WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:03 AM GMT

PDB ID	:	3D45
Title	:	Crystal structure of mouse PARN in complex with m7GpppG
Authors	:	Wu, M; Song, H
Deposited on	:	2008-05-13
Resolution	:	3.00 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.00 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	Percentile Ranks	Value
Clashscore		21
Ramachandran outliers		2.4%
Sidechain outliers		14.6%
RSRZ outliers		2.5%

Worse ⟵ ⟶ *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
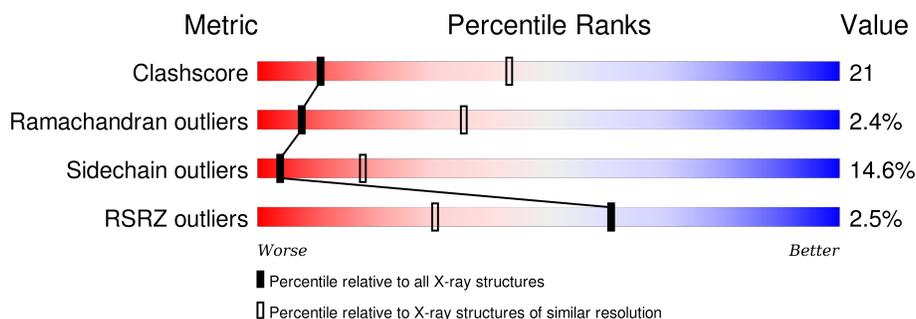
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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. 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	507	2% · 45% · 25% · 5% · 24%
1	B	507	2% · 39% · 27% · 7% · 26%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6307 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 Poly(A)-specific ribonuclease PARN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	S	0	0	0
			3109	2005	503	586	15			
1	B	373	Total	C	N	O	S	0	0	0
			3016	1947	488	567	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	901	GLY	-	EXPRESSION TAG	UNP Q8VDG3
A	900	PRO	-	EXPRESSION TAG	UNP Q8VDG3
B	901	GLY	-	EXPRESSION TAG	UNP Q8VDG3
B	900	PRO	-	EXPRESSION TAG	UNP Q8VDG3

- Molecule 2 is 7N-METHYL-8-HYDROGUANOSINE-5'-MONOPHOSPHATE (three-letter code: GDP, 7MG) (formula: $C_{10}H_{15}N_5O_{11}P_2$, $C_{11}H_{18}N_5O_8P$).
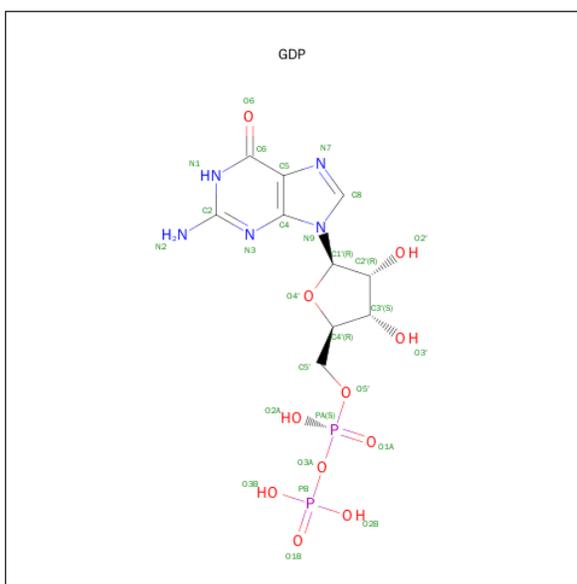
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	2	Total	C	N	O	P	0	0
			52	21	10	18	3		
2	B	2	Total	C	N	O	P	0	0
			52	21	10	18	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	34	Total	O	0	0
			34	34		
3	B	44	Total	O	0	0
			44	44		

