	LYS	conflict	UNP Q10567
B	476	LYS	GLU	conflict	UNP Q10567

- Molecule 3 is a protein called ADP-ribosylation factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	165	Total	C	N	O	S	0	0
			1330	842	233	249	6		
3	H	163	Total	C	N	O	S	0	0
			1312	831	229	246	6		

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-11	MET	-	expression tag	UNP P84077
C	-10	SER	-	expression tag	UNP P84077
C	-9	TYR	-	expression tag	UNP P84077
C	-8	TYR	-	expression tag	UNP P84077

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	HIS	-	expression tag	UNP P84077
C	-6	HIS	-	expression tag	UNP P84077
C	-5	HIS	-	expression tag	UNP P84077
C	-4	HIS	-	expression tag	UNP P84077
C	-3	HIS	-	expression tag	UNP P84077
C	-2	HIS	-	expression tag	UNP P84077
C	-1	ASP	-	expression tag	UNP P84077
C	0	TYR	-	expression tag	UNP P84077
C	1	ASP	-	expression tag	UNP P84077
C	2	ILE	-	expression tag	UNP P84077
C	3	PRO	-	expression tag	UNP P84077
C	4	THR	-	expression tag	UNP P84077
C	5	THR	-	expression tag	UNP P84077
C	6	GLU	-	expression tag	UNP P84077
C	7	ASN	-	expression tag	UNP P84077
C	8	LEU	-	expression tag	UNP P84077
C	9	TYR	-	expression tag	UNP P84077
C	10	PHE	-	expression tag	UNP P84077
C	11	GLN	-	expression tag	UNP P84077
C	12	GLY	-	expression tag	UNP P84077
C	13	ALA	-	expression tag	UNP P84077
C	14	MET	-	expression tag	UNP P84077
C	15	GLY	-	expression tag	UNP P84077
C	16	SER	-	expression tag	UNP P84077
C	71	LEU	GLN	conflict	UNP P84077
H	-11	MET	-	expression tag	UNP P84077
H	-10	SER	-	expression tag	UNP P84077
H	-9	TYR	-	expression tag	UNP P84077
H	-8	TYR	-	expression tag	UNP P84077
H	-7	HIS	-	expression tag	UNP P84077
H	-6	HIS	-	expression tag	UNP P84077
H	-5	HIS	-	expression tag	UNP P84077
H	-4	HIS	-	expression tag	UNP P84077
H	-3	HIS	-	expression tag	UNP P84077
H	-2	HIS	-	expression tag	UNP P84077
H	-1	ASP	-	expression tag	UNP P84077
H	0	TYR	-	expression tag	UNP P84077
H	1	ASP	-	expression tag	UNP P84077
H	2	ILE	-	expression tag	UNP P84077
H	3	PRO	-	expression tag	UNP P84077
H	4	THR	-	expression tag	UNP P84077
H	5	THR	-	expression tag	UNP P84077

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Chain	Residue	Modelled	Actual	Comment	Reference
H	6	GLU	-	expression tag	UNP P84077
H	7	ASN	-	expression tag	UNP P84077
H	8	LEU	-	expression tag	UNP P84077
H	9	TYR	-	expression tag	UNP P84077
H	10	PHE	-	expression tag	UNP P84077
H	11	GLN	-	expression tag	UNP P84077
H	12	GLY	-	expression tag	UNP P84077
H	13	ALA	-	expression tag	UNP P84077
H	14	MET	-	expression tag	UNP P84077
H	15	GLY	-	expression tag	UNP P84077
H	16	SER	-	expression tag	UNP P84077
H	71	LEU	GLN	conflict	UNP P84077

- Molecule 4 is a protein called AP-1 complex subunit gamma-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	585	Total	C	N	O	S	0	0
			4633	2914	815	865	39		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	596	GLU	-	expression tag	UNP P22892
G	597	ASN	-	expression tag	UNP P22892
G	598	LEU	-	expression tag	UNP P22892
G	599	TYR	-	expression tag	UNP P22892
G	600	PHE	-	expression tag	UNP P22892
G	601	GLN	-	expression tag	UNP P22892

- Molecule 5 is a protein called AP-1 complex subunit mu-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	415	Total	C	N	O	S	0	0
			3362	2161	566	621	14		

