



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2026 – 08:52 AM EDT

PDB ID : 3Q24 / pdb_00003q24
Title : X-ray crystal structure of the N4 mini-VRNAP and P2_7a promoter transcription initiation complex with pppGpG and pyrophosphate: product complex
Authors : Gleghorn, M.L.; Murakami, K.S.
Deposited on : 2010-12-19
Resolution : 1.81 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

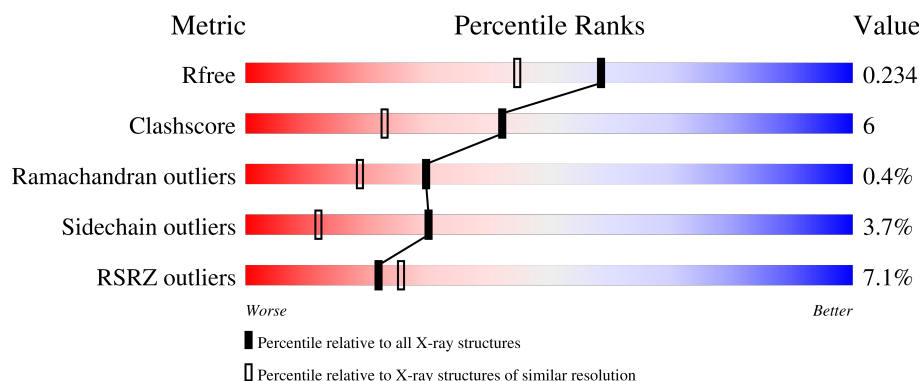
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.81 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}	180053	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1117	6% 84% 12% ..
1	B	1117	8% 85% 12% ..
2	C	36	3% 50% 8% 42%
2	D	36	6% 47% 14% 39%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20260 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 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			

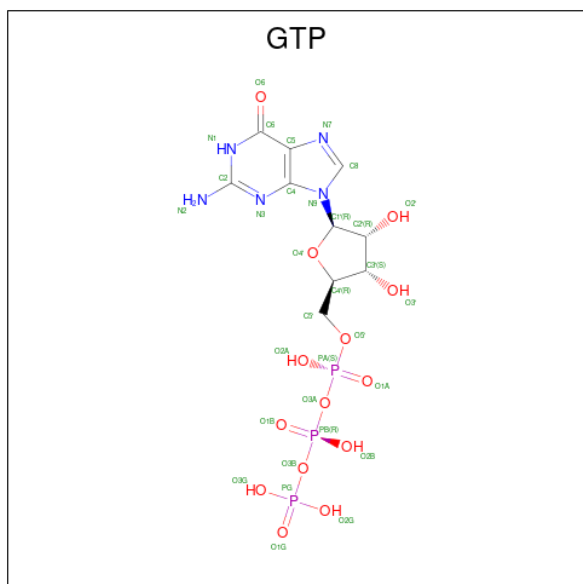
There are 24 discrepancies between the modelled and reference sequences:

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').

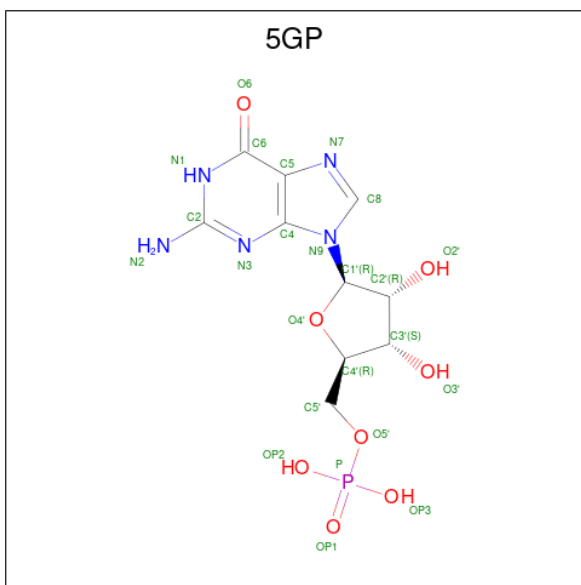
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	21	Total	C	N	O	P	0	0	0
			432	205	83	123	21			
2	D	22	Total	C	N	O	P	0	0	0
			449	215	88	125	21			

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



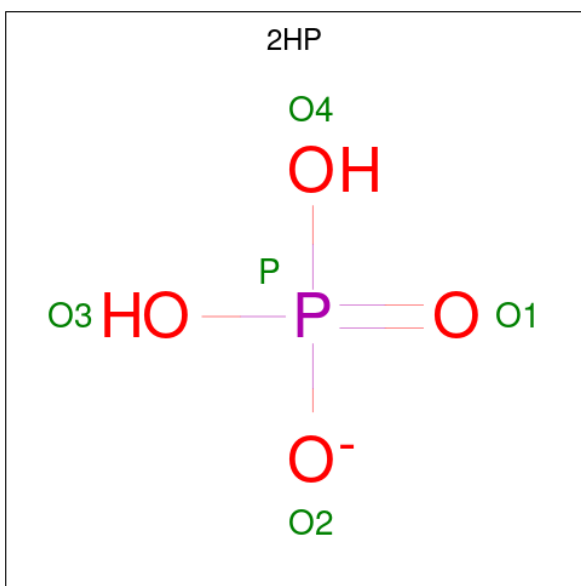
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 4 is GUANOSINE-5'-MONOPHOSPHATE (CCD ID: 5GP) (formula: C₁₀H₁₄N₅O₈P).



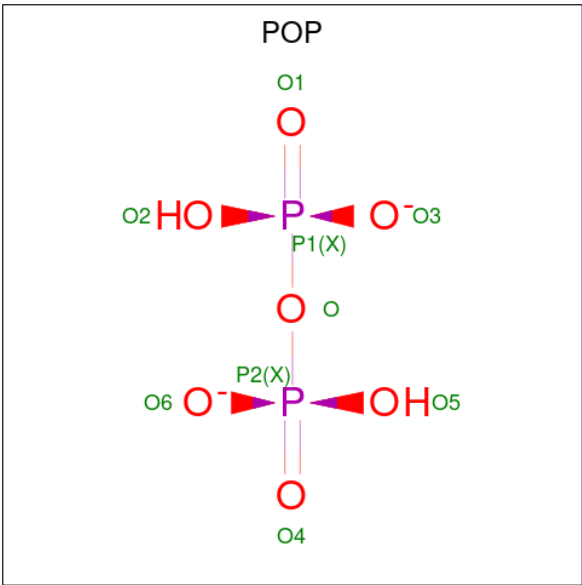
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 5 is DIHYDROGENPHOSPHATE ION (CCD ID: 2HP) (formula: $\text{H}_2\text{O}_4\text{P}$).