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 errors 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: Poly(A)-specific ribonuclease PARN
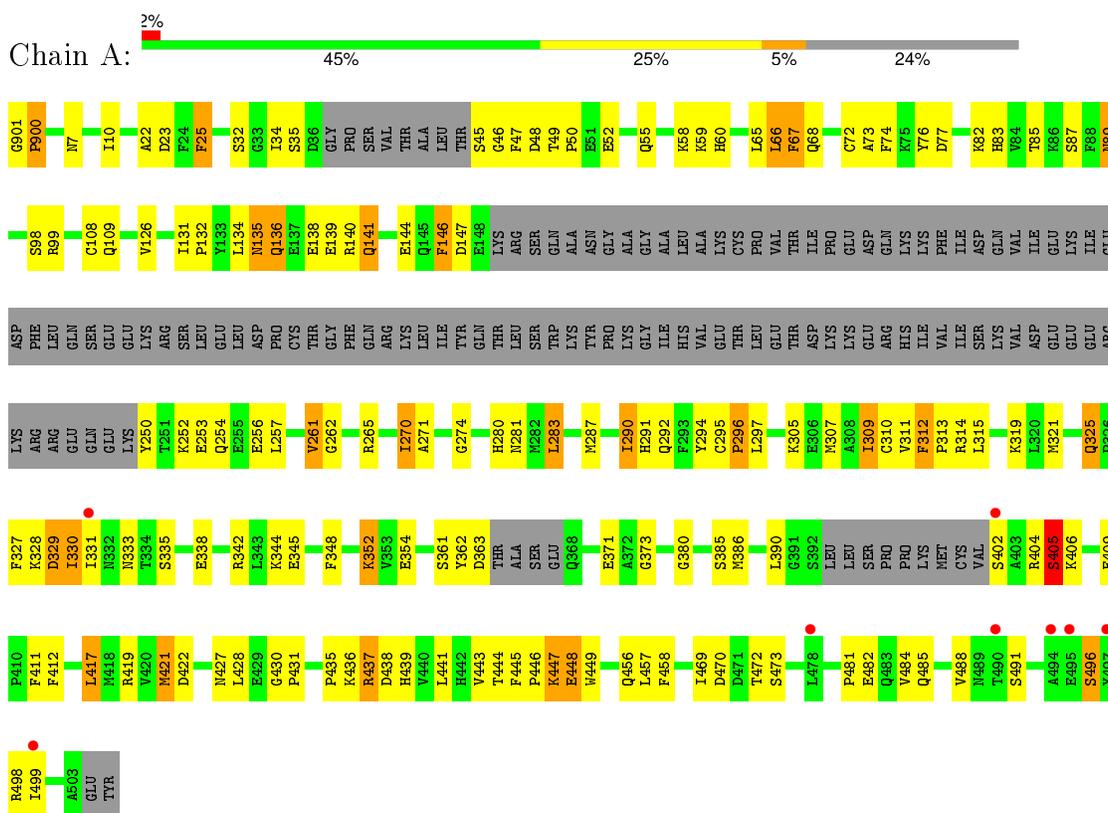
- Molecule 1: Poly(A)-specific ribonuclease PARN
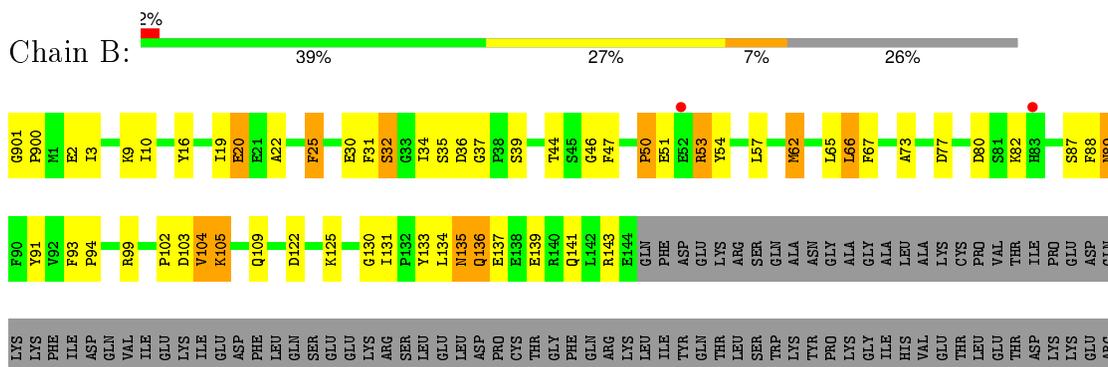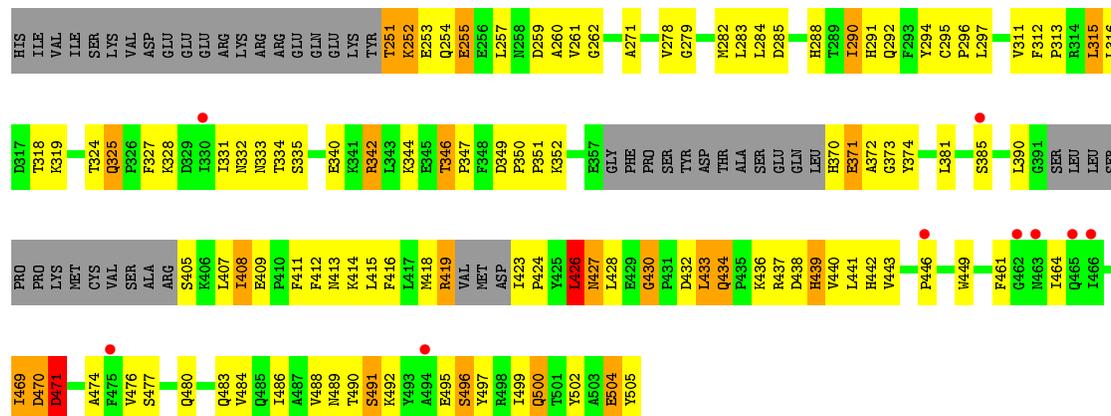
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	58.01Å　　128.35Å　　176.84Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	103.69　−　3.00 72.82　−　2.92	Depositor EDS
% Data completeness (in resolution range)	94.7 (103.69-3.00) 94.0 (72.82-2.92)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.78 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.299　,　　0.334 0.294　,　(Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	78.7	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 71.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.51$, $<L^2> = 0.34$	Xtriage
Outliers	4 of 27821 reflections (0.014%)	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	6307	wwPDB-VP
Average B, all atoms (Å^2)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, 7MG

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	0.65	2/3189 (0.1%)	0.73	0/4306
1	B	0.67	0/3093	0.74	0/4179
All	All	0.66	2/6282 (0.0%)	0.74	0/8485

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	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	CYS	CB-SG	-5.96	1.72	1.81
1	A	310	CYS	CB-SG	-5.18	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	430	GLY	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	3109	0	2999	112	0
1	B	3016	0	2926	138	0
2	A	52	0	28	5	0
2	B	52	0	28	7	0
3	A	34	0	0	6	0
3	B	44	0	0	9	0
All	All	6307	0	5981	257	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 21.