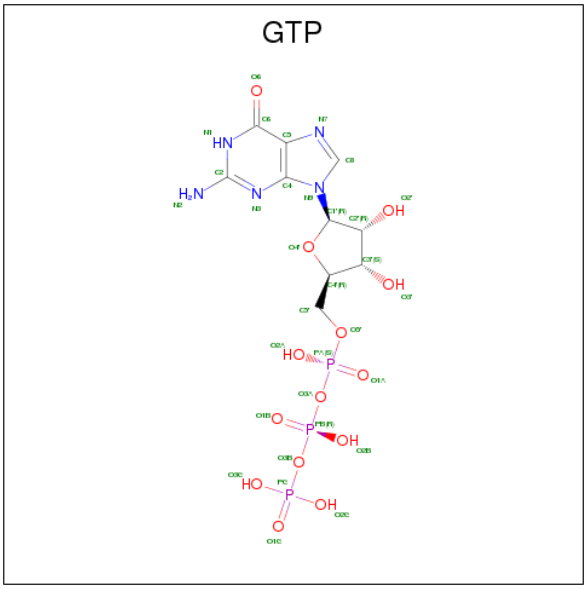
- Molecule 6 is a protein called AP-1 complex subunit sigma-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S	142	Total	C	N	O	S	0	0
			1197	782	197	213	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	148	CYS	SER	conflict	UNP Q96PC3

- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
7	C	1	Total	C	N	O	P	0
			32	10	5	14	3	
7	H	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

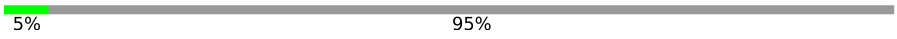
Mol	Chain	Residues	Atoms		AltConf
8	H	1	Total	Mg	0
			1	1	
8	C	1	Total	Mg	0
			1	1	

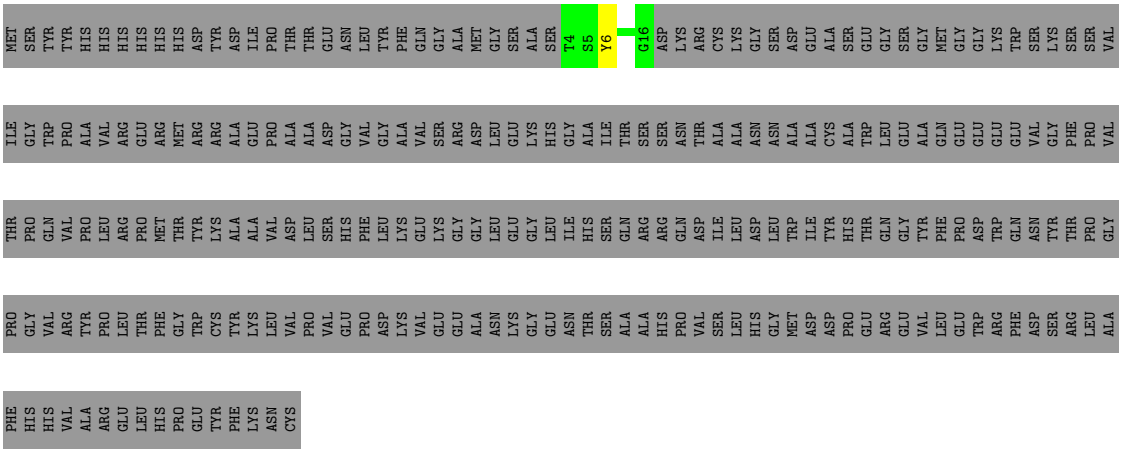
3 Residue-property plots (i)

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: Bone marrow stromal antigen 2,Protein Nef

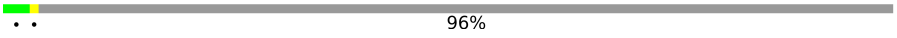
Chain T:

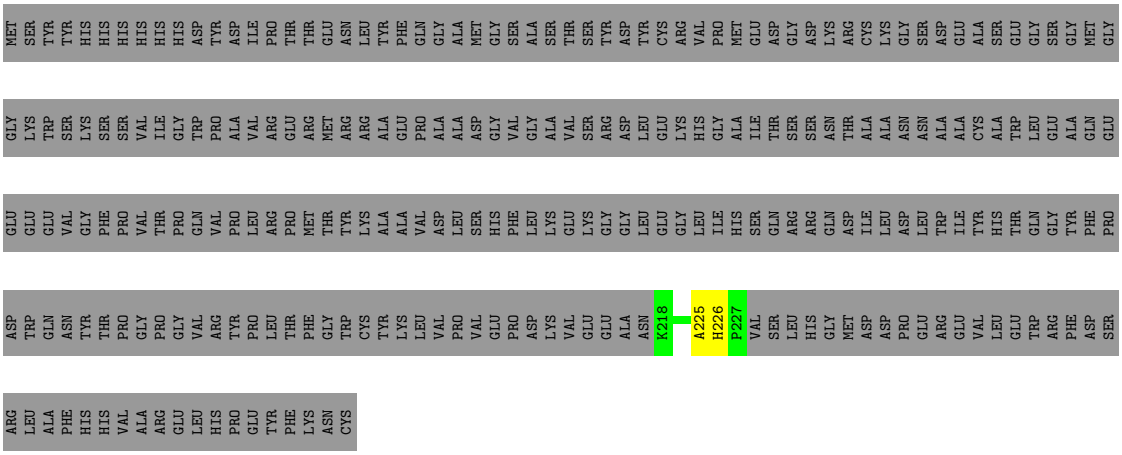




• Molecule 1: Bone marrow stromal antigen 2,Protein Nef

Chain L:



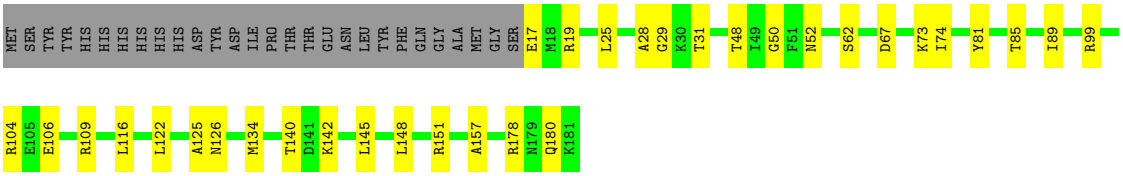


• Molecule 2: AP-1 complex subunit beta-1

Chain B:

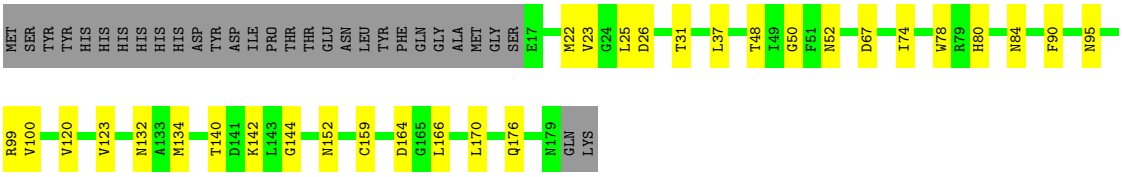
• Molecule 3: ADP-ribosylation factor 1

Chain C:



• Molecule 3: ADP-ribosylation factor 1

Chain H:

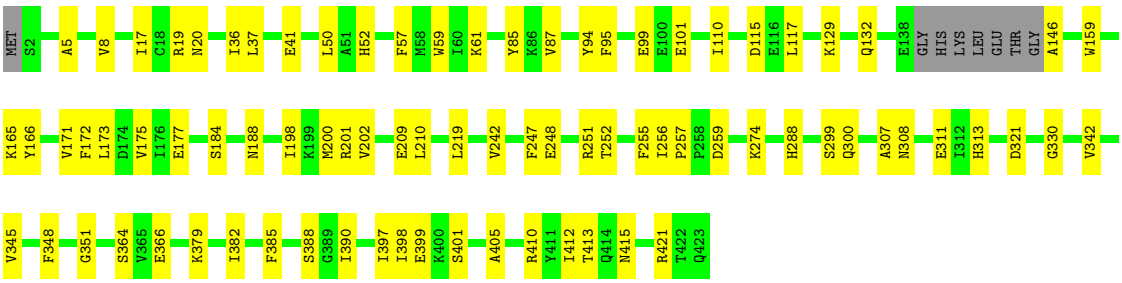


• Molecule 4: AP-1 complex subunit gamma-1

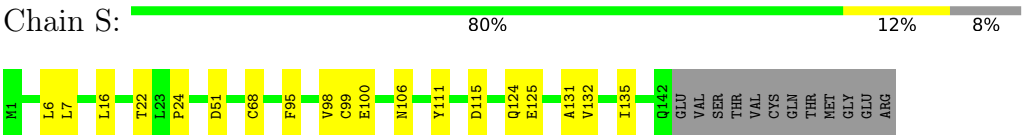
Chain G:

• Molecule 5: AP-1 complex subunit mu-1

Chain M:



• Molecule 6: AP-1 complex subunit sigma-3



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	85592	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	39.7	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: GTP, MG

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	L	0.22	0/71	0.49	0/95
1	T	0.36	0/107	0.55	0/144
2	B	0.30	0/4583	0.53	0/6216
3	C	0.27	0/1353	0.52	0/1831
3	H	0.29	0/1335	0.55	0/1808
4	G	0.29	0/4697	0.53	0/6338
5	M	0.32	0/3439	0.54	0/4648
6	S	0.29	0/1220	0.55	0/1639
All	All	0.30	0/16805	0.54	0/22719

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	295	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	L	70	0	63	0	0
1	T	105	0	89	1	0
2	B	4513	0	4647	55	0
3	C	1330	0	1328	22	0
3	H	1312	0	1307	21	0
4	G	4633	0	4756	60	0
5	M	3362	0	3373	49	0
6	S	1197	0	1229	13	0
7	C	32	0	12	3	0
7	H	32	0	12	2	0
8	C	1	0	0	0	0
8	H	1	0	0	0	0
All	All	16588	0	16816	202	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 (202) 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)
3:C:25:LEU:HD21	3:C:99:ARG:HE	1.58	0.67
2:B:304:ARG:HH21	2:B:575:HIS:HD2	1.44	0.66
4:G:31:CYS:SG	4:G:35:ARG:NH2	2.69	0.65
4:G:289:LEU:HD21	4:G:312:ILE:HD12	1.79	0.64
5:M:288:HIS:HE1	5:M:366:GLU:HB3	1.62	0.64
2:B:63:LEU:HD23	5:M:146:ALA:HB3	1.80	0.63
2:B:74:MET:SD	5:M:19:ARG:NH1	2.73	0.62
5:M:311:GLU:HB2	5:M:379:LYS:HB2	1.80	0.62
3:C:178:ARG:HD2	3:C:180:GLN:HE21	1.66	0.61
3:C:31:THR:HG21	3:C:48:THR:HG21	1.82	0.61
5:M:307:ALA:HB3	5:M:348:PHE:HB3	1.82	0.60
2:B:246:PRO:HB3	5:M:248:GLU:HB2	1.83	0.60
4:G:223:LEU:HD23	4:G:270:ILE:HD12	1.84	0.60
3:C:140:THR:HG23	3:C:145:LEU:HB2	1.84	0.59
4:G:258:ARG:HA	4:G:299:ILE:HA	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:25:LEU:HB3	3:H:99:ARG:HH21	1.67	0.59
2:B:308:LEU:HD11	2:B:563:LEU:HB3	1.85	0.58
4:G:148:THR:O	4:G:154:ARG:NH1	2.36	0.58
2:B:138:ARG:NH1	2:B:171:ASP:OD2	2.37	0.58
2:B:439:LEU:O	2:B:445:ARG:NH1	2.35	0.58
2:B:522:ARG:NH2	2:B:526:TYR:OH	2.37	0.58
4:G:450:GLU:HG2	4:G:451:MET:HG2	1.84	0.58
2:B:473:PHE:O	2:B:481:GLN:NE2	2.36	0.58
4:G:503:ASP:HA	4:G:543:ARG:HH22	1.69	0.57
2:B:386:GLN:O	2:B:390:ARG:NH2	2.37	0.57
4:G:482:GLU:O	4:G:583:ARG:NH1	2.38	0.57
2:B:92:VAL:HG12	2:B:125:PRO:HG3	1.87	0.56
4:G:35:ARG:HB3	5:M:321:ASP:HB3	1.87	0.56
3:H:22:MET:HB2	3:H:67:ASP:HA	1.86	0.56
6:S:99:CYS:SG	6:S:100:GLU:N	2.78	0.56
2:B:292:LEU:O	2:B:299:GLN:NE2	2.39	0.56
5:M:177:GLU:HB2	5:M:413:THR:HA	1.86	0.56
4:G:96:ARG:HD2	6:S:24:PRO:HB3	1.87	0.56
2:B:454:GLU:O	2:B:494:LYS:NZ	2.38	0.55
5:M:219:LEU:HD13	5:M:251:ARG:HB2	1.89	0.55
3:C:28:ALA:O	3:C:126:ASN:ND2	2.39	0.55
4:G:536:ARG:NH1	4:G:581:LEU:O	2.39	0.55
3:H:52:ASN:HB2	3:H:67:ASP:HB3	1.89	0.55
3:C:125:ALA:HB3	3:C:157:ALA:HA	1.89	0.55
2:B:359:ARG:HE	2:B:394:THR:HG23	1.71	0.55
4:G:88:GLY:O	4:G:92:LEU:HB2	2.07	0.55
2:B:551:GLU:HB2	4:G:555:ILE:HD13	1.90	0.54
4:G:146:LEU:HD12	4:G:154:ARG:HE	1.72	0.54
2:B:18:LEU:HD13	2:B:36:LYS:HD3	1.90	0.54
3:C:106:GLU:OE2	3:C:109:ARG:NH1	2.39	0.54
1:T:6:TYR:OH	5:M:308:ASN:ND2	2.40	0.54
2:B:127:ARG:NH2	2:B:159:GLN:O	2.36	0.54
5:M:175:VAL:HG22	5:M:198:ILE:HG12	1.90	0.54
4:G:539:CYS:SG	4:G:540:THR:N	2.81	0.53
3:H:159:CYS:HB2	3:H:164:ASP:HB2	1.90	0.53
3:C:104:ARG:NH1	3:C:142:LYS:O	2.41	0.53
2:B:297:GLU:OE1	5:M:85:TYR:OH	2.26	0.53
2:B:493:LEU:HD21	2:B:538:LYS:HA	1.91	0.53
5:M:385:PHE:O	5:M:413:THR:OG1	2.25	0.53
5:M:299:SER:OG	5:M:351:GLY:N	2.39	0.53
