



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:55 PM GMT

PDB ID : 3Q22
Title : X-ray crystal structure of the N4 mini-VRNAP and P2_7a promoter transcription initiation complex with GTP and Magnesium: substrate complex I
Authors : Gleghorn, M.L.; Murakami, K.S.
Deposited on : 2010-12-19
Resolution : 2.11 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

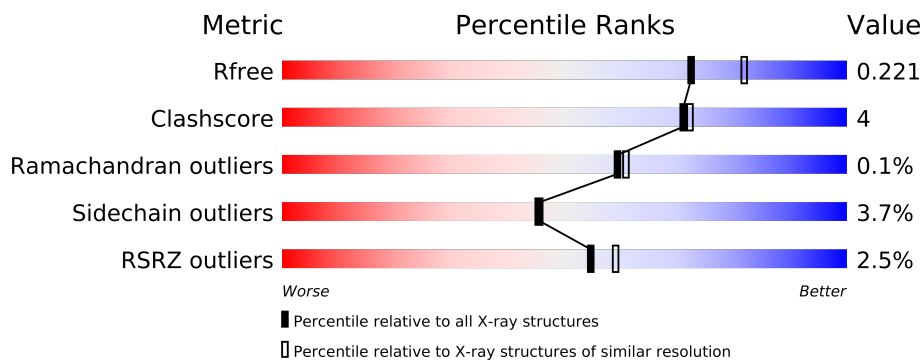
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.11 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}	66092	3409 (2.14-2.10)
Clashscore	79885	4090 (2.14-2.10)
Ramachandran outliers	78287	4048 (2.14-2.10)
Sidechain outliers	78261	4049 (2.14-2.10)
RSRZ outliers	66119	3410 (2.14-2.10)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1118	
1	B	1118	
2	C	36	
2	D	36	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19285 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Virion RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1095	Total	C	N	O	S	0	0	0
			8454	5306	1435	1672	41			
1	B	1094	Total	C	N	O	S	0	0	0
			8443	5299	1432	1671	41			

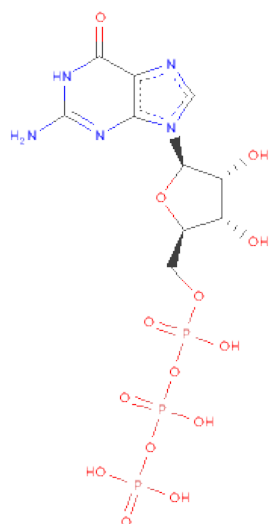
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	EXPRESSION TAG	UNP Q859P9
A	-10	GLY	-	EXPRESSION TAG	UNP Q859P9
A	-9	GLY	-	EXPRESSION TAG	UNP Q859P9
A	-8	SER	-	EXPRESSION TAG	UNP Q859P9
A	-7	HIS	-	EXPRESSION TAG	UNP Q859P9
A	-6	HIS	-	EXPRESSION TAG	UNP Q859P9
A	-5	HIS	-	EXPRESSION TAG	UNP Q859P9
A	-4	HIS	-	EXPRESSION TAG	UNP Q859P9
A	-3	HIS	-	EXPRESSION TAG	UNP Q859P9
A	-2	HIS	-	EXPRESSION TAG	UNP Q859P9
A	-1	ARG	-	EXPRESSION TAG	UNP Q859P9
A	0	SER	-	EXPRESSION TAG	UNP Q859P9
B	-11	MET	-	EXPRESSION TAG	UNP Q859P9
B	-10	GLY	-	EXPRESSION TAG	UNP Q859P9
B	-9	GLY	-	EXPRESSION TAG	UNP Q859P9
B	-8	SER	-	EXPRESSION TAG	UNP Q859P9
B	-7	HIS	-	EXPRESSION TAG	UNP Q859P9
B	-6	HIS	-	EXPRESSION TAG	UNP Q859P9
B	-5	HIS	-	EXPRESSION TAG	UNP Q859P9
B	-4	HIS	-	EXPRESSION TAG	UNP Q859P9
B	-3	HIS	-	EXPRESSION TAG	UNP Q859P9
B	-2	HIS	-	EXPRESSION TAG	UNP Q859P9
B	-1	ARG	-	EXPRESSION TAG	UNP Q859P9
B	0	SER	-	EXPRESSION TAG	UNP Q859P9

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*GP*CP*CP*TP*CP*CP*CP*AP*GP*GP*CP*AP*TP*CP*CP*AP*AP*AP*AP*GP*AP*AP*GP*CP*GP*GP*AP*GP*CP*TP*TP*CP*TP*TP*C)-3').