All (257) 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:B:325:GLN:HE21	1:B:325:GLN:HA	1.07	1.09
1:B:484:VAL:O	1:B:488:VAL:HG23	1.71	0.90
1:A:470:ASP:HB2	1:A:473:SER:OG	1.70	0.90
1:B:66:LEU:H	1:B:292:GLN:HE22	1.03	0.90
1:B:325:GLN:CA	1:B:325:GLN:HE21	1.86	0.89
1:B:66:LEU:H	1:B:292:GLN:NE2	1.70	0.88
1:B:66:LEU:N	1:B:292:GLN:HE22	1.72	0.87
1:B:342:ARG:HD2	3:B:1158:HOH:O	1.75	0.86
1:B:325:GLN:NE2	1:B:325:GLN:HA	1.91	0.86
1:B:35:SER:H	1:B:109:GLN:HE22	1.23	0.85
1:B:31:PHE:HE2	1:B:66:LEU:HD22	1.42	0.84
1:B:89:ASN:HD21	1:B:373:GLY:H	1.27	0.82
1:A:900:PRO:HB3	1:A:87:SER:OG	1.80	0.81
1:B:319:LYS:HD3	1:B:416:PHE:CE2	2.15	0.81
1:B:901:GLY:N	1:B:900:PRO:HD3	1.96	0.81
1:B:441:LEU:HD12	1:B:499:ILE:HG23	1.64	0.80
1:A:333:ASN:HD22	1:A:338:GLU:HB2	1.46	0.79
1:B:900:PRO:HG2	1:B:373:GLY:HA3	1.64	0.79
2:A:651:7MG:P	2:A:652:GDP:O3B	2.41	0.78
2:B:1152:7MG:P	2:B:1151:GDP:O3B	2.42	0.78
1:A:325:GLN:NE2	1:A:325:GLN:H	1.81	0.78
1:A:35:SER:H	1:A:109:GLN:HE22	1.32	0.78
1:B:480:GLN:H	1:B:483:GLN:HE21	1.31	0.77
1:B:413:ASN:O	1:B:427:ASN:ND2	2.18	0.75
1:A:325:GLN:H	1:A:325:GLN:CD	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:ILE:H	1:B:109:GLN:NE2	1.85	0.74
1:B:427:ASN:HB2	1:B:430:GLY:H	1.53	0.74
1:B:102:PRO:O	3:B:1184:HOH:O	2.05	0.74
1:A:470:ASP:HB3	1:A:472:THR:H	1.53	0.73
1:A:333:ASN:ND2	1:A:338:GLU:HB2	2.03	0.73
1:B:135:ASN:HD21	1:B:137:GLU:HB2	1.54	0.73
1:B:441:LEU:HD12	1:B:499:ILE:CG2	2.18	0.73
1:B:346:THR:HG22	1:B:347:PRO:HA	1.71	0.72
1:A:34:ILE:H	1:A:109:GLN:HE21	1.37	0.72
1:A:333:ASN:HD22	1:A:338:GLU:CB	2.02	0.72
1:B:433:LEU:HG	1:B:434:GLN:H	1.54	0.72
1:A:274:GLY:HA2	1:A:313:PRO:HG3	1.71	0.71
1:A:89:ASN:HD21	1:A:373:GLY:H	1.37	0.71
1:A:305:LYS:HE2	1:A:427:ASN:O	1.91	0.70
1:A:901:GLY:N	3:A:929:HOH:O	2.24	0.70
1:A:348:PHE:HB2	3:A:907:HOH:O	1.92	0.70
1:A:271:ALA:HA	1:A:311:VAL:O	1.93	0.69
1:B:333:ASN:HA	3:B:1195:HOH:O	1.92	0.69
1:B:432:ASP:O	1:B:433:LEU:HB2	1.92	0.68
1:B:469:ILE:HG23	1:B:474:ALA:HA	1.75	0.68
1:A:333:ASN:OD1	2:A:651:7MG:HM72	1.95	0.66
1:B:480:GLN:HB2	1:B:483:GLN:HG3	1.78	0.66
1:A:49:THR:OG1	1:A:52:GLU:HG3	1.96	0.65
1:A:253:GLU:CD	1:A:256:GLU:HG3	2.17	0.65
1:B:2:GLU:OE1	1:B:125:LYS:HE2	1.97	0.65
1:A:253:GLU:OE1	1:A:256:GLU:HG3	1.96	0.64
1:B:490:THR:O	1:B:491:SER:HB3	1.99	0.63
1:B:16:TYR:O	1:B:20:GLU:HB2	1.99	0.63
1:A:419:ARG:HG2	1:A:469:ILE:HA	1.81	0.63
1:B:80:ASP:HB2	1:B:82:LYS:HG2	1.81	0.63
1:B:139:GLU:HG3	1:B:261:VAL:CG1	2.29	0.63
1:B:32:SER:HB2	1:B:65:LEU:H	1.64	0.63
1:A:254:GLN:HB3	3:A:924:HOH:O	1.98	0.62
1:B:31:PHE:CD2	1:B:288:HIS:HD2	2.17	0.62
2:A:651:7MG:P	2:A:652:GDP:PB	2.97	0.62
1:A:34:ILE:H	1:A:109:GLN:NE2	1.97	0.62
1:A:900:PRO:HD3	1:A:371:GLU:OE1	2.00	0.61
1:B:371:GLU:OE1	1:B:374:TYR:HB2	2.00	0.61
1:B:419:ARG:NH1	3:B:1181:HOH:O	2.34	0.61
1:B:490:THR:O	1:B:491:SER:CB	2.49	0.60
1:A:281:ASN:HB2	1:A:319:LYS:HD2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:901:GLY:HA2	1:A:362:TYR:CE1	2.37	0.59
1:B:34:ILE:H	1:B:109:GLN:HE21	1.50	0.59
1:A:283:LEU:O	1:A:287:MET:HG3	2.02	0.59
1:A:321:MET:HG2	1:A:386:MET:SD	2.42	0.59
1:A:352:LYS:HD2	1:A:352:LYS:H	1.68	0.58
1:B:19:ILE:HA	1:B:25:PHE:CE2	2.38	0.58
1:B:427:ASN:H	1:B:427:ASN:HD22	1.50	0.58
1:A:98:SER:HA	3:A:919:HOH:O	2.04	0.58
1:B:470:ASP:C	2:B:1152:7MG:H1'	2.24	0.58
1:A:437:ARG:C	1:A:439:HIS:H	2.07	0.58
1:B:316:LEU:HD12	1:B:411:PHE:HB2	1.84	0.57
1:B:446:PRO:HD3	1:B:496:SER:O	2.05	0.57
1:A:484:VAL:O	1:A:488:VAL:HG23	2.04	0.57
1:B:282:MET:HG3	1:B:415:LEU:HD22	1.86	0.57
1:B:89:ASN:ND2	1:B:373:GLY:H	1.98	0.57
1:B:31:PHE:CE2	1:B:288:HIS:HD2	2.23	0.57
1:B:449:TRP:CH2	1:B:497:TYR:HB3	2.40	0.56
1:B:315:LEU:H	1:B:413:ASN:ND2	2.03	0.56
1:A:146:PHE:HE2	1:A:254:GLN:HA	1.71	0.56
2:A:651:7MG:P	2:A:652:GDP:O2B	2.65	0.55
