Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2024 – 04:44 PM EST

PDB ID	:	3Q24
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 (i) 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 (i)) were used in the production of this report:

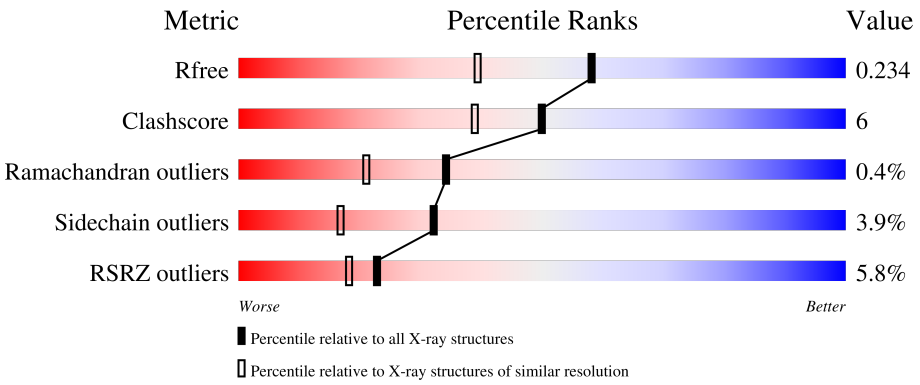
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 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}	130704	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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 <=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	5% 85% 12% • •
1	B	1117	6% 85% 11% • •
2	C	36	6% 42% 14% • 42%
2	D	36	6% 44% 17% 39%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	1095	8454	5306	1435	1672	41	0	0	0
1	B	1094	8443	5299	1432	1671	41	0	0	0

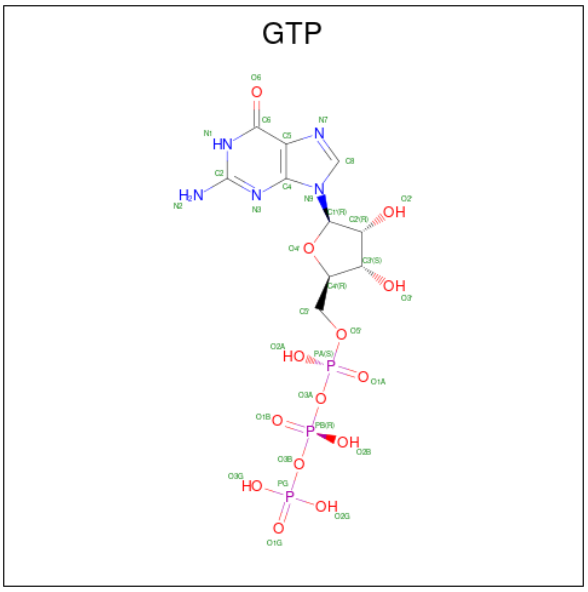
There are 24 discrepancies between the modelled and reference sequences:

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').

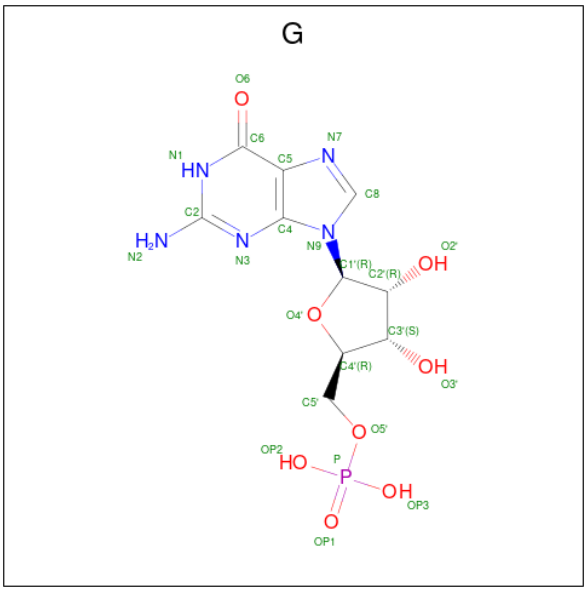
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	21	432	205	83	123	21	0	0	0
2	D	22	449	215	88	125	21	0	0	0