4:G:528:THR:OG1	4:G:562:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:24:ARG:HG2	4:G:61:TYR:HE1	1.74	0.52
4:G:68:LEU:HD21	3:H:80:HIS:HB3	1.91	0.52
5:M:379:LYS:HD3	5:M:415:ASN:HD21	1.74	0.52
2:B:211:LEU:O	2:B:219:GLN:NE2	2.43	0.52
4:G:67:GLN:NE2	4:G:92:LEU:O	2.43	0.52
4:G:152:TYR:HA	4:G:155:LYS:HE2	1.92	0.52
2:B:520:ARG:NH2	4:G:585:PRO:O	2.39	0.52
3:C:48:THR:OG1	7:C:1001:GTP:O1G	2.27	0.51
2:B:312:LYS:HG3	2:B:313:ARG:HG2	1.92	0.51
4:G:443:GLN:NE2	4:G:587:MET:O	2.43	0.51
5:M:19:ARG:NH2	5:M:115:ASP:OD1	2.42	0.51
4:G:485:ASP:OD2	4:G:583:ARG:NH2	2.44	0.51
3:C:52:ASN:HB2	3:C:67:ASP:HB3	1.92	0.51
4:G:113:HIS:O	4:G:119:GLN:NE2	2.42	0.51
3:H:26:ASP:OD1	3:H:99:ARG:NH2	2.43	0.51
2:B:268:GLU:OE2	2:B:312:LYS:NZ	2.37	0.51
4:G:241:SER:O	4:G:246:GLN:NE2	2.44	0.51
2:B:357:GLU:OE2	5:M:421:ARG:NH2	2.36	0.50
2:B:89:ASN:HB2	3:C:50:GLY:H	1.76	0.50
5:M:184:SER:OG	5:M:188:ASN:OD1	2.28	0.50
5:M:95:PHE:HE2	5:M:110:ILE:HD11	1.76	0.50
2:B:482:LEU:HD11	2:B:522:ARG:HG3	1.94	0.50
3:C:19:ARG:HE	3:C:85:THR:HA	1.76	0.50
3:C:73:LYS:HG3	3:C:74:ILE:HG23	1.94	0.50
5:M:274:LYS:HD2	5:M:300:GLN:HE21	1.76	0.50
2:B:58:MET:O	2:B:66:LYS:NZ	2.40	0.50
5:M:242:VAL:HA	5:M:255:PHE:HB3	1.94	0.49
2:B:530:LEU:HD12	2:B:534:PRO:HB3	1.95	0.49
4:G:364:ARG:NH2	6:S:51:ASP:OD1	2.45	0.49
4:G:54:LEU:HD21	4:G:88:GLY:HA2	1.93	0.49
5:M:307:ALA:HA	5:M:382:ILE:HG12	1.95	0.49
4:G:257:GLY:HA2	4:G:260:ASP:HB3	1.94	0.49
3:C:116:LEU:O	3:C:151:ARG:NH2	2.42	0.49
4:G:192:HIS:HA	4:G:245:LEU:HD13	1.95	0.48
3:H:90:PHE:HB3	3:H:123:VAL:HG22	1.94	0.48
4:G:574:ASP:OD1	4:G:577:ARG:NE	2.44	0.48
3:H:37:LEU:HD21	3:H:166:LEU:HB3	1.96	0.48
2:B:78:LYS:HD3	2:B:114:ARG:HH12	1.77	0.48
3:C:29:GLY:N	7:C:1001:GTP:O2B	2.47	0.48
3:H:100:VAL:HG11	3:H:142:LYS:HD2	1.94	0.48
5:M:209:GLU:HB3	5:M:398:ILE:HB	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:151:SER:HB3	4:G:187:ASN:HD22	1.78	0.48
5:M:5:ALA:HA	5:M:20:ASN:HA	1.95	0.48
2:B:515:ASP:HA	2:B:520:ARG:HD2	1.95	0.48
4:G:115:THR:HG22	4:G:117:PHE:H	1.79	0.48
2:B:162:LEU:HD11	2:B:187:ILE:HG21	1.95	0.48
3:C:48:THR:HG1	7:C:1001:GTP:PG	2.37	0.48
3:H:120:VAL:HG12	3:H:152:ASN:HB2	1.95	0.48
5:M:37:LEU:O	5:M:41:GLU:HB2	2.14	0.48
5:M:99:GLU:HB2	5:M:101:GLU:HG2	1.95	0.48
3:C:81:TYR:O	3:C:85:THR:OG1	2.31	0.47
5:M:172:PHE:HB2	5:M:201:ARG:HB2	1.95	0.47
6:S:115:ASP:O	6:S:124:GLN:NE2	2.47	0.47
5:M:50:LEU:HB2	5:M:57:PHE:HB2	1.96	0.47
6:S:95:PHE:HD2	6:S:98:VAL:HG23	1.79	0.47
2:B:545:LYS:HD2	4:G:560:GLN:HE22	1.80	0.47
2:B:174:PRO:HB3	2:B:210:ALA:HB1	1.96	0.47
3:C:17:GLU:N	3:C:62:SER:HG	2.12	0.47
5:M:173:LEU:HG	5:M:200:MET:HG2	1.96	0.47
2:B:452:VAL:HG11	2:B:465:LEU:HD11	1.97	0.47
4:G:220:VAL:HG13	4:G:270:ILE:HD13	1.97	0.47
5:M:330:GLY:HA3	5:M:345:VAL:HG22	1.96	0.47
2:B:174:PRO:HG2	2:B:213:GLU:HB2	1.97	0.47
2:B:466:LEU:HD13	2:B:488:ILE:HG12	1.98	0.47
3:C:134:MET:SD	3:C:134:MET:N	2.88	0.46
3:C:148:LEU:HB3	3:C:151:ARG:HB2	1.96	0.46
5:M:129:LYS:NZ	5:M:259:ASP:OD2	2.48	0.46
4:G:83:ARG:HE	4:G:121:LEU:HD11	1.80	0.46
3:H:48:THR:HG1	7:H:1001:GTP:PG	2.39	0.46
6:S:7:LEU:HD13	6:S:16:LEU:HD22	1.98	0.46
5:M:87:VAL:HG22	5:M:117:LEU:HD13	1.96	0.46
6:S:132:VAL:HA	6:S:135:ILE:HG22	1.98	0.46
5:M:94:TYR:HE1	5:M:132:GLN:HG2	1.80	0.46
2:B:374:VAL:HG12	2:B:413:VAL:HG21	1.98	0.46
4:G:457:GLN:HE22	4:G:500:VAL:HG11	1.80	0.46
4:G:491:GLN:HE21	4:G:498:ILE:HD12	1.81	0.45
6:S:7:LEU:HB2	6:S:16:LEU:HB3	1.97	0.45
5:M:410:ARG:HE	5:M:412:ILE:HD11	1.82	0.45
3:H:120:VAL:HG11	3:H:176:GLN:HB3	1.99	0.45
4:G:257:GLY:O	4:G:264:SER:OG	2.34	0.45