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

- Molecule 6 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: $\text{H}_2\text{O}_7\text{P}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			9	7	2		
6	B	1	Total	O	P	0	0
			9	7	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1055	Total	O	0	0
			1055	1055		
7	B	1167	Total	O	0	0
			1167	1167		
7	C	81	Total	O	0	0
			81	81		
7	D	96	Total	O	0	0
			96	96		

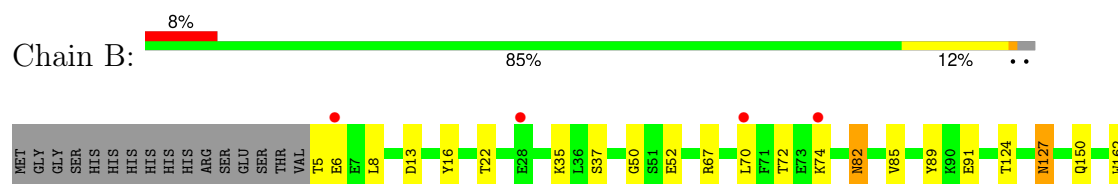
3 Residue-property plots [i](#)

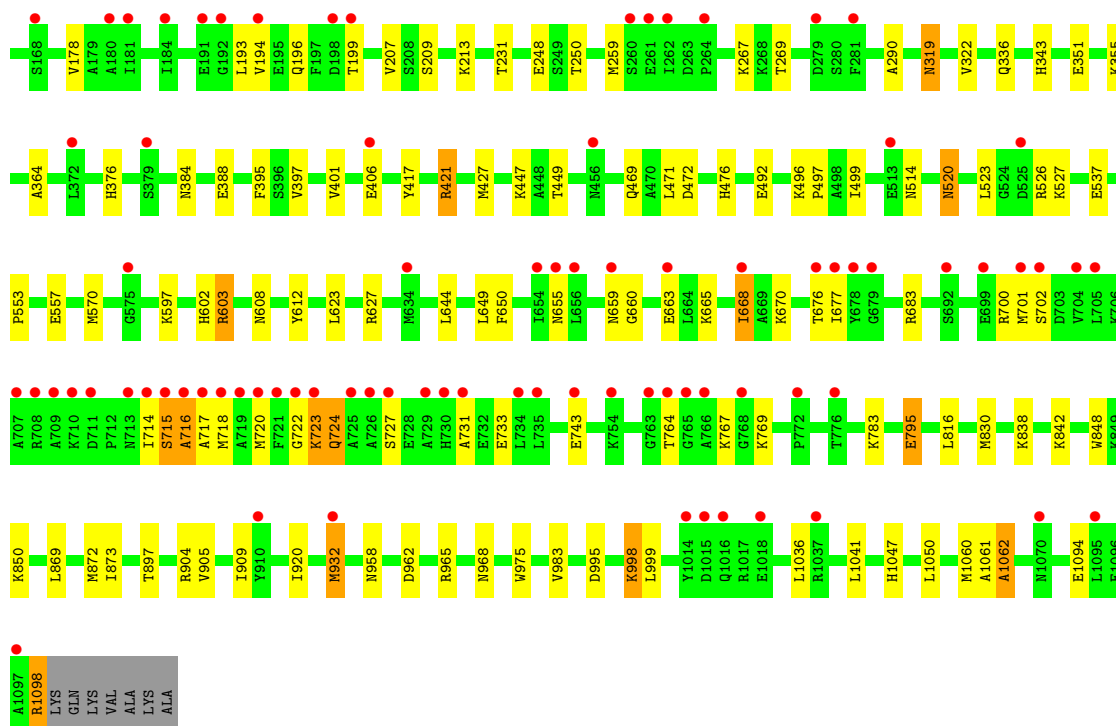
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Virion RNA polymerase

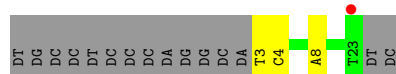


• Molecule 1: Virion RNA polymerase

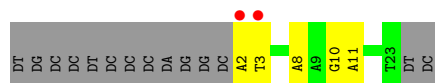




- Molecule 2: DNA (5'-D(*TP*GP*CP*CP*TP*CP*CP*CP*AP*GP*GP*CP*AP*TP*CP*CP*AP*AP*AP*AP*GP*AP*AP*GP*CP*GP*GP*AP*GP*CP*TP*TP*CP*TP*TP*C)-3')



- 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')



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.46Å 111.79Å 277.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.49 – 1.81 41.49 – 1.81	Depositor EDS
% Data completeness (in resolution range)	98.9 (41.49-1.81) 99.0 (41.49-1.81)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019, CNS	Depositor
R, R_{free}	0.201 , 0.235 0.199 , 0.234	Depositor DCC
R_{free} test set	11698 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20260	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: POP, 5GP, 2HP, GTP

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	0.48	0/8583	0.80	1/11609 (0.0%)
1	B	0.49	0/8572	0.80	2/11596 (0.0%)
2	C	0.29	0/485	0.91	0/746
2	D	0.26	0/505	0.86	0/778
All	All	0.48	0/18145	0.81	3/24729 (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	B	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	852	ASP	N-CA-C	-6.96	99.98	110.28
1	B	660	GLY	N-CA-C	-6.24	107.07	115.36
1	B	676	THR	N-CA-C	6.10	117.60	111.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	727	SER	Peptide