1:B:423:ILE:HG13	1:B:424:PRO:HD3	1.88	0.55
1:B:271:ALA:HA	1:B:311:VAL:O	2.06	0.55
1:A:457:LEU:HD23	1:A:458:PHE:CE2	2.41	0.55
1:A:253:GLU:HA	1:A:256:GLU:HG3	1.88	0.55
1:B:133:TYR:O	1:B:134:LEU:HD23	2.06	0.55
1:A:437:ARG:O	1:A:439:HIS:N	2.39	0.55
1:A:294:TYR:O	1:A:295:CYS:HB3	2.07	0.55
1:B:408:ILE:HG23	1:B:412:PHE:CE2	2.42	0.55
1:A:446:PRO:HD3	1:A:496:SER:O	2.06	0.55
1:B:423:ILE:HD12	3:B:1181:HOH:O	2.07	0.55
1:B:319:LYS:HD3	1:B:416:PHE:CD2	2.41	0.55
1:B:442:HIS:CD2	1:B:500:GLN:OE1	2.60	0.55
1:B:34:ILE:N	1:B:109:GLN:NE2	2.53	0.54
1:B:901:GLY:N	1:B:900:PRO:CD	2.67	0.54
1:B:443:VAL:HG12	1:B:499:ILE:HG12	1.88	0.54
1:B:295:CYS:HB2	1:B:296:PRO:HD2	1.88	0.54
1:B:91:TYR:O	1:B:131:ILE:HD12	2.07	0.54
1:B:44:THR:HA	1:B:53:ARG:NH2	2.23	0.54
1:B:344:LYS:HA	1:B:350:PRO:HG3	1.90	0.54
1:B:91:TYR:CZ	1:B:125:LYS:HD2	2.43	0.53
1:A:46:GLY:O	1:A:421:MET:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:LEU:O	1:A:261:VAL:HG13	2.09	0.53
1:B:32:SER:CB	1:B:65:LEU:H	2.22	0.53
1:A:74:PHE:CD2	1:A:85:THR:HG22	2.43	0.52
1:A:32:SER:HB2	1:A:65:LEU:H	1.74	0.52
1:B:82:LYS:HB3	1:B:352:LYS:HD2	1.91	0.52
1:B:900:PRO:HB3	1:B:88:PHE:CA	2.40	0.52
1:A:309:ILE:HA	1:A:312:PHE:O	2.09	0.52
1:A:59:LYS:HE3	1:A:60:HIS:CE1	2.45	0.52
1:A:281:ASN:HB2	1:A:319:LYS:CD	2.39	0.51
1:B:135:ASN:HD22	1:B:137:GLU:H	1.57	0.51
1:B:489:ASN:HA	1:B:492:LYS:HE3	1.92	0.51
1:B:135:ASN:HD22	1:B:137:GLU:N	2.09	0.51
1:A:49:THR:O	1:A:50:PRO:C	2.49	0.51
1:A:144:GLU:O	1:A:147:ASP:CB	2.58	0.51
1:B:35:SER:N	1:B:109:GLN:HE22	2.01	0.51
1:B:346:THR:CG2	1:B:347:PRO:HA	2.40	0.51
1:B:135:ASN:ND2	1:B:137:GLU:N	2.58	0.51
1:B:31:PHE:CE2	1:B:66:LEU:HD22	2.33	0.51
1:A:333:ASN:ND2	1:A:338:GLU:CB	2.70	0.51
1:B:311:VAL:HG12	1:B:312:PHE:CZ	2.46	0.50
1:B:440:VAL:HG12	1:B:477:SER:HA	1.92	0.50
1:A:55:GLN:HE21	1:A:58:LYS:NZ	2.10	0.50
1:A:35:SER:H	1:A:109:GLN:NE2	2.04	0.50
1:B:433:LEU:HG	1:B:434:GLN:N	2.23	0.50
1:A:491:SER:HB3	1:A:499:ILE:HD12	1.94	0.50
1:B:9:LYS:HB3	1:B:9:LYS:NZ	2.27	0.49
1:A:82:LYS:HD2	1:A:354:GLU:HB2	1.94	0.49
1:B:135:ASN:ND2	1:B:137:GLU:H	2.10	0.49
1:B:443:VAL:HG12	1:B:499:ILE:CG1	2.42	0.49
1:B:279:GLY:HA3	1:B:282:MET:SD	2.52	0.49
1:A:136:GLN:HE21	1:A:136:GLN:HA	1.77	0.49
1:A:25:PHE:CE1	1:A:270:ILE:CG2	2.95	0.49
1:A:291:HIS:CD2	1:A:297:LEU:HD13	2.48	0.49
1:B:22:ALA:HB2	1:B:73:ALA:HB1	1.94	0.49
1:A:327:PHE:CZ	1:A:390:LEU:HD13	2.47	0.48
1:A:280:HIS:CE1	1:A:319:LYS:HB2	2.48	0.48
1:B:471:ASP:HA	2:B:1152:7MG:H82	1.94	0.48
1:A:446:PRO:HD2	1:A:449:TRP:NE1	2.28	0.48
1:A:23:ASP:OD2	1:A:76:TYR:N	2.47	0.48
1:B:900:PRO:HG3	1:B:87:SER:HB2	1.96	0.48
1:A:45:SER:HA	1:A:48:ASP:OD1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:ILE:N	1:B:109:GLN:HE21	2.12	0.48
1:A:327:PHE:HB3	1:A:331:ILE:HD12	1.96	0.48
1:B:291:HIS:HB2	1:B:297:LEU:HD13	1.95	0.48
1:A:443:VAL:HG23	1:A:445:PHE:HE1	1.79	0.48
1:A:319:LYS:NZ	2:A:652:GDP:O2A	2.46	0.47
2:B:1152:7MG:P	2:B:1151:GDP:PB	3.12	0.47
1:B:471:ASP:HA	2:B:1152:7MG:C8	2.50	0.47
1:A:25:PHE:HB3	1:A:73:ALA:HA	1.96	0.47
1:A:443:VAL:HG23	1:A:445:PHE:CE1	2.48	0.47
1:B:469:ILE:HG23	1:B:474:ALA:CA	2.45	0.47
1:A:447:LYS:HD2	1:A:448:GLU:OE2	2.15	0.47
1:A:89:ASN:ND2	1:A:373:GLY:H	2.09	0.47
1:B:44:THR:HG23	1:B:53:ARG:HH12	1.80	0.47
1:A:441:LEU:HD23	1:A:484:VAL:HG13	1.97	0.47
1:B:62:MET:HG3	1:B:291:HIS:CG	2.50	0.47
1:B:93:PHE:HB3	1:B:130:GLY:HA3	1.96	0.47
1:B:331:ILE:HG23	1:B:342:ARG:HG2	1.96	0.46
1:A:144:GLU:O	1:A:147:ASP:HB2	2.15	0.46
1:A:290:ILE:CD1	1:A:307:MET:SD	3.03	0.46
1:A:344:LYS:C	3:A:907:HOH:O	2.54	0.46
1:A:76:TYR:HD1	1:A:83:HIS:CE1	2.34	0.46
1:A:135:ASN:HD21	1:A:138:GLU:H	1.62	0.46
1:B:370:HIS:N	3:B:1168:HOH:O	2.48	0.46
1:A:405:SER:OG	1:A:406:LYS:N	2.48	0.46
1:B:134:LEU:HG	1:B:260:ALA:O	2.14	0.46
1:B:53:ARG:O	1:B:54:TYR:C	2.54	0.46