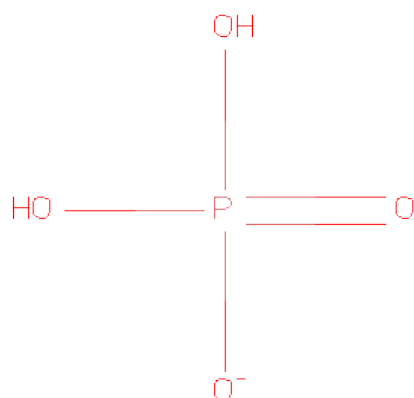
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	20	Total	C	N	O	P	0	0	0
			396	185	79	112	20			
2	D	21	Total	C	N	O	P	0	0	0
			432	205	83	123	21			

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 4 is DIHYDROGENPHOSPHATE ION (three-letter code: 2HP) (formula: H₂O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

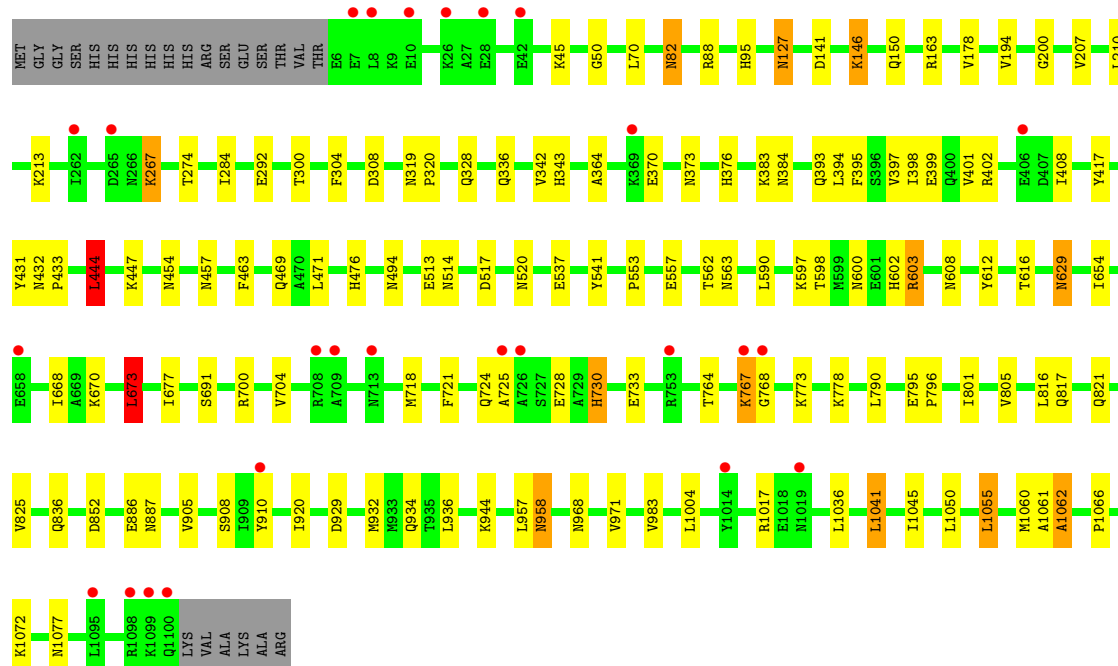
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	610	Total	O	0	0
			610	610		
6	C	50	Total	O	0	0
			50	50		
6	B	692	Total	O	0	0
			692	692		
6	D	68	Total	O	0	0
			68	68		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

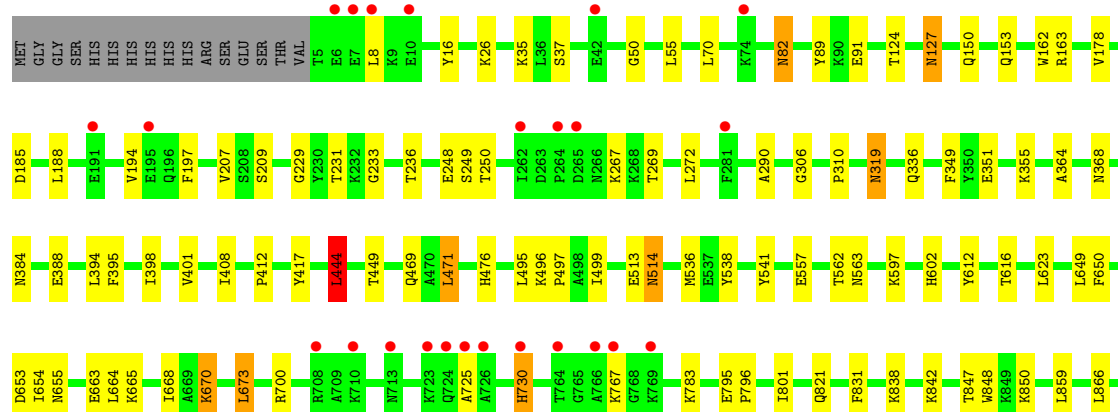
• Molecule 1: Virion RNA polymerase

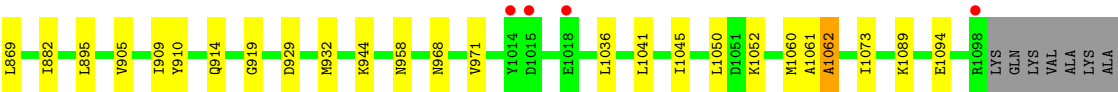
Chain A: 