5.2 Too-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 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	8454	0	8479	123	0
1	B	8443	0	8465	96	0
2	C	432	0	236	2	0
2	D	449	0	245	4	0
3	A	32	0	11	0	0
4	A	23	0	12	2	0
5	A	5	0	0	0	0
5	B	5	0	0	1	0
6	A	9	0	0	2	0
6	B	9	0	0	0	0
7	A	1055	0	0	10	0
7	B	1167	0	0	15	0
7	C	81	0	0	3	0
7	D	96	0	0	3	0
All	All	20260	0	17448	222	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 (222) 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:469:GLN:HE22	1:B:557:GLU:H	1.11	0.98
1:B:701:MET:HE1	1:B:720:MET:HE2	1.45	0.97
1:A:561:VAL:HA	6:A:1109:POP:O6	1.68	0.93
1:A:469:GLN:HE22	1:A:557:GLU:H	1.11	0.93
1:A:866:LEU:HD12	7:A:2137:HOH:O	1.70	0.91
1:B:499:ILE:HG13	7:B:2872:HOH:O	1.67	0.91
1:A:701:MET:HE1	1:A:720:MET:HE2	1.53	0.90
1:A:603:ARG:NH1	1:A:608:ASN:OD1	2.07	0.88
1:B:322:VAL:HG22	1:B:872:MET:HE1	1.54	0.88
1:A:1017:ARG:HG2	1:A:1017:ARG:HH11	1.39	0.87
1:A:336:GLN:HE21	1:A:417:TYR:H	1.24	0.85
1:B:603:ARG:NH1	1:B:608:ASN:OD1	2.10	0.84
1:A:701:MET:HA	1:A:701:MET:HE2	1.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:790:LEU:O	1:A:795:GLU:HG2	1.82	0.79
1:B:700:ARG:CZ	1:B:723:LYS:HG3	2.15	0.77
1:A:1017:ARG:HG2	1:A:1017:ARG:NH1	1.98	0.77
1:B:850:LYS:O	7:B:2876:HOH:O	2.02	0.77
1:B:830:MET:HE3	1:B:999:LEU:HD23	1.67	0.75
1:A:351:GLU:HG3	1:A:395:PHE:CE2	2.22	0.74
1:B:476:HIS:ND1	5:B:1106:2HP:O4	2.17	0.74
1:B:336:GLN:HE21	1:B:417:TYR:H	1.34	0.73
1:A:421:ARG:HD2	7:C:68:HOH:O	1.86	0.73
1:A:364:ALA:H	1:A:384:ASN:HD21	1.37	0.72
1:A:364:ALA:H	1:A:384:ASN:ND2	1.89	0.71
1:B:724:GLN:HA	1:B:724:GLN:OE1	1.88	0.71
1:B:650:PHE:HE2	1:B:700:ARG:HG3	1.55	0.70
1:A:656:LEU:HD23	7:A:2091:HOH:O	1.90	0.70
1:A:603:ARG:HB3	1:A:603:ARG:HH11	1.59	0.68
1:B:91:GLU:HG3	7:B:2063:HOH:O	1.92	0.68
1:A:127:ASN:HD22	1:A:127:ASN:H	1.42	0.66
1:A:597:LYS:NZ	1:A:602:HIS:HD2	1.92	0.66
1:B:700:ARG:NE	1:B:723:LYS:HG3	2.11	0.66
1:A:778:LYS:N	1:A:778:LYS:HD3	2.11	0.65
1:A:82:ASN:HD22	1:A:82:ASN:C	2.04	0.64
1:A:150:GLN:HG2	7:A:2134:HOH:O	1.97	0.64
1:B:127:ASN:HD22	1:B:127:ASN:H	1.44	0.64
1:B:364:ALA:H	1:B:384:ASN:ND2	1.96	0.64
1:A:968:ASN:HD21	1:A:1060:MET:H	1.46	0.63
1:A:191:GLU:HG2	1:A:375:ASN:HB3	1.81	0.63
1:B:449:THR:H	1:B:958:ASN:HD21	1.45	0.63
1:A:958:ASN:H	1:A:958:ASN:HD22	1.45	0.62
1:A:207:VAL:HG11	1:A:905:VAL:HG21	1.81	0.62
1:B:16:TYR:O	1:B:35:LYS:HE3	2.00	0.62
1:A:830:MET:O	1:A:834:ARG:HG2	2.00	0.61
1:A:597:LYS:HZ1	1:A:602:HIS:HD2	1.48	0.61
1:A:718:MET:HE2	1:A:728:GLU:HA	1.80	0.61
1:B:1094:GLU:O	1:B:1098:ARG:HG2	2.01	0.60
1:A:370:GLU:HA	1:A:773:LYS:HE2	1.82	0.60
1:B:570:MET:HE3	1:B:975:TRP:HB3	1.83	0.60
1:A:1017:ARG:HH11	1:A:1017:ARG:CG	2.13	0.60
1:B:82:ASN:C	1:B:82:ASN:HD22	2.10	0.59
1:A:627:ARG:NH2	1:A:641:ASP:OD1	2.33	0.59
1:B:364:ALA:H	1:B:384:ASN:HD21	1.51	0.59
1:A:1017:ARG:O	1:A:1018:GLU:C	2.45	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:795:GLU:HB2	1:A:796:PRO:HD3	1.85	0.59
1:B:968:ASN:HD21	1:B:1060:MET:H	1.49	0.58
1:B:447:LYS:HE2	7:B:2219:HOH:O	2.03	0.58
1:A:730:HIS:O	1:A:733:GLU:HG2	2.03	0.58
1:A:358:ILE:HD12	1:A:391:TYR:CE1	2.40	0.57
1:A:616:THR:HG22	1:A:620:MET:HE2	1.85	0.57
1:A:402:ARG:HA	1:A:408:ILE:HG22	1.86	0.57
1:B:701:MET:HE2	1:B:701:MET:HA	1.88	0.56
1:B:207:VAL:HG11	1:B:905:VAL:HG21	1.88	0.56
1:B:421:ARG:HD2	7:D:95:HOH:O	2.05	0.56
1:A:778:LYS:HD3	1:A:778:LYS:H	1.70	0.55
1:B:998:LYS:HD2	7:B:2793:HOH:O	2.07	0.55