1:B:284:LEU:O	1:B:285:ASP:C	2.53	0.46
1:A:49:THR:O	1:A:52:GLU:N	2.49	0.46
1:B:409:GLU:HG2	3:B:1173:HOH:O	2.14	0.46
1:B:319:LYS:HE3	1:B:334:THR:OG1	2.16	0.45
1:A:135:ASN:ND2	1:A:138:GLU:H	2.14	0.45
1:A:295:CYS:HB2	1:A:296:PRO:HD2	1.97	0.45
1:B:442:HIS:HD2	1:B:500:GLN:OE1	1.99	0.45
1:B:94:PRO:HB2	1:B:104:VAL:HG21	1.99	0.45
1:A:25:PHE:CE1	1:A:270:ILE:HG23	2.50	0.45
1:A:72:CYS:SG	1:A:87:SER:HB3	2.57	0.45
1:B:251:THR:HB	1:B:252:LYS:H	1.44	0.45
1:B:426:LEU:HA	1:B:426:LEU:HD23	1.84	0.45
1:B:327:PHE:CZ	1:B:390:LEU:HD13	2.52	0.45
1:B:441:LEU:HD12	1:B:499:ILE:HG21	1.98	0.45
1:A:321:MET:HA	1:A:411:PHE:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:GLY:O	1:B:419:ARG:HB2	2.17	0.44
1:A:330:ILE:HG22	1:A:342:ARG:NH1	2.32	0.44
1:B:290:ILE:HG13	1:B:291:HIS:N	2.32	0.44
1:B:103:ASP:O	1:B:105:LYS:NZ	2.25	0.44
1:A:305:LYS:HZ1	1:A:431:PRO:HA	1.82	0.44
1:A:305:LYS:HB3	1:A:428:LEU:O	2.17	0.44
1:B:315:LEU:HB2	1:B:413:ASN:HD22	1.82	0.44
1:A:253:GLU:HA	1:A:256:GLU:CG	2.47	0.44
1:A:439:HIS:CE1	1:A:481:PRO:HD3	2.53	0.44
1:A:32:SER:CB	1:A:65:LEU:H	2.30	0.44
1:A:22:ALA:HB2	1:A:73:ALA:HB1	2.00	0.44
1:B:414:LYS:HE3	1:B:428:LEU:HG	1.99	0.44
1:A:331:ILE:HG12	1:A:342:ARG:HG2	2.00	0.44
1:B:324:THR:O	1:B:327:PHE:N	2.51	0.44
1:B:278:VAL:HA	1:B:316:LEU:O	2.17	0.44
1:B:294:TYR:CE1	1:B:311:VAL:HG13	2.52	0.43
1:B:436:LYS:HG2	1:B:438:ASP:HB2	1.99	0.43
1:A:305:LYS:NZ	1:A:431:PRO:HA	2.33	0.43
1:B:405:SER:N	3:B:1192:HOH:O	2.50	0.43
1:B:136:GLN:CA	1:B:136:GLN:HE21	2.31	0.43
1:B:122:ASP:HB3	1:B:125:LYS:HG3	1.99	0.43
1:B:350:PRO:HA	1:B:351:PRO:HD2	1.67	0.43
2:B:1152:7MG:H3'	2:B:1151:GDP:O4'	2.19	0.43
1:B:93:PHE:CD1	1:B:94:PRO:HD2	2.53	0.43
1:B:143:ARG:HH21	1:B:257:LEU:HD21	1.84	0.43
2:B:1151:GDP:H5"	2:B:1151:GDP:O3B	2.19	0.43
1:A:146:PHE:CE2	1:A:254:GLN:HA	2.51	0.43
1:A:435:PRO:O	1:A:436:LYS:HB2	2.19	0.43
1:B:412:PHE:N	1:B:412:PHE:CD2	2.87	0.42
1:B:427:ASN:N	1:B:427:ASN:HD22	2.10	0.42
1:B:139:GLU:HG3	1:B:261:VAL:HG11	2.00	0.42
1:A:7:ASN:C	1:A:7:ASN:OD1	2.58	0.42
1:B:504:GLU:C	1:B:504:GLU:OE1	2.58	0.42
1:A:134:LEU:HD22	1:A:138:GLU:HB3	2.02	0.42
1:A:417:LEU:HA	1:A:417:LEU:HD12	1.68	0.42
1:A:409:GLU:HA	1:A:412:PHE:CE1	2.54	0.42
1:B:294:TYR:CZ	1:B:311:VAL:HG13	2.55	0.42
1:B:279:GLY:CA	1:B:282:MET:SD	3.08	0.41
1:A:139:GLU:HG3	1:A:261:VAL:CG1	2.50	0.41
1:B:253:GLU:C	1:B:255:GLU:H	2.23	0.41
1:A:333:ASN:HD21	1:A:335:SER:HB2	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:LEU:HD22	1:A:287:MET:HG3	2.02	0.41
1:A:74:PHE:CE2	1:A:85:THR:CG2	3.03	0.41
1:A:342:ARG:HH21	1:A:345:GLU:HB2	1.85	0.41
1:A:329:ASP:OD1	1:A:329:ASP:N	2.53	0.41
1:B:30:GLU:HG2	1:B:372:ALA:HB2	2.02	0.41
1:B:440:VAL:HG23	1:B:502:TYR:HB2	2.02	0.41
1:B:135:ASN:HD22	1:B:136:GLN:N	2.17	0.41
1:B:480:GLN:H	1:B:483:GLN:NE2	2.09	0.41
1:B:415:LEU:HA	1:B:415:LEU:HD23	1.88	0.41
1:A:74:PHE:CE1	1:A:380:GLY:HA3	2.55	0.41
1:A:67:PHE:HB2	1:A:126:VAL:HG11	2.03	0.41
1:A:325:GLN:HE21	1:A:328:LYS:HD2	1.85	0.41
1:B:57:LEU:O	1:B:62:MET:HE2	2.21	0.41
1:B:414:LYS:NZ	3:B:1171:HOH:O	2.53	0.41
1:B:312:PHE:HA	1:B:313:PRO:HD2	1.84	0.41
1:A:59:LYS:O	1:A:59:LYS:HG2	2.21	0.41
1:B:50:PRO:O	1:B:51:GLU:C	2.59	0.41
1:A:140:ARG:O	1:A:141:GLN:C	2.58	0.41
1:A:131:ILE:HA	1:A:132:PRO:HD3	1.98	0.41
1:B:381:LEU:HD23	1:B:381:LEU:HA	1.87	0.40
1:A:74:PHE:CD2	1:A:85:THR:CG2	3.05	0.40
1:B:412:PHE:HD2	1:B:412:PHE:N	2.19	0.40
1:A:66:LEU:H	1:A:292:GLN:HE22	1.70	0.40
1:B:3:ILE:O	1:B:131:ILE:HD11	2.22	0.40
1:A:291:HIS:HD2	1:A:297:LEU:HD13	1.87	0.40
1:A:436:LYS:HE3	3:A:904:HOH:O	2.22	0.40
1:A:262:GLY:O	1:A:265:ARG:HG3	2.22	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	373/507 (74%)	322 (86%)	43 (12%)	8 (2%)	9 40
1	B	363/507 (72%)	316 (87%)	37 (10%)	10 (3%)	6 30
All	All	736/1014 (73%)	638 (87%)	80 (11%)	18 (2%)	7 35