• Molecule 1: Virion RNA polymerase

Chain B: 

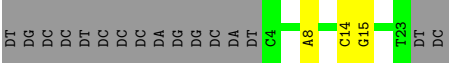




ARG

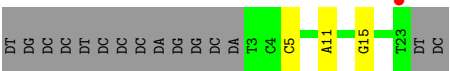
● Molecule 2: DNA (5'-D(*TP*GP*CP*CP*TP*CP*CP*CP*AP*GP*GP*CP*AP*TP*CP*CP*AP*AP*AP*AP*GP*AP*AP*GP*CP*GP*GP*AP*GP*CP*TP*TP*CP*TP*TP*C)-3')

Chain C:



● Molecule 2: DNA (5'-D(*TP*GP*CP*CP*TP*CP*CP*CP*AP*GP*GP*CP*AP*TP*CP*CP*AP*AP*AP*AP*GP*AP*AP*GP*CP*GP*GP*AP*GP*CP*TP*TP*CP*TP*TP*C)-3')

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.30Å 111.79Å 276.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.11 47.81 – 2.11	Depositor EDS
% Data completeness (in resolution range)	89.1 (50.00-2.11) 89.1 (47.81-2.11)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.208 , 0.219 0.209 , 0.221	Depositor DCC
R_{free} test set	6713 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 29.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 133426 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	19285	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, 2HP, 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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.40	0/8583	0.55	2/11609 (0.0%)
1	B	0.40	0/8572	0.54	1/11596 (0.0%)
2	C	0.66	0/445	1.23	2/685 (0.3%)
2	D	0.66	0/485	1.21	2/746 (0.3%)
All	All	0.42	0/18085	0.60	7/24636 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	444	LEU	CA-CB-CG	7.95	133.57	115.30
1	B	444	LEU	CA-CB-CG	7.82	133.29	115.30
1	A	673	LEU	CA-CB-CG	5.86	128.78	115.30
2	C	14	DC	O4'-C1'-N1	5.50	111.85	108.00
2	C	15	DG	P-O3'-C3'	5.24	125.99	119.70
2	D	5	DC	O4'-C4'-C3'	-5.17	102.43	104.50
2	D	15	DG	P-O3'-C3'	5.01	125.72	119.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8454	0	8479	81	0
1	B	8443	0	8465	77	0
2	C	396	0	211	1	0
2	D	432	0	236	1	0
3	A	64	0	24	2	0
3	B	32	0	12	0	0
3	D	32	0	12	0	0
4	A	5	0	0	1	0
4	B	5	0	0	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	610	0	0	7	0
6	B	692	0	0	6	1
6	C	50	0	0	0	0
6	D	68	0	0	0	1
All	All	19285	0	17439	157	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (157) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:469:GLN:HE22	1:A:557:GLU:H	1.12	0.91
1:B:469:GLN:HE22	1:B:557:GLU:H	1.14	0.91
1:A:336:GLN:HE21	1:A:417:TYR:H	1.21	0.88
1:B:336:GLN:HE21	1:B:417:TYR:H	1.16	0.87
1:B:850:LYS:O	6:B:2046:HOH:O	1.96	0.82
1:B:932:MET:CE	1:B:971:VAL:HG22	2.12	0.80
1:B:673:LEU:HD13	1:B:801:ILE:HG23	1.65	0.77
1:A:932:MET:CE	6:A:1630:HOH:O	2.33	0.77
1:A:932:MET:HE2	6:A:1630:HOH:O	1.86	0.74
1:B:932:MET:SD	6:B:1714:HOH:O	2.45	0.74
1:A:603:ARG:NH1	1:A:608:ASN:OD1	2.23	0.72
1:A:127:ASN:H	1:A:127:ASN:HD22	1.37	0.72
1:B:932:MET:HE3	6:B:2048:HOH:O	1.90	0.71
1:A:958:ASN:HD22	1:A:958:ASN:H	1.37	0.71
1:A:364:ALA:H	1:A:384:ASN:HD21	1.38	0.71
1:B:449:THR:H	1:B:958:ASN:HD21	1.38	0.70
1:B:650:PHE:HE2	1:B:700:ARG:HG3	1.57	0.70
1:B:932:MET:HE1	1:B:971:VAL:HG22	1.76	0.68
1:A:852:ASP:O	6:A:1632:HOH:O	2.11	0.68
1:B:932:MET:HE2	1:B:971:VAL:HG22	1.76	0.67
1:A:141:ASP:HB2	1:A:146:LYS:HG2	1.75	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:469:GLN:NE2	1:A:557:GLU:H	1.90	0.67