1:A:1045:ILE:HD12	1:A:1094:GLU:HG3	1.89	0.54
1:A:968:ASN:ND2	1:A:1060:MET:H	2.05	0.54
1:A:373:ASN:HD22	1:A:376:HIS:H	1.56	0.54
1:B:178:VAL:HG21	1:B:194:VAL:HA	1.87	0.54
1:A:603:ARG:NH1	1:A:603:ARG:HB3	2.22	0.54
1:B:13:ASP:HA	1:B:35:LYS:HE2	1.90	0.53
1:A:421:ARG:CD	7:C:68:HOH:O	2.50	0.53
1:B:848:TRP:CH2	1:B:850:LYS:HA	2.43	0.53
1:A:617:ASN:HA	1:A:620:MET:HE3	1.91	0.52
1:A:178:VAL:HG21	1:A:194:VAL:HA	1.91	0.52
1:A:752:LYS:HE3	1:A:755:GLY:HA2	1.91	0.52
1:B:677:ILE:O	1:B:920:ILE:HG21	2.09	0.52
1:B:722:GLY:O	1:B:723:LYS:C	2.52	0.52
1:A:570:MET:O	1:A:1047:HIS:HE1	1.93	0.52
1:B:421:ARG:CD	7:D:95:HOH:O	2.58	0.52
1:B:650:PHE:CE2	1:B:700:ARG:HG3	2.41	0.51
1:A:771:ASN:C	1:A:771:ASN:HD22	2.16	0.51
1:B:665:LYS:O	1:B:668:ILE:HG13	2.10	0.51
1:B:715:SER:HB3	1:B:718:MET:H	1.76	0.51
1:B:250:THR:O	1:B:250:THR:HG22	2.10	0.51
1:A:767:LYS:HE3	1:A:767:LYS:HA	1.93	0.51
1:B:469:GLN:HE22	1:B:557:GLU:N	1.93	0.51
1:B:72:THR:O	1:B:74:LYS:HE3	2.11	0.51
1:A:863:GLN:CD	7:A:2137:HOH:O	2.53	0.51
1:A:1018:GLU:HG3	1:A:1019:ASN:H	1.75	0.50
1:A:816:LEU:HD13	1:A:983:VAL:HG21	1.93	0.50
1:B:5:THR:HG23	1:B:6:GLU:H	1.76	0.50
1:A:514:ASN:HD22	1:A:514:ASN:H	1.59	0.50
1:A:673:LEU:HD22	1:A:801:ILE:HG23	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:816:LEU:HD13	1:B:983:VAL:HG21	1.93	0.50
1:A:52:GLU:H	1:A:52:GLU:CD	2.20	0.50
1:B:469:GLN:NE2	1:B:557:GLU:H	1.94	0.49
1:B:492:GLU:HG3	7:B:2367:HOH:O	2.13	0.49
1:A:351:GLU:HG3	1:A:395:PHE:HE2	1.74	0.49
1:B:597:LYS:NZ	1:B:602:HIS:HD2	2.10	0.49
1:A:747:SER:HB3	1:A:765:GLY:HA3	1.94	0.49
1:A:127:ASN:HD22	1:A:127:ASN:N	2.11	0.49
1:A:600:ASN:ND2	1:A:600:ASN:H	2.11	0.49
1:A:1061:ALA:O	1:A:1062:ALA:HB2	2.12	0.48
1:B:962:ASP:HB3	7:B:2877:HOH:O	2.13	0.48
1:B:968:ASN:ND2	1:B:1060:MET:H	2.11	0.48
1:B:82:ASN:ND2	1:B:85:VAL:H	2.11	0.48
1:B:127:ASN:HD22	1:B:127:ASN:N	2.12	0.48
1:B:343:HIS:HE1	1:B:537:GLU:OE2	1.96	0.48
2:D:8:DA:H1'	7:D:2361:HOH:O	2.13	0.48
1:A:351:GLU:HG3	1:A:395:PHE:CZ	2.49	0.47
1:B:1061:ALA:O	1:B:1062:ALA:HB2	2.14	0.47
1:B:520:ASN:HD21	1:B:527:LYS:NZ	2.12	0.47
1:A:597:LYS:NZ	1:A:602:HIS:CD2	2.78	0.47
1:A:816:LEU:CD1	1:A:983:VAL:HG21	2.45	0.47
1:A:1012:LEU:HD11	1:A:1025:ILE:HG22	1.95	0.47
1:A:176:LYS:HE3	7:C:2363:HOH:O	2.14	0.47
1:B:873:ILE:HD13	1:B:983:VAL:HG22	1.96	0.47
1:A:701:MET:CE	1:A:720:MET:HE2	2.33	0.47
1:B:717:ALA:HB1	1:B:731:ALA:C	2.40	0.46
1:A:721:PHE:HA	1:A:724:GLN:NE2	2.30	0.46
1:B:764:THR:HG23	7:B:2597:HOH:O	2.16	0.46
1:A:393:GLN:HG2	1:A:431:TYR:HB2	1.98	0.46
1:B:523:LEU:O	1:B:526:ARG:HG3	2.15	0.46
1:A:654:ILE:HD11	1:A:668:ILE:HG21	1.98	0.46
1:A:886:GLU:O	2:C:8:DA:H4'	2.15	0.46
1:B:715:SER:O	1:B:716:ALA:HB2	2.15	0.46
1:A:753:ARG:HH21	1:A:760:GLN:HE22	1.64	0.46
1:A:343:HIS:HE1	1:A:537:GLU:OE2	1.98	0.46
1:B:724:GLN:OE1	1:B:724:GLN:CA	2.59	0.46
1:B:743:GLU:HG3	7:B:2891:HOH:O	2.15	0.45
1:A:82:ASN:C	1:A:82:ASN:ND2	2.74	0.45
1:B:355:LYS:HD2	1:B:388:GLU:HG3	1.97	0.45
1:A:47:ARG:NE	7:A:2103:HOH:O	2.49	0.45
1:A:619:LEU:HD22	1:A:797:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:GLY:H	1:B:150:GLN:NE2	2.14	0.45
1:A:791:HIS:HA	1:A:795:GLU:HG3	1.98	0.45
1:A:267:LYS:HB2	1:A:267:LYS:HE2	1.72	0.45
2:D:2:DA:H2''	2:D:3:DT:C6	2.52	0.45
1:A:469:GLN:NE2	1:A:557:GLU:H	1.95	0.44
1:A:721:PHE:HA	1:A:724:GLN:HE21	1.81	0.44
1:B:714:ILE:HG13	1:B:715:SER:N	2.33	0.44
1:A:563:ASN:HD21	1:A:929:ASP:HB3	1.83	0.44