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	405	SER
1	A	438	ASP
1	B	433	LEU
1	B	491	SER
1	A	252	LYS
1	B	36	ASP
1	B	37	GLY
1	A	421	MET
1	B	471	ASP
1	B	439	HIS
1	A	900	PRO
1	A	146	PHE
1	B	254	GLN
1	B	426	LEU
1	B	50	PRO
1	A	296	PRO
1	B	262	GLY
1	A	430	GLY

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	345/458 (75%)	303 (88%)	42 (12%)	6 25
1	B	335/458 (73%)	278 (83%)	57 (17%)	2 13
All	All	680/916 (74%)	581 (85%)	99 (15%)	4 18

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ILE
1	A	25	PHE
1	A	47	PHE
1	A	66	LEU
1	A	67	PHE
1	A	68	GLN
1	A	77	ASP
1	A	89	ASN
1	A	99	ARG
1	A	135	ASN
1	A	136	GLN
1	A	141	GLN
1	A	250	TYR
1	A	261	VAL
1	A	270	ILE
1	A	283	LEU
1	A	290	ILE
1	A	309	ILE
1	A	312	PHE
1	A	314	ARG
1	A	315	LEU
1	A	325	GLN
1	A	329	ASP
1	A	330	ILE
1	A	352	LYS
1	A	361	SER
1	A	363	ASP
1	A	385	SER
1	A	402	SER
1	A	404	ARG
1	A	405	SER
1	A	417	LEU
1	A	422	ASP
1	A	437	ARG
1	A	444	THR
1	A	447	LYS
1	A	448	GLU
1	A	456	GLN
1	A	482	GLU
1	A	485	GLN
1	A	496	SER
1	A	498	ARG
1	B	10	ILE