1:B:364:ALA:H	1:B:384:ASN:ND2	1.93	0.67
1:A:816:LEU:HD13	1:A:983:VAL:HG21	1.76	0.66
1:A:968:ASN:HD21	1:A:1060:MET:H	1.44	0.66
1:A:469:GLN:HE22	1:A:557:GLU:N	1.92	0.64
1:A:364:ALA:H	1:A:384:ASN:ND2	1.95	0.64
1:B:469:GLN:HE22	1:B:557:GLU:N	1.92	0.64
1:B:932:MET:CE	6:B:2048:HOH:O	2.44	0.64
1:B:469:GLN:NE2	1:B:557:GLU:H	1.92	0.63
1:B:207:VAL:HG11	1:B:905:VAL:HG21	1.80	0.63
1:A:654:ILE:HD11	1:A:668:ILE:HG21	1.81	0.63
1:A:767:LYS:HE3	1:A:768:GLY:H	1.64	0.62
1:A:597:LYS:NZ	1:A:602:HIS:HD2	1.97	0.62
1:A:82:ASN:HD22	1:A:82:ASN:C	2.05	0.60
1:B:882:ILE:HD13	1:B:919:GLY:HA2	1.85	0.59
1:B:616:THR:HG23	1:B:664:LEU:HB2	1.84	0.58
1:B:562:THR:HG22	1:B:612:TYR:CE1	2.38	0.58
1:B:351:GLU:HG3	1:B:395:PHE:CE2	2.39	0.57
1:B:91:GLU:HG3	6:B:1574:HOH:O	2.03	0.57
1:A:821:GLN:O	1:A:825:VAL:HG23	2.05	0.57
1:B:1045:ILE:HD12	1:B:1094:GLU:HG3	1.87	0.57
1:A:393:GLN:HG2	1:A:431:TYR:HB2	1.87	0.57
1:B:127:ASN:H	1:B:127:ASN:HD22	1.52	0.56
1:B:16:TYR:O	1:B:35:LYS:HE3	2.05	0.56
1:B:162:TRP:HE1	1:B:209:SER:HB2	1.71	0.56
1:A:1077:ASN:HB3	6:A:1426:HOH:O	2.06	0.55
1:B:654:ILE:HD11	1:B:668:ILE:HG21	1.87	0.55
1:A:932:MET:HE3	6:A:1630:HOH:O	2.02	0.55
1:A:402:ARG:HA	1:A:408:ILE:HG22	1.88	0.55
1:B:932:MET:HE1	1:B:971:VAL:CG2	2.36	0.55
1:A:397:VAL:O	1:A:401:VAL:HG23	2.06	0.55
1:B:82:ASN:C	1:B:82:ASN:HD22	2.09	0.54
1:B:364:ALA:H	1:B:384:ASN:HD21	1.54	0.54
1:B:655:ASN:HB2	1:B:663:GLU:HB3	1.90	0.54
1:A:886:GLU:O	2:C:8:DA:H4'	2.07	0.54
1:B:563:ASN:HD21	1:B:929:ASP:HB3	1.73	0.54
1:A:342:VAL:HG11	1:A:408:ILE:HD12	1.91	0.53
1:B:185:ASP:HB3	1:B:188:LEU:HD12	1.91	0.53
1:B:50:GLY:H	1:B:150:GLN:HE22	1.55	0.53
1:A:795:GLU:HB2	1:A:796:PRO:HD3	1.90	0.53
1:A:1072:LYS:HE2	1:A:1072:LYS:HA	1.91	0.53
1:A:213:LYS:HE3	1:A:292:GLU:OE1	2.10	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:968:ASN:ND2	1:A:1060:MET:H	2.06	0.52
3:A:1107:GTP:H5'	3:A:1107:GTP:PB	2.50	0.52
1:A:721:PHE:HA	1:A:724:GLN:HE21	1.73	0.52
1:A:178:VAL:HG21	1:A:194:VAL:HA	1.91	0.52
1:B:612:TYR:CD1	1:B:670:LYS:HG2	2.45	0.51
1:A:444:LEU:HG	1:A:553:PRO:HB2	1.93	0.51
1:A:513:GLU:HB3	1:B:513:GLU:OE2	2.11	0.51
1:B:229:GLY:O	1:B:233:GLY:HA3	2.11	0.51
1:B:178:VAL:HG21	1:B:194:VAL:HA	1.93	0.51
1:B:650:PHE:CE2	1:B:700:ARG:HG3	2.41	0.51
1:A:395:PHE:O	1:A:399:GLU:HG2	2.11	0.51
1:B:968:ASN:HD21	1:B:1060:MET:H	1.57	0.50
1:B:37:SER:HB3	1:B:231:THR:HG22	1.93	0.50
1:B:336:GLN:NE2	1:B:417:TYR:H	1.98	0.49
1:A:127:ASN:N	1:A:127:ASN:HD22	2.08	0.49
1:B:249:SER:O	1:B:250:THR:HB	2.11	0.49
1:A:45:LYS:HE3	6:A:1377:HOH:O	2.12	0.49
1:A:320:PRO:HD2	1:A:910:TYR:CE2	2.48	0.49
1:B:449:THR:H	1:B:958:ASN:ND2	2.08	0.48
1:B:50:GLY:H	1:B:150:GLN:NE2	2.12	0.48
1:B:267:LYS:HE2	1:B:267:LYS:HA	1.94	0.48
1:A:958:ASN:ND2	1:A:958:ASN:H	2.10	0.48
1:A:932:MET:CE	1:A:971:VAL:HG22	2.44	0.48
1:A:207:VAL:HG11	1:A:905:VAL:HG21	1.95	0.48
1:B:26:LYS:HG2	1:B:847:THR:HG21	1.96	0.47
1:B:401:VAL:HG12	1:B:408:ILE:HG13	1.95	0.47
1:A:95:HIS:HA	1:B:248:GLU:O	2.15	0.47
1:B:236:THR:HG21	1:B:895:LEU:HD23	1.96	0.47