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



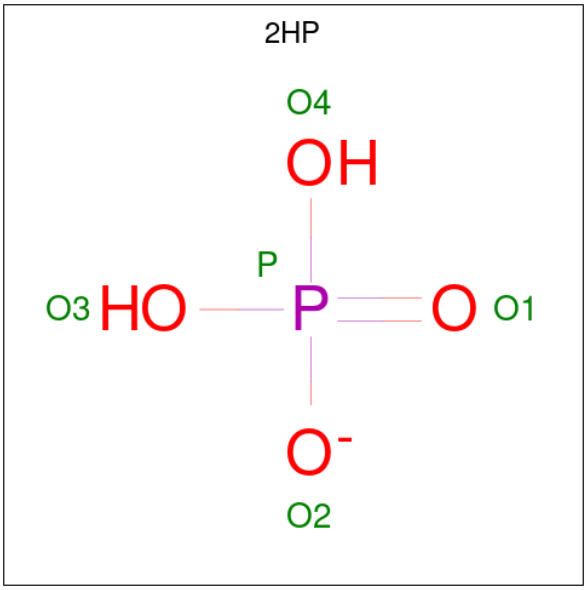
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	32	10	5	14	3	0	0

- Molecule 4 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: G) (formula: $C_{10}H_{14}N_5O_8P$).



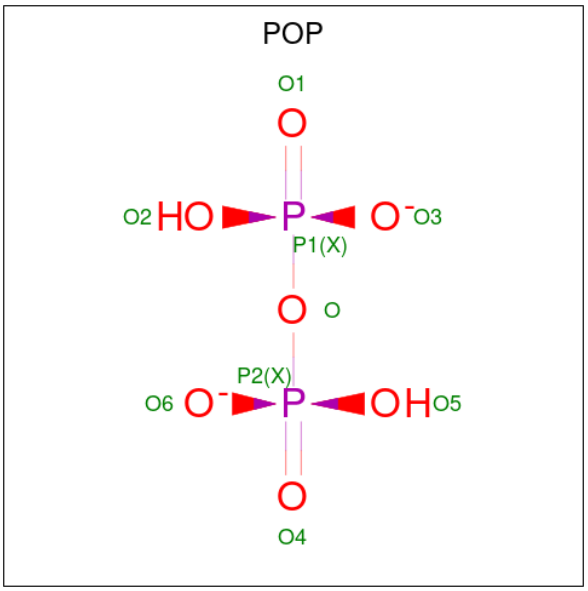
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	23	10	5	7	1	0	0

- Molecule 5 is DIHYDROGENPHOSPHATE ION (three-letter code: 2HP) (formula: H_2O_4P).



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

- Molecule 6 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $H_2O_7P_2$).



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

- Molecule 7 is water.