4:G:322:LYS:HD3	4:G:325:ARG:HD2	1.99	0.45
4:G:471:PRO:HA	4:G:474:GLN:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:36:ILE:HD11	5:M:52:HIS:HD2	1.81	0.45
4:G:456:VAL:HG12	4:G:487:LEU:HD13	1.99	0.45
5:M:210:LEU:HD13	5:M:257:PRO:HG3	1.99	0.45
4:G:149:SER:HA	4:G:154:ARG:HH11	1.81	0.44
4:G:217:PRO:HA	4:G:220:VAL:HB	1.99	0.44
2:B:408:GLN:HE21	2:B:440:ASP:H	1.66	0.44
2:B:522:ARG:NH2	4:G:565:GLU:OE1	2.50	0.44
4:G:581:LEU:HA	4:G:581:LEU:HD23	1.86	0.44
4:G:39:ARG:HH21	3:H:84:ASN:HD21	1.65	0.44
5:M:59:TRP:HZ3	5:M:61:LYS:HB2	1.82	0.44
2:B:502:LEU:HD12	2:B:505:GLN:HE21	1.82	0.44
3:H:95:ASN:O	3:H:132:ASN:ND2	2.51	0.44
3:H:31:THR:OG1	7:H:1001:GTP:O1A	2.33	0.44
2:B:426:GLU:HB2	2:B:458:ARG:HG2	1.99	0.44
4:G:34:ILE:HG21	4:G:53:LEU:HD12	2.00	0.44
5:M:288:HIS:ND1	5:M:364:SER:O	2.51	0.43
5:M:382:ILE:HB	5:M:413:THR:HB	1.98	0.43
4:G:161:ALA:HA	4:G:164:VAL:HG22	2.00	0.43
2:B:135:PRO:HG2	2:B:173:ASN:HD22	1.83	0.43
2:B:97:ASP:H	2:B:103:ARG:HD3	1.83	0.43
5:M:171:VAL:HG13	5:M:202:VAL:HG22	2.01	0.43
5:M:388:SER:HB2	5:M:390:ILE:HG22	2.01	0.43
2:B:304:ARG:HD2	2:B:304:ARG:HA	1.86	0.43
2:B:135:PRO:HA	2:B:138:ARG:HE	1.84	0.42
5:M:165:LYS:NZ	5:M:166:TYR:O	2.45	0.42
6:S:16:LEU:HG	6:S:111:TYR:CZ	2.54	0.42
2:B:63:LEU:HD21	2:B:101:LEU:HD23	2.02	0.42
3:C:89:ILE:HG12	3:C:122:LEU:HB3	2.00	0.42
5:M:399:GLU:HG3	5:M:401:SER:H	1.85	0.42
2:B:577:PRO:HA	2:B:578:PRO:HD3	1.92	0.42
5:M:8:VAL:HB	5:M:17:ILE:HG22	2.02	0.42
6:S:6:LEU:HB2	6:S:68:CYS:HB3	2.01	0.42
4:G:336:VAL:HG11	4:G:371:ALA:HB1	2.02	0.42
2:B:569:THR:O	2:B:572:SER:OG	2.33	0.41
3:H:37:LEU:HD13	3:H:170:LEU:HD11	2.01	0.41
4:G:130:GLY:O	4:G:163:HIS:NE2	2.42	0.41
4:G:8:ARG:NH2	6:S:106:ASN:OD1	2.44	0.41
5:M:379:LYS:HA	5:M:415:ASN:ND2	2.35	0.41
2:B:446:ALA:HB1	2:B:483:GLN:HG3	2.02	0.41
2:B:40:SER:HB3	2:B:45:LYS:HB2	2.01	0.41
5:M:159:TRP:NE1	5:M:256:ILE:O	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:488:ILE:HD12	2:B:506:VAL:HG21	2.03	0.41
4:G:293:VAL:HG11	4:G:313:LEU:HD21	2.03	0.41
4:G:105:ASN:HB2	3:H:50:GLY:H	1.85	0.41
4:G:154:ARG:HH21	4:G:182:LEU:HD22	1.86	0.41
4:G:513:LEU:HD23	4:G:513:LEU:HA	1.90	0.41
4:G:94:ASP:HB2	6:S:22:THR:HB	2.03	0.41
3:H:134:MET:N	3:H:134:MET:SD	2.94	0.41
4:G:491:GLN:HE22	4:G:500:VAL:HG23	1.86	0.41
3:H:23:VAL:HG23	3:H:90:PHE:HD1	1.86	0.41
5:M:313:HIS:CD2	5:M:342:VAL:HG22	2.56	0.41
2:B:326:VAL:HG12	2:B:338:LYS:HD2	2.02	0.41
3:C:25:LEU:HD11	3:C:99:ARG:HB3	2.03	0.41
4:G:46:ARG:HE	4:G:73:LEU:HD23	1.84	0.41
5:M:397:ILE:HG13	5:M:405:ALA:HB3	2.03	0.41
6:S:125:GLU:HG2	6:S:131:ALA:HB2	2.03	0.40
2:B:201:PRO:HA	2:B:204:ILE:HD12	2.03	0.40
5:M:247:PHE:HA	5:M:252:THR:H	1.86	0.40
2:B:24:SER:OG	2:B:25:ASP:N	2.53	0.40
2:B:477:SER:OG	2:B:478:THR:N	2.54	0.40
4:G:278:THR:HG21	4:G:289:LEU:HD22	2.02	0.40
4:G:456:VAL:HG21	4:G:483:TYR:HB2	2.03	0.40
3:H:74:ILE:HG22	3:H:78:TRP:HE1	1.85	0.40
3:H:140:THR:O	3:H:144:GLY:N	2.51	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	L	8/264 (3%)	5 (62%)	2 (25%)	1 (12%)	0 6
1	T	11/264 (4%)	10 (91%)	1 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	568/586 (97%)	537 (94%)	31 (6%)	0	100	100
3	C	163/193 (84%)	154 (94%)	9 (6%)	0	100	100
3	H	161/193 (83%)	152 (94%)	9 (6%)	0	100	100
4	G	583/601 (97%)	559 (96%)	24 (4%)	0	100	100
5	M	411/423 (97%)	393 (96%)	18 (4%)	0	100	100
6	S	140/154 (91%)	131 (94%)	9 (6%)	0	100	100
All	All	2045/2678 (76%)	1941 (95%)	103 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	225	ALA