1:B:821:GLN:HE22	1:B:914:GLN:HE21	1.63	0.47
1:A:677:ILE:HD11	1:A:805:VAL:HG11	1.97	0.46
1:A:670:LYS:NZ	3:A:1108:GTP:O3A	2.48	0.46
1:B:616:THR:CG2	1:B:664:LEU:HB2	2.45	0.46
1:B:514:ASN:H	1:B:514:ASN:HD22	1.63	0.46
1:B:653:ASP:HA	1:B:665:LYS:HD2	1.96	0.46
1:B:310:PRO:HG2	1:B:336:GLN:HB3	1.98	0.46
1:B:471:LEU:HG	1:B:495:LEU:HD11	1.97	0.46
1:B:496:LYS:HB3	1:B:497:PRO:HD3	1.98	0.46
1:A:393:GLN:HG2	1:A:431:TYR:CB	2.45	0.46
1:B:795:GLU:HB3	1:B:796:PRO:HD3	1.98	0.46
1:B:16:TYR:O	1:B:35:LYS:CE	2.64	0.46
1:A:1061:ALA:O	1:A:1062:ALA:HB2	2.17	0.45
1:B:499:ILE:HD12	1:B:538:TYR:HD2	1.82	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:370:GLU:HA	1:A:773:LYS:HE2	1.98	0.45
1:A:200:GLY:HA2	1:A:274:THR:HG22	1.99	0.45
1:A:373:ASN:HD22	1:A:376:HIS:H	1.63	0.45
1:B:725:ALA:HB1	1:B:730:HIS:HB3	1.97	0.45
1:B:394:LEU:O	1:B:398:ILE:HG12	2.17	0.45
1:A:600:ASN:H	1:A:600:ASN:ND2	2.14	0.45
1:A:1041:LEU:O	1:A:1045:ILE:HG12	2.17	0.45
1:A:563:ASN:HD21	1:A:929:ASP:HB3	1.82	0.45
1:B:55:LEU:HD12	1:B:153:GLN:HG2	1.99	0.44
1:B:269:THR:O	2:D:11:DA:H5'	2.17	0.44
1:A:454:ASN:HB3	1:A:457:ASN:ND2	2.32	0.44
1:B:355:LYS:HD2	1:B:388:GLU:HG3	1.99	0.44
1:A:328:GLN:HG2	1:A:934:GLN:OE1	2.16	0.44
1:A:304:PHE:HB3	1:A:308:ASP:O	2.17	0.44
1:B:319:ASN:HD22	1:B:910:TYR:HE1	1.64	0.44
1:B:444:LEU:HB3	6:B:1423:HOH:O	2.18	0.44
1:A:50:GLY:H	1:A:150:GLN:NE2	2.16	0.44
1:B:1061:ALA:O	1:B:1062:ALA:HB2	2.18	0.43
1:A:700:ARG:O	1:A:704:VAL:HG23	2.19	0.43
1:B:127:ASN:N	1:B:127:ASN:HD22	2.16	0.43
1:A:673:LEU:HD22	1:A:801:ILE:HG23	2.00	0.43
1:B:476:HIS:ND1	4:B:1108:2HP:O2	2.32	0.43
1:A:790:LEU:O	1:A:795:GLU:HG2	2.19	0.43
1:A:677:ILE:O	1:A:920:ILE:HG21	2.18	0.43
1:A:432:ASN:HB2	1:A:433:PRO:HD2	2.01	0.43
1:A:447:LYS:HE3	6:A:1345:HOH:O	2.18	0.43
1:A:725:ALA:HB1	1:A:730:HIS:HB3	2.01	0.42
1:B:842:LYS:HB3	1:B:848:TRP:CD2	2.55	0.42
1:A:598:THR:HG22	1:A:1066:PRO:HD3	2.02	0.42
1:A:562:THR:HG22	1:A:612:TYR:CE1	2.54	0.42
1:A:718:MET:HG2	1:A:728:GLU:HG3	2.00	0.42
1:A:394:LEU:O	1:A:398:ILE:HG12	2.19	0.42
1:A:384:ASN:HD22	1:A:384:ASN:HA	1.65	0.42
1:A:816:LEU:CD1	1:A:983:VAL:HG21	2.47	0.42
1:A:597:LYS:HZ1	1:A:602:HIS:HD2	1.68	0.42
1:B:197:PHE:CD1	1:B:272:LEU:HD21	2.55	0.42
1:A:932:MET:HE2	1:A:971:VAL:HG22	2.00	0.41
1:A:730:HIS:O	1:A:733:GLU:HG2	2.21	0.41
1:A:590:LEU:HD11	1:A:1055:LEU:HG	2.02	0.41
1:B:1052:LYS:HB3	1:B:1073:ILE:HD12	2.02	0.41
1:A:463:PHE:HA	1:A:957:LEU:HD13	2.03	0.41
1:A:343:HIS:HE1	1:A:537:GLU:OE2	2.04	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:629:ASN:HD22	1:A:629:ASN:N	2.18	0.41
1:A:616:THR:HG23	1:A:668:ILE:HD11	2.02	0.41
1:B:306:GLY:HA2	1:B:412:PRO:HG2	2.03	0.41
1:A:476:HIS:ND1	4:A:1109:2HP:O2	2.35	0.41
1:B:831:PHE:HD2	1:B:866:LEU:HD11	1.85	0.41
1:B:89:TYR:CZ	1:B:290:ALA:HB3	2.56	0.41
1:B:597:LYS:NZ	1:B:602:HIS:HD2	2.18	0.41
1:A:82:ASN:ND2	1:A:82:ASN:C	2.70	0.41
1:A:267:LYS:HB2	1:A:267:LYS:HE2	1.73	0.41
1:B:349:PHE:HB2	1:B:536:MET:CE	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:B:1460:HOH:O	6:D:93:HOH:O[4_527]	1.81	0.39