1:A:50:GLY:H	1:A:150:GLN:NE2	2.15	0.44
1:B:269:THR:O	2:D:11:DA:H5'	2.17	0.44
1:A:951:ASP:CG	4:A:1107:5GP:H5'1	2.43	0.44
1:A:673:LEU:C	1:A:673:LEU:HD13	2.42	0.44
1:B:193:LEU:HD12	1:B:196:GLN:HE21	1.83	0.44
1:B:196:GLN:O	1:B:199:THR:HG22	2.17	0.44
1:A:454:ASN:HB3	1:A:457:ASN:ND2	2.33	0.44
1:B:838:LYS:O	1:B:842:LYS:HG2	2.18	0.44
1:A:499:ILE:HD12	1:A:538:TYR:HD2	1.83	0.43
1:A:764:THR:HG21	1:A:780:GLU:HB3	2.00	0.43
1:A:7:GLU:H	1:A:7:GLU:HG2	1.69	0.43
1:B:376:HIS:HD2	1:B:702:SER:OG	2.01	0.43
1:A:426:GLN:NE2	7:A:2073:HOH:O	2.52	0.43
1:A:170:THR:HG22	1:A:201:MET:HE3	2.00	0.43
1:A:965:ARG:HD2	7:A:2035:HOH:O	2.18	0.43
1:B:655:ASN:HB2	1:B:663:GLU:HB3	2.01	0.43
1:A:1045:ILE:HD12	1:A:1094:GLU:CG	2.48	0.43
1:B:319:ASN:HD22	1:B:319:ASN:HA	1.67	0.43
1:B:715:SER:O	1:B:716:ALA:CB	2.66	0.43
1:A:562:THR:HG22	1:A:612:TYR:CZ	2.54	0.43
1:B:50:GLY:H	1:B:150:GLN:HE22	1.67	0.43
2:C:3:DT:H4'	2:C:4:DC:OP1	2.19	0.43
1:A:82:ASN:ND2	1:A:85:VAL:H	2.17	0.42
1:A:492:GLU:HG3	7:A:2077:HOH:O	2.19	0.42
1:B:16:TYR:O	1:B:35:LYS:CE	2.66	0.42
1:B:496:LYS:HB3	1:B:497:PRO:HD3	2.00	0.42
1:A:1061:ALA:O	1:A:1062:ALA:CB	2.67	0.42
1:B:520:ASN:HD21	1:B:527:LYS:HZ2	1.66	0.42
1:B:162:TRP:HE1	1:B:209:SER:HB3	1.84	0.42
1:A:668:ILE:H	1:A:668:ILE:HG13	1.66	0.42
1:B:259:MET:HA	1:B:259:MET:HE2	2.01	0.42
1:B:965:ARG:HG2	7:B:2065:HOH:O	2.20	0.42
1:B:1061:ALA:O	1:B:1062:ALA:CB	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:PRO:CG	1:A:673:LEU:HD12	2.50	0.42
1:A:951:ASP:OD2	4:A:1107:5GP:H5'1	2.20	0.42
1:A:972:TYR:OH	1:A:1051:ASP:OD1	2.25	0.42
1:B:612:TYR:CZ	1:B:670:LYS:HG2	2.55	0.42
1:A:454:ASN:OD1	1:A:456:ASN:HB2	2.20	0.42
1:A:707:ALA:HA	1:A:710:LYS:HE3	2.01	0.42
7:B:2871:HOH:O	2:D:10:DG:H5''	2.19	0.42
1:A:1047:HIS:HD2	7:A:1249:HOH:O	2.01	0.42
1:A:113:THR:HG22	1:A:114:LYS:HG3	2.02	0.41
1:A:267:LYS:HD3	1:A:267:LYS:H	1.85	0.41
1:A:677:ILE:HD11	1:A:805:VAL:HG11	2.01	0.41
1:B:677:ILE:HG22	7:B:2870:HOH:O	2.19	0.41
1:B:932:MET:HE2	7:B:1771:HOH:O	2.19	0.41
1:A:201:MET:HE2	1:A:205:GLU:HG2	2.03	0.41
1:A:342:VAL:HG11	1:A:408:ILE:HD12	2.02	0.41
1:A:393:GLN:HG2	1:A:431:TYR:CB	2.50	0.41
1:A:598:THR:HG22	1:A:1066:PRO:HD3	2.03	0.41
1:A:771:ASN:C	1:A:771:ASN:ND2	2.78	0.41
1:B:670:LYS:HD3	1:B:670:LYS:C	2.44	0.41
1:A:304:PHE:HB3	1:A:308:ASP:O	2.20	0.41
1:A:95:HIS:HA	1:B:248:GLU:O	2.21	0.41
1:A:562:THR:N	6:A:1109:POP:O6	2.50	0.41
1:B:5:THR:HG23	1:B:6:GLU:N	2.35	0.41
1:B:897:THR:HG22	1:B:904:ARG:HG2	2.02	0.41
1:B:995:ASP:OD2	1:B:998:LYS:HE3	2.21	0.41
1:A:351:GLU:CG	1:A:395:PHE:CE2	3.01	0.41
1:A:397:VAL:O	1:A:401:VAL:HG23	2.20	0.41
1:A:677:ILE:O	1:A:920:ILE:HG21	2.21	0.41
1:B:37:SER:HB3	1:B:231:THR:HG22	2.03	0.41
1:B:267:LYS:HA	1:B:267:LYS:HE2	2.03	0.41
1:B:351:GLU:HG2	1:B:395:PHE:CE2	2.56	0.41
1:B:397:VAL:O	1:B:401:VAL:HG23	2.21	0.41
1:A:6:GLU:HG2	7:A:2104:HOH:O	2.21	0.41
1:A:603:ARG:HD2	1:A:603:ARG:HA	1.90	0.40
1:A:649:LEU:HD13	1:A:737:ARG:NH2	2.35	0.40
1:B:89:TYR:CZ	1:B:290:ALA:HB3	2.56	0.40
1:B:627:ARG:HH21	1:B:644:LEU:HD12	1.86	0.40
1:A:393:GLN:HG2	1:A:431:TYR:CD2	2.56	0.40
1:A:141:ASP:HB2	1:A:146:LYS:HG2	2.03	0.40
1:A:384:ASN:HD22	1:A:384:ASN:HA	1.66	0.40
1:B:22:THR:HG23	7:B:2299:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:HIS:CD2	1:B:553:PRO:HG3	2.57	0.40
1:B:570:MET:O	1:B:1047:HIS:HE1	2.03	0.40
1:A:261:GLU:H	1:A:261:GLU:HG2	1.70	0.40
1:B:795:GLU:HB2	7:B:2854:HOH:O	2.21	0.40