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Mol	Chain	Res	Type
1	B	20	GLU
1	B	25	PHE
1	B	32	SER
1	B	39	SER
1	B	47	PHE
1	B	53	ARG
1	B	62	MET
1	B	66	LEU
1	B	67	PHE
1	B	77	ASP
1	B	89	ASN
1	B	99	ARG
1	B	104	VAL
1	B	105	LYS
1	B	135	ASN
1	B	136	GLN
1	B	141	GLN
1	B	251	THR
1	B	252	LYS
1	B	255	GLU
1	B	259	ASP
1	B	283	LEU
1	B	290	ILE
1	B	315	LEU
1	B	318	THR
1	B	325	GLN
1	B	328	LYS
1	B	332	ASN
1	B	335	SER
1	B	340	GLU
1	B	342	ARG
1	B	346	THR
1	B	349	ASP
1	B	371	GLU
1	B	385	SER
1	B	407	LEU
1	B	408	ILE
1	B	418	MET
1	B	419	ARG
1	B	426	LEU
1	B	427	ASN
1	B	434	GLN

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Mol	Chain	Res	Type
1	B	437	ARG
1	B	439	HIS
1	B	461	PHE
1	B	464	ILE
1	B	469	ILE
1	B	470	ASP
1	B	471	ASP
1	B	476	VAL
1	B	486	ILE
1	B	495	GLU
1	B	496	SER
1	B	500	GLN
1	B	504	GLU
1	B	505	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	60	HIS
1	A	89	ASN
1	A	109	GLN
1	A	124	ASN
1	A	135	ASN
1	A	136	GLN
1	A	145	GLN
1	A	254	GLN
1	A	291	HIS
1	A	325	GLN
1	A	333	ASN
1	A	368	GLN
1	A	439	HIS
1	A	463	ASN
1	A	483	GLN
1	A	485	GLN
1	B	17	GLN
1	B	89	ASN
1	B	109	GLN
1	B	135	ASN
1	B	136	GLN
1	B	280	HIS
1	B	288	HIS

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Mol	Chain	Res	Type
1	B	291	HIS
1	B	292	GLN
1	B	325	GLN
1	B	370	HIS
1	B	413	ASN
1	B	427	ASN
1	B	442	HIS
1	B	483	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 ⓘ