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	1093/1118 (98%)	1068 (98%)	24 (2%)	1 (0%)	59	61
1	B	1092/1118 (98%)	1067 (98%)	24 (2%)	1 (0%)	59	61
All	All	2185/2236 (98%)	2135 (98%)	48 (2%)	2 (0%)	59	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1062	ALA
1	B	1062	ALA

5.3.2 Protein sidechains ⓘ

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	916/935 (98%)	876 (96%)	40 (4%)	39	36
1	B	915/935 (98%)	887 (97%)	28 (3%)	52	54
All	All	1831/1870 (98%)	1763 (96%)	68 (4%)	45	45

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	LEU
1	A	82	ASN
1	A	88	ARG
1	A	127	ASN
1	A	146	LYS
1	A	163	ARG
1	A	210	LEU
1	A	267	LYS
1	A	284	ILE
1	A	300	THR
1	A	319	ASN
1	A	383	LYS
1	A	444	LEU
1	A	471	LEU
1	A	494	ASN
1	A	514	ASN
1	A	517	ASP
1	A	520	ASN
1	A	541	TYR
1	A	603	ARG
1	A	629	ASN
1	A	673	LEU
1	A	691	SER
1	A	730	HIS
1	A	764	THR
1	A	767	LYS
1	A	778	LYS
1	A	817	GLN
1	A	836	GLN

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Mol	Chain	Res	Type
1	A	887	ASN
1	A	908	SER
1	A	936	LEU
1	A	944	LYS
1	A	958	ASN
1	A	1004	LEU
1	A	1017	ARG
1	A	1036	LEU
1	A	1041	LEU
1	A	1050	LEU
1	A	1055	LEU
1	B	8	LEU
1	B	70	LEU
1	B	82	ASN
1	B	124	THR
1	B	127	ASN
1	B	163	ARG
1	B	319	ASN
1	B	368	ASN
1	B	444	LEU
1	B	471	LEU
1	B	514	ASN
1	B	541	TYR
1	B	623	LEU
1	B	649	LEU
1	B	670	LYS
1	B	673	LEU
1	B	730	HIS
1	B	767	LYS
1	B	783	LYS
1	B	838	LYS
1	B	859	LEU
1	B	869	LEU
1	B	909	ILE
1	B	944	LYS
1	B	1036	LEU
1	B	1041	LEU
1	B	1050	LEU
1	B	1089	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	82	ASN
1	A	127	ASN
1	A	150	GLN
1	A	169	ASN
1	A	186	GLN
1	A	212	GLN
1	A	316	GLN
1	A	319	ASN
1	A	324	ASN
1	A	336	GLN
1	A	343	HIS
1	A	348	GLN
1	A	373	ASN
1	A	375	ASN
1	A	384	ASN
1	A	414	HIS
1	A	457	ASN
1	A	469	GLN
1	A	506	ASN
1	A	514	ASN
1	A	563	ASN
1	A	600	ASN
1	A	602	HIS
1	A	629	ASN
1	A	639	GLN
1	A	724	GLN
1	A	781	GLN
1	A	815	GLN
1	A	817	GLN
1	A	823	GLN
1	A	833	GLN
1	A	863	GLN
1	A	893	GLN
1	A	954	ASN
1	A	958	ASN
1	A	968	ASN
1	A	1035	ASN
1	A	1038	ASN
1	A	1047	HIS
1	A	1059	GLN
1	B	82	ASN
1	B	122	GLN