There are no symmetry-related clashes.

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	1093/1117 (98%)	1067 (98%)	23 (2%)	3 (0%)	36	26
1	B	1092/1117 (98%)	1063 (97%)	23 (2%)	6 (0%)	24	14
All	All	2185/2234 (98%)	2130 (98%)	46 (2%)	9 (0%)	30	19

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1018	GLU
1	B	716	ALA
1	B	723	LYS
1	B	769	LYS
1	A	370	GLU
1	A	1062	ALA
1	B	1062	ALA
1	B	659	ASN
1	B	767	LYS

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	916/934 (98%)	882 (96%)	34 (4%)	30	12
1	B	915/934 (98%)	881 (96%)	34 (4%)	30	12
All	All	1831/1868 (98%)	1763 (96%)	68 (4%)	30	12

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	228	LEU
1	A	250	THR
1	A	261	GLU
1	A	267	LYS
1	A	272	LEU
1	A	319	ASN
1	A	372	LEU
1	A	421	ARG
1	A	472	ASP
1	A	494	ASN
1	A	514	ASN
1	A	600	ASN
1	A	603	ARG
1	A	623	LEU
1	A	649	LEU
1	A	668	ILE
1	A	708	ARG
1	A	728	GLU
1	A	767	LYS
1	A	778	LYS
1	A	936	LEU
1	A	958	ASN
1	A	1004	LEU

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Mol	Chain	Res	Type
1	A	1017	ARG
1	A	1019	ASN
1	A	1025	ILE
1	A	1036	LEU
1	A	1041	LEU
1	A	1050	LEU
1	A	1055	LEU
1	B	8	LEU
1	B	52	GLU
1	B	67	ARG
1	B	70	LEU
1	B	82	ASN
1	B	124	THR
1	B	127	ASN
1	B	213	LYS
1	B	319	ASN
1	B	406	GLU
1	B	421	ARG
1	B	427	MET
1	B	471	LEU
1	B	472	ASP
1	B	514	ASN
1	B	520	ASN
1	B	603	ARG
1	B	623	LEU
1	B	649	LEU
1	B	668	ILE
1	B	683	ARG
1	B	715	SER
1	B	724	GLN
1	B	733	GLU
1	B	783	LYS
1	B	795	GLU
1	B	869	LEU
1	B	909	ILE
1	B	932	MET
1	B	998	LYS
1	B	1036	LEU
1	B	1041	LEU
1	B	1050	LEU
1	B	1098	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	A	127	ASN
1	A	150	GLN
1	A	225	ASN
1	A	316	GLN
1	A	319	ASN
1	A	336	GLN
1	A	343	HIS
1	A	348	GLN
1	A	368	ASN
1	A	373	ASN
1	A	375	ASN
1	A	384	ASN
1	A	404	GLN
1	A	414	HIS
1	A	455	GLN
1	A	457	ASN
1	A	469	GLN
1	A	506	ASN
1	A	514	ASN
1	A	596	ASN
1	A	600	ASN
1	A	602	HIS
1	A	629	ASN
1	A	639	GLN
1	A	724	GLN
1	A	730	HIS
1	A	760	GLN
1	A	771	ASN
1	A	791	HIS
1	A	803	GLN
1	A	815	GLN
1	A	817	GLN
1	A	823	GLN
1	A	833	GLN
1	A	856	GLN
1	A	863	GLN
1	A	954	ASN
1	A	958	ASN
1	A	968	ASN
1	A	982	ASN
1	A	1016	GLN

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Mol	Chain	Res	Type
1	A	1035	ASN
1	A	1038	ASN
1	A	1047	HIS
1	A	1100	GLN
1	B	82	ASN
1	B	112	ASN
1	B	122	GLN
1	B	127	ASN
1	B	140	GLN
1	B	150	GLN
1	B	186	GLN
1	B	196	GLN
1	B	255	ASN
1	B	324	ASN
1	B	336	GLN
1	B	343	HIS
1	B	348	GLN
1	B	376	HIS
1	B	384	ASN
1	B	414	HIS
1	B	455	GLN
1	B	469	GLN
1	B	506	ASN
1	B	514	ASN
1	B	520	ASN
1	B	602	HIS
1	B	609	ASN
1	B	613	GLN
1	B	629	ASN
1	B	639	GLN
1	B	760	GLN
1	B	781	GLN
1	B	786	GLN
1	B	817	GLN
1	B	833	GLN
1	B	856	GLN
1	B	914	GLN
1	B	954	ASN
1	B	958	ASN
1	B	968	ASN
1	B	982	ASN
1	B	1047	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	5GP	A	1107	3	22,25,26	0.37	0	32,37,40	0.63	0
5	2HP	B	1106	-	4,4,4	5.81	2 (50%)	6,6,6	0.98	0
3	GTP	A	1106	4	33,34,34	0.98	3 (9%)	50,54,54	1.60	11 (22%)
6	POP	B	1107	-	6,8,8	0.74	0	12,13,13	0.96	0
5	2HP	A	1108	-	4,4,4	5.81	2 (50%)	6,6,6	0.81	0
6	POP	A	1109	-	6,8,8	0.82	0	12,13,13	0.99	0

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
6	POP	A	1109	-	-	2/6/6/6	-
4	5GP	A	1107	3	-	0/7/25/26	0/3/3/3
3	GTP	A	1106	4	-	4/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	POP	B	1107	-	-	0/6/6/6	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1108	2HP	P-O3	8.26	1.78	1.54
5	B	1106	2HP	P-O3	8.23	1.78	1.54
5	B	1106	2HP	P-O4	8.13	1.78	1.54
5	A	1108	2HP	P-O4	8.12	1.78	1.54
3	A	1106	GTP	PB-O3A	2.49	1.62	1.59
3	A	1106	GTP	C2-N3	2.17	1.38	1.33
3	A	1106	GTP	PA-O3A	2.05	1.61	1.59

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1106	GTP	C2-N3-C4	4.71	120.41	112.30
3	A	1106	GTP	C5-C4-N3	-4.54	121.17	128.39
3	A	1106	GTP	N9-C8-N7	-2.69	108.42	113.40
3	A	1106	GTP	C2-N1-C6	-2.68	120.25	125.11
3	A	1106	GTP	N9-C4-N3	2.56	131.07	125.95
3	A	1106	GTP	C8-N7-C5	2.50	108.72	104.26
3	A	1106	GTP	C5-C6-N1	2.45	119.50	113.25
3	A	1106	GTP	C2'-C1'-N9	-2.42	106.53	113.25
3	A	1106	GTP	O2B-PB-O3A	2.33	113.58	107.27
3	A	1106	GTP	O6-C6-C5	-2.31	120.43	126.53
3	A	1106	GTP	O4'-C1'-N9	2.00	112.90	108.36

There are no chirality outliers.