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	L	7/220 (3%)	6 (86%)	1 (14%)	3	22
1	T	12/220 (6%)	12 (100%)	0	100	100
2	B	510/523 (98%)	510 (100%)	0	100	100
3	C	143/168 (85%)	143 (100%)	0	100	100
3	H	141/168 (84%)	141 (100%)	0	100	100
4	G	520/534 (97%)	520 (100%)	0	100	100
5	M	377/383 (98%)	377 (100%)	0	100	100
6	S	132/143 (92%)	132 (100%)	0	100	100
All	All	1842/2359 (78%)	1841 (100%)	1 (0%)	94	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	226	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	205	ASN
2	B	299	GLN
2	B	408	GLN
2	B	483	GLN
2	B	505	GLN
2	B	575	HIS
3	C	86	GLN
3	C	128	GLN
3	C	150	HIS
3	C	180	GLN
4	G	67	GLN
4	G	97	GLN
4	G	218	GLN
4	G	235	HIS
4	G	443	GLN
4	G	447	ASN
4	G	457	GLN
4	G	491	GLN
3	H	176	GLN
5	M	32	HIS
5	M	52	HIS
5	M	239	HIS
5	M	300	GLN
5	M	308	ASN
6	S	3	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	GTP	C	1001	8	27,34,34	0.93	1 (3%)	29,54,54	1.91	6 (20%)
7	GTP	H	1001	8	27,34,34	0.91	1 (3%)	29,54,54	1.85	6 (20%)