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Mol	Chain	Res	Type
1	B	127	ASN
1	B	150	GLN
1	B	196	GLN
1	B	255	ASN
1	B	314	ASN
1	B	316	GLN
1	B	319	ASN
1	B	324	ASN
1	B	336	GLN
1	B	343	HIS
1	B	348	GLN
1	B	368	ASN
1	B	376	HIS
1	B	384	ASN
1	B	414	HIS
1	B	469	GLN
1	B	506	ASN
1	B	514	ASN
1	B	520	ASN
1	B	563	ASN
1	B	602	HIS
1	B	629	ASN
1	B	639	GLN
1	B	724	GLN
1	B	815	GLN
1	B	817	GLN
1	B	892	ASN
1	B	893	GLN
1	B	914	GLN
1	B	958	ASN
1	B	968	ASN
1	B	1035	ASN
1	B	1047	HIS
1	B	1059	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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$
3	GTP	A	1107	-	34,34,34	1.02	1 (2%)	51,54,54	2.08	6 (11%)
3	GTP	A	1108	5	34,34,34	0.96	1 (2%)	51,54,54	1.73	10 (19%)
4	2HP	A	1109	-	4,4,4	4.32	2 (50%)	6,6,6	0.92	0
3	GTP	B	1107	5	34,34,34	0.98	1 (2%)	51,54,54	1.93	10 (19%)
4	2HP	B	1108	-	4,4,4	4.45	2 (50%)	6,6,6	0.81	0
3	GTP	D	26	-	34,34,34	1.02	1 (2%)	51,54,54	2.16	9 (17%)

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
3	GTP	A	1107	-	-	0/22/38/38	0/1/3/3
3	GTP	A	1108	5	-	0/22/38/38	0/1/3/3
4	2HP	A	1109	-	-	0/0/0/0	0/0/0/0
3	GTP	B	1107	5	-	0/22/38/38	0/1/3/3
4	2HP	B	1108	-	-	0/0/0/0	0/0/0/0
3	GTP	D	26	-	-	0/22/38/38	0/1/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1108	2HP	P-O4	6.32	1.79	1.55
4	B	1108	2HP	P-O3	6.27	1.78	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1109	2HP	P-O3	6.13	1.78	1.55
4	A	1109	2HP	P-O4	6.08	1.78	1.55
3	D	26	GTP	C2-N3	3.98	1.38	1.33
3	A	1107	GTP	C2-N3	3.98	1.38	1.33
3	B	1107	GTP	C2-N3	3.95	1.38	1.33
3	A	1108	GTP	C2-N3	3.50	1.37	1.33