All (6) torsion outliers are listed below:

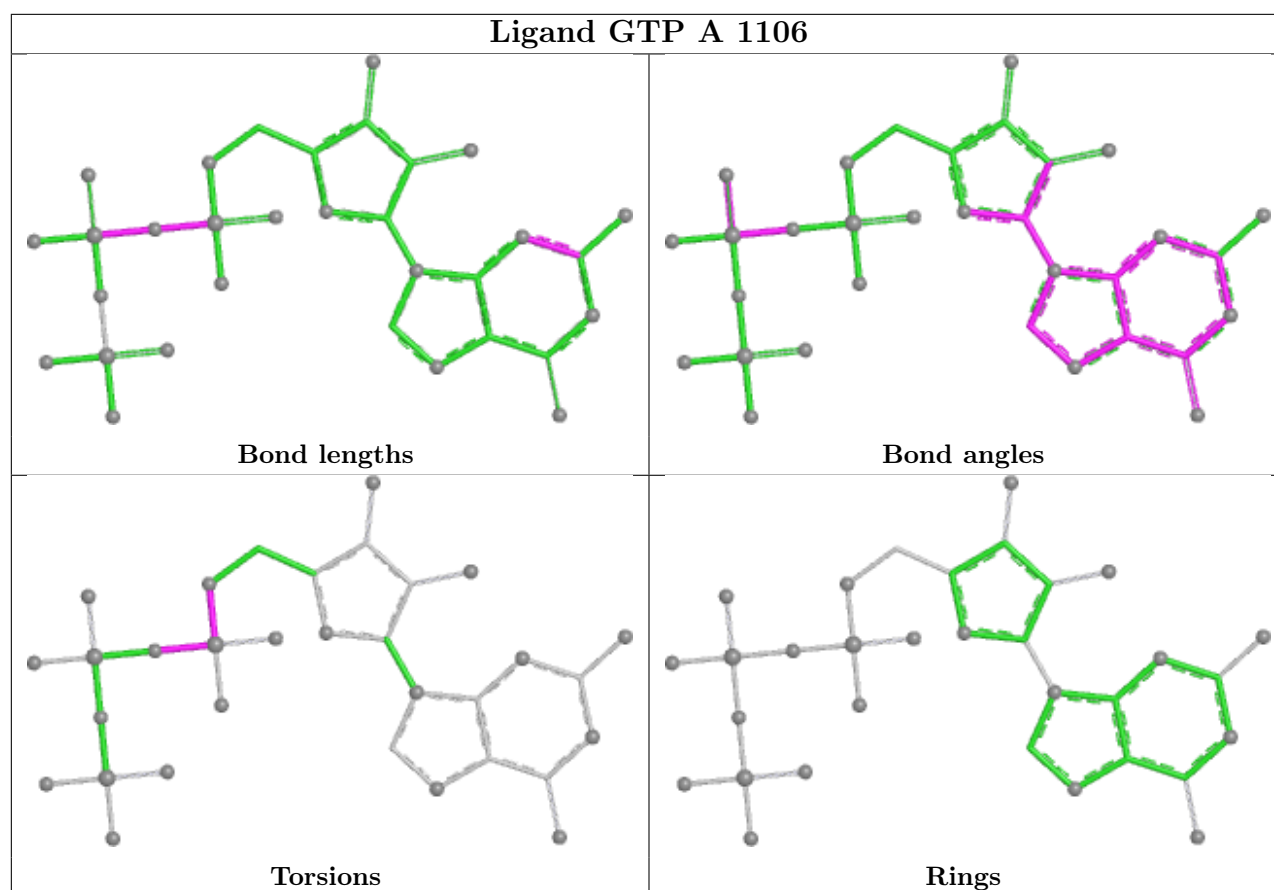
Mol	Chain	Res	Type	Atoms
3	A	1106	GTP	C5'-O5'-PA-O1A
3	A	1106	GTP	C5'-O5'-PA-O2A
6	A	1109	POP	P2-O-P1-O3
3	A	1106	GTP	C5'-O5'-PA-O3A
3	A	1106	GTP	PB-O3A-PA-O1A
6	A	1109	POP	P2-O-P1-O1