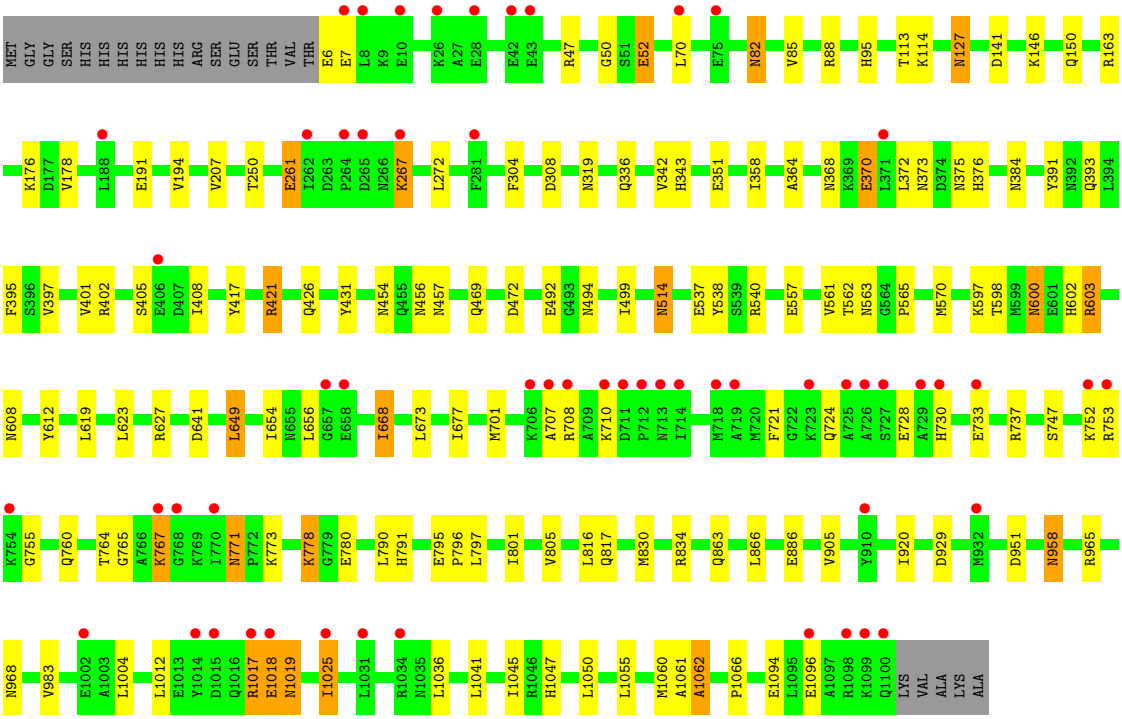
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1055	Total O 1055 1055	0	0
7	B	1167	Total O 1167 1167	0	0
7	C	81	Total O 81 81	0	0
7	D	96	Total O 96 96	0	0

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.

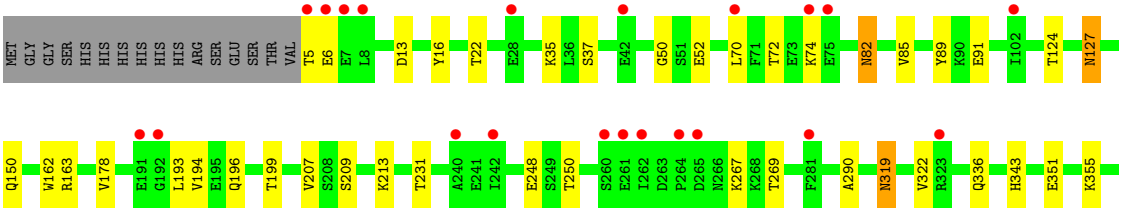
• Molecule 1: Virion RNA polymerase

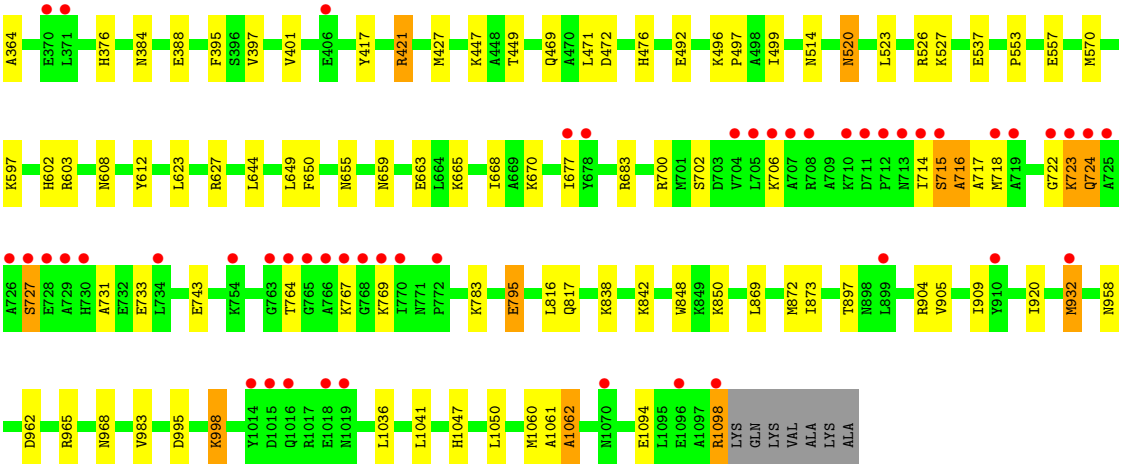
Chain A:



• Molecule 1: Virion RNA polymerase