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	GTP	C	1001	8	-	0/18/38/38	0/3/3/3
7	GTP	H	1001	8	-	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	H	1001	GTP	C6-N1	2.73	1.37	1.33
7	C	1001	GTP	C6-N1	2.94	1.38	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	1001	GTP	N3-C2-N1	-4.90	120.23	127.41
7	H	1001	GTP	N3-C2-N1	-4.74	120.46	127.41
7	C	1001	GTP	PB-O3B-PG	-4.38	117.92	132.63
7	H	1001	GTP	PB-O3B-PG	-3.96	119.31	132.63
7	H	1001	GTP	PA-O3A-PB	-3.89	119.56	132.63
7	C	1001	GTP	PA-O3A-PB	-3.69	120.24	132.63
7	H	1001	GTP	C5-C6-N1	-2.77	119.54	123.47
7	C	1001	GTP	C5-C6-N1	-2.70	119.63	123.47
7	C	1001	GTP	C6-N1-C2	2.58	119.77	116.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	H	1001	GTP	C6-N1-C2	2.60	119.79	116.06
7	H	1001	GTP	C2-N3-C4	4.17	120.03	115.16
7	C	1001	GTP	C2-N3-C4	4.40	120.29	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1001	GTP	3	0
7	H	1001	GTP	2	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.