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1107	GTP	C6-C5-N7	-11.20	132.63	134.14
3	D	26	GTP	C6-C5-N7	-11.01	132.66	134.14
3	B	1107	GTP	C6-C5-N7	-8.53	132.99	134.14
3	A	1108	GTP	C6-C5-N7	-5.16	133.44	134.14
3	A	1108	GTP	O4'-C1'-N9	4.59	112.71	108.44
3	D	26	GTP	C5-C4-N3	-4.20	119.85	125.94
3	A	1107	GTP	PB-O3B-PG	-4.20	119.38	131.68
3	D	26	GTP	C2-N3-C4	4.19	120.98	115.09
3	B	1107	GTP	O4'-C1'-N9	4.05	112.21	108.44
3	A	1108	GTP	C2'-C1'-N9	-3.97	103.06	113.27
3	B	1107	GTP	C2-N3-C4	3.79	120.42	115.09
3	D	26	GTP	N3-C4-N9	3.69	132.32	126.91
3	B	1107	GTP	C2'-C1'-N9	-3.60	104.03	113.27
3	B	1107	GTP	C5-C4-N3	-3.58	120.76	125.94
3	A	1108	GTP	C2-N3-C4	3.57	120.10	115.09
3	D	26	GTP	PB-O3B-PG	-3.56	121.24	131.68
3	A	1107	GTP	C5-C4-N3	-3.50	120.87	125.94
3	A	1107	GTP	C2-N3-C4	3.49	120.00	115.09
3	B	1107	GTP	N3-C4-N9	3.14	131.52	126.91
3	A	1107	GTP	N3-C4-N9	3.11	131.47	126.91
3	D	26	GTP	PA-O3A-PB	-3.02	122.83	131.68
3	A	1108	GTP	N2-C2-N1	3.02	121.18	117.86
3	A	1108	GTP	C5-C4-N3	-3.00	121.60	125.94
3	A	1108	GTP	N3-C4-N9	2.83	131.06	126.91
3	B	1107	GTP	N2-C2-N1	2.82	120.96	117.86
3	D	26	GTP	N2-C2-N1	2.58	120.69	117.86
3	B	1107	GTP	PB-O3B-PG	-2.40	124.63	131.68
3	A	1107	GTP	N2-C2-N1	2.40	120.50	117.86
3	B	1107	GTP	O2B-PB-O3A	2.29	116.03	105.14
3	A	1108	GTP	O2B-PB-O3A	2.29	116.02	105.14
3	D	26	GTP	C3'-C2'-C1'	2.29	104.49	100.91
3	B	1107	GTP	C4-C5-N7	-2.24	107.60	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	26	GTP	C4-C5-N7	-2.23	107.61	109.52
3	A	1108	GTP	N7-C8-N9	-2.22	108.09	114.36
3	A	1108	GTP	C1'-N9-C4	-2.07	123.05	126.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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(Å ²)	Q<0.9
1	A	1095/1118 (97%)	-0.02	26 (2%) 56 61	15, 29, 53, 69	0
1	B	1094/1118 (97%)	0.02	28 (2%) 53 58	15, 27, 48, 78	0
2	C	20/36 (55%)	-0.49	0 100 100	22, 33, 53, 60	0
2	D	21/36 (58%)	-0.37	1 (4%) 29 32	23, 27, 46, 67	0
All	All	2230/2308 (96%)	-0.01	55 (2%) 54 59	15, 28, 51, 78	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	725	ALA	5.9
1	B	723	LYS	5.1
1	A	8	LEU	5.1
1	B	726	ALA	4.8
1	B	713	ASN	4.8
1	A	1019	ASN	4.5
1	B	764	THR	4.2
1	A	1098	ARG	4.1
1	B	724	GLN	4.1
1	A	7	GLU	3.9
1	B	264	PRO	3.8
1	A	1014	TYR	3.6
1	A	369	LYS	3.2
1	A	910	TYR	3.2
1	A	767	LYS	3.1
1	B	730	HIS	3.1
1	A	658	GLU	2.9
1	B	710	LYS	2.9
1	B	1015	ASP	2.7
1	A	10	GLU	2.7
1	B	8	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	265	ASP	2.6
1	B	42	GLU	2.6
1	B	281	PHE	2.6
1	B	769	LYS	2.6
1	B	1014	TYR	2.6
1	B	7	GLU	2.5
1	A	262	ILE	2.5
1	B	1098	ARG	2.5
1	A	768	GLY	2.4
1	B	10	GLU	2.4
1	B	708	ARG	2.4
1	B	262	ILE	2.4
1	B	766	ALA	2.4
1	A	713	ASN	2.4
1	A	1099	LYS	2.4
1	A	406	GLU	2.4
1	A	708	ARG	2.3
1	A	753	ARG	2.3
1	A	26	LYS	2.3
1	B	74	LYS	2.3
1	A	709	ALA	2.3
1	A	42	GLU	2.3
1	B	1018	GLU	2.3
1	A	1095	LEU	2.1
2	D	23	DT	2.1
1	A	265	ASP	2.1
1	A	725	ALA	2.1
1	A	1100	GLN	2.1
1	A	726	ALA	2.1
1	B	767	LYS	2.1
1	B	6	GLU	2.0
1	B	195	GLU	2.0
1	B	191	GLU	2.0
1	A	28	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	2HP	A	1109	5/5	0.15	1.68	45,45,45,46	0
3	GTP	D	26	32/32	0.15	0.91	37,44,70,70	0
3	GTP	A	1107	32/32	0.13	0.52	25,33,60,60	0
4	2HP	B	1108	5/5	0.10	0.08	44,44,44,44	0
3	GTP	A	1108	32/32	0.10	-0.49	18,21,27,28	0
5	MG	A	1110	1/1	0.09	-1.34	22,22,22,22	0
3	GTP	B	1107	32/32	0.08	-1.34	23,26,34,35	0
5	MG	B	1109	1/1	0.07	-2.17	27,27,27,27	0

6.5 Other polymers ⓘ

There are no such residues in this entry.