4 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	$\#|Z| > 2$
2	7MG	A	651	-	19,26,27	1.76	3 (15%)	24,39,42	2.77	6 (25%)
2	GDP	A	652	-	23,30,30	1.14	2 (8%)	30,47,47	1.72	7 (23%)
2	GDP	B	1151	-	23,30,30	1.29	2 (8%)	30,47,47	1.95	7 (23%)
2	7MG	B	1152	-	19,26,27	1.69	4 (21%)	24,39,42	2.37	5 (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
2	7MG	A	651	-	-	0/7/37/38	0/3/3/3
2	GDP	A	652	-	-	0/12/32/32	0/3/3/3
2	GDP	B	1151	-	-	0/12/32/32	0/3/3/3
2	7MG	B	1152	-	-	0/7/37/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	651	7MG	C8-N9	-5.22	1.37	1.45
2	B	1152	7MG	C8-N9	-3.94	1.39	1.45
2	A	651	7MG	C8-N7	-2.76	1.30	1.43
2	B	1152	7MG	C8-N7	-2.52	1.32	1.43
2	B	1152	7MG	C2-N3	-2.46	1.31	1.35
2	A	652	GDP	C5-C4	2.94	1.47	1.40
2	B	1151	GDP	C5-C4	3.20	1.47	1.40
2	A	652	GDP	C6-C5	3.51	1.48	1.41
2	A	651	7MG	C6-N1	3.52	1.39	1.33
2	B	1152	7MG	C6-N1	3.99	1.40	1.33
2	B	1151	GDP	C6-C5	4.37	1.50	1.41

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	651	7MG	C5-C6-N1	-7.72	111.59	123.46
2	B	1152	7MG	C5-C6-N1	-7.00	112.70	123.46
2	B	1151	GDP	PA-O3A-PB	-4.19	118.62	132.67
2	B	1151	GDP	C5-C6-N1	-3.98	118.15	123.59
2	A	652	GDP	C6-C5-C4	-3.57	116.63	120.90
2	B	1151	GDP	C4-C5-N7	-3.56	106.20	109.48
2	B	1151	GDP	C6-C5-C4	-3.38	116.86	120.90
2	A	652	GDP	C5-C6-N1	-3.09	119.37	123.59
2	B	1151	GDP	N3-C2-N1	-3.06	122.79	127.44
2	A	652	GDP	PA-O3A-PB	-3.01	122.56	132.67
2	A	652	GDP	N3-C2-N1	-2.62	123.45	127.44
2	A	652	GDP	C4-C5-N7	-2.53	107.15	109.48
2	A	651	7MG	N1-C2-N3	-2.50	121.44	125.53
2	B	1152	7MG	O4'-C4'-C3'	-2.21	100.69	105.15
2	B	1151	GDP	C5'-C4'-C3'	-2.15	106.66	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1152	7MG	N3-C4-N9	-2.06	123.67	126.75
2	A	652	GDP	O2A-PA-O3A	2.09	114.59	105.09
2	A	651	7MG	CM7-N7-C8	3.11	129.34	120.52
2	A	651	7MG	C5-C4-N3	3.15	129.89	126.82
2	A	651	7MG	N2-C2-N3	3.33	122.72	117.20
2	A	652	GDP	C6-N1-C2	3.68	121.05	115.94
2	B	1152	7MG	C5-C4-N3	3.85	130.58	126.82
2	B	1151	GDP	C6-N1-C2	4.63	122.37	115.94
2	B	1152	7MG	C6-N1-C2	6.40	124.82	115.94
2	A	651	7MG	C6-N1-C2	7.76	126.70	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	651	7MG	4	0
2	A	652	GDP	4	0
2	B	1151	GDP	4	0
2	B	1152	7MG	6	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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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(Å²)	Q<0.9
1	A	383/507 (75%)	0.44	8 (2%)	67	36	58, 75, 95, 110	0
1	B	373/507 (73%)	0.38	11 (2%)	55	26	57, 76, 95, 107	0
All	All	756/1014 (74%)	0.41	19 (2%)	61	30	57, 75, 95, 110	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	385	SER	3.5
1	A	494	ALA	3.5
1	B	465	GLN	3.2
1	A	497	TYR	3.0
1	A	495	GLU	2.8
1	B	466	ILE	2.7
1	B	494	ALA	2.6
1	A	490	THR	2.5
1	B	52	GLU	2.5
1	B	463	ASN	2.5
1	B	475	PHE	2.5
1	A	402	SER	2.4
1	A	478	LEU	2.3
1	B	462	GLY	2.3
1	A	499	ILE	2.3
1	A	331	ILE	2.3
1	B	83	HIS	2.2
1	B	446	PRO	2.2
1	B	330	ILE	2.1

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 (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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors($Å^2$)	Q<0.9
2	GDP	B	1151	28/28	0.81	0.23	-0.45	114,118,121,122	0
2	7MG	B	1152	24/25	0.91	0.19	-0.72	61,68,75,76	0
2	7MG	A	651	24/25	0.93	0.21	-0.87	54,64,65,68	0
2	GDP	A	652	28/28	0.96	0.20	-1.53	57,60,64,65	0

6.5 Other polymers (i)

There are no such residues in this entry.