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1107	5GP	2	0
5	B	1106	2HP	1	0
6	A	1109	POP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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	1095/1117 (98%)	0.47	69 (6%)	26 30	16, 29, 53, 79	0
1	B	1094/1117 (97%)	0.40	86 (7%)	18 20	17, 27, 54, 84	0
2	C	21/36 (58%)	0.18	1 (4%)	35 41	29, 33, 59, 102	0
2	D	22/36 (61%)	0.37	2 (9%)	15 16	24, 38, 60, 88	0
All	All	2232/2306 (96%)	0.43	158 (7%)	22 25	16, 28, 54, 102	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	677	ILE	6.7
1	A	910	TYR	5.9
1	B	678	TYR	5.1
1	B	910	TYR	4.7
1	B	705	LEU	4.2
1	A	1097	ALA	4.1
1	A	707	ALA	4.0
1	B	714	ILE	4.0
1	A	661	ALA	4.0
1	A	1018	GLU	3.9
1	A	719	ALA	3.8
1	B	716	ALA	3.8
1	B	264	PRO	3.7
1	B	764	THR	3.7
1	A	264	PRO	3.7
1	B	727	SER	3.6
1	B	679	GLY	3.5
1	B	707	ALA	3.5
1	B	721	PHE	3.4
1	B	726	ALA	3.4
1	A	1015	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	766	ALA	3.4
1	B	704	VAL	3.3
2	D	2	DA	3.3
1	B	734	LEU	3.3
1	A	1012	LEU	3.2
1	B	1014	TYR	3.2
1	A	1016	GLN	3.2
1	B	765	GLY	3.2
1	A	729	ALA	3.1
1	B	659	ASN	3.1
1	A	1011	ALA	3.1
1	A	1014	TYR	3.1
1	B	722	GLY	3.1
1	B	711	ASP	3.1
1	A	1025	ILE	3.0
1	B	372	LEU	3.0
2	C	23	DT	3.0
1	B	406	GLU	3.0
1	B	719	ALA	3.0
1	B	718	MET	3.0
1	B	28	GLU	3.0
1	A	731	ALA	3.0
1	B	725	ALA	3.0
1	A	42	GLU	3.0
1	A	8	LEU	2.9
1	B	729	ALA	2.9
1	B	192	GLY	2.9
1	A	1034	ARG	2.8
1	A	726	ALA	2.8
1	A	1093	GLU	2.8
1	B	717	ALA	2.8
1	A	199	THR	2.8
1	A	717	ALA	2.8
1	B	708	ARG	2.8
1	A	714	ILE	2.8
1	B	932	MET	2.8
1	B	731	ALA	2.7
1	B	260	SER	2.7
1	B	525	ASP	2.7
1	B	730	HIS	2.7
1	A	1020	ALA	2.7
1	A	767	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	702	SER	2.6
1	B	763	GLY	2.6
1	A	675	ILE	2.6
1	B	198	ASP	2.5
1	A	716	ALA	2.5
1	B	199	THR	2.5
1	A	712	PRO	2.5
1	B	723	LYS	2.5
1	B	1016	GLN	2.5
1	A	52	GLU	2.5
1	B	701	MET	2.5
1	B	668	ILE	2.5
1	A	704	VAL	2.5
1	B	1070	ASN	2.4
1	A	75	GLU	2.4
1	B	379	SER	2.4
1	A	447	LYS	2.4
1	A	657	GLY	2.4
1	B	191	GLU	2.4
1	A	677	ILE	2.4
1	B	181	ILE	2.4
1	B	772	PRO	2.4
1	A	1031	LEU	2.3
1	B	70	LEU	2.3
1	B	281	PHE	2.3
1	A	1021	THR	2.3
1	B	709	ALA	2.3
1	B	768	GLY	2.3
1	A	300	THR	2.3
1	A	678	TYR	2.3
1	A	764	THR	2.3
1	B	184	ILE	2.3
1	B	262	ILE	2.3
1	B	6	GLU	2.3
1	A	1095	LEU	2.3
1	B	735	LEU	2.3
1	B	676	THR	2.3
1	B	720	MET	2.3
1	B	180	ALA	2.3
1	A	755	GLY	2.3
1	A	710	LYS	2.3
1	A	708	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	513	GLU	2.2
1	B	743	GLU	2.2
1	B	715	SER	2.2
1	A	525	ASP	2.2
1	B	279	ASP	2.2
1	A	655	ASN	2.2
1	B	655	ASN	2.2
1	A	406	GLU	2.2
1	A	999	LEU	2.2
1	A	1004	LEU	2.2
1	B	261	GLU	2.2
1	B	634	MET	2.2
1	B	194	VAL	2.2
1	A	29	GLY	2.2
1	B	575	GLY	2.2
1	B	710	LYS	2.2
1	B	699	GLU	2.2
1	B	1015	ASP	2.2
1	A	431	TYR	2.1
1	A	743	GLU	2.1
1	A	262	ILE	2.1
1	B	168	SER	2.1
1	A	267	LYS	2.1
1	B	663	GLU	2.1
2	D	3	DT	2.1
1	A	279	ASP	2.1
1	B	754	LYS	2.1
1	A	6	GLU	2.1
1	A	1002	GLU	2.1
1	B	656	LEU	2.1
1	B	713	ASN	2.1
1	B	1095	LEU	2.1
1	B	1097	ALA	2.1
1	B	1018	GLU	2.1
1	A	183	GLY	2.1
1	A	656	LEU	2.1
1	A	753	ARG	2.1
1	A	7	GLU	2.0
1	A	621	GLU	2.0
1	A	654	ILE	2.0
1	A	658	GLU	2.0
1	B	692	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	634	MET	2.0
1	B	776	THR	2.0
1	B	456	ASN	2.0
1	A	711	ASP	2.0
1	B	1037	ARG	2.0
1	A	940	LYS	2.0
1	B	74	LYS	2.0
1	A	932	MET	2.0
1	B	654	ILE	2.0
1	A	624	GLY	2.0
1	A	297	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

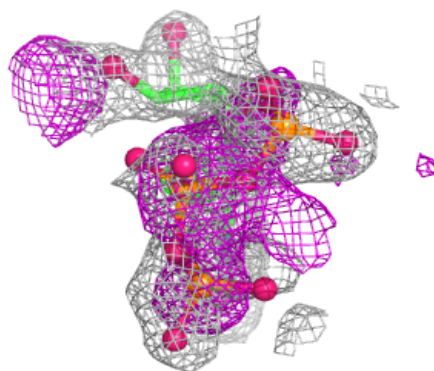
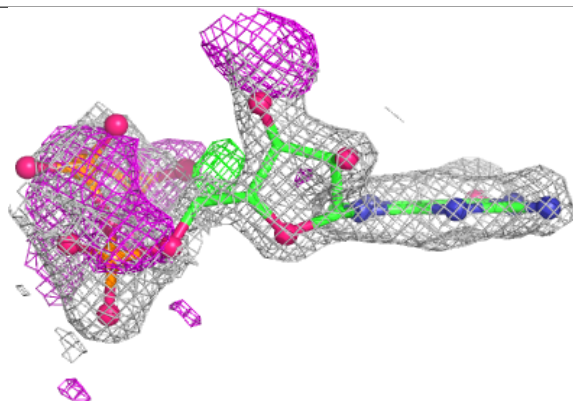
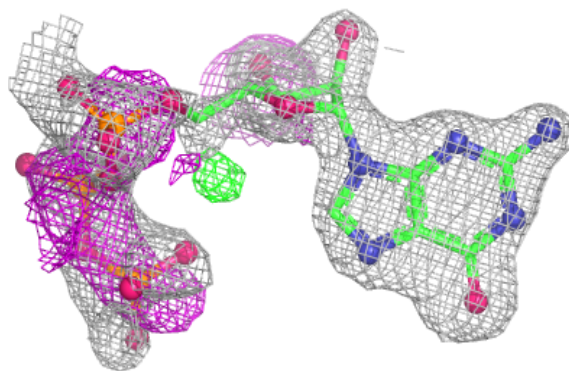
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	POP	A	1109	9/9	0.66	0.19	95,95,95,95	0
3	GTP	A	1106	32/32	0.70	0.15	44,51,72,73	0
6	POP	B	1107	9/9	0.71	0.20	72,72,73,73	0
4	5GP	A	1107	23/24	0.77	0.14	36,39,48,49	0
5	2HP	B	1106	5/5	0.84	0.14	42,43,43,43	0
5	2HP	A	1108	5/5	0.95	0.09	32,32,34,34	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GTP A 1106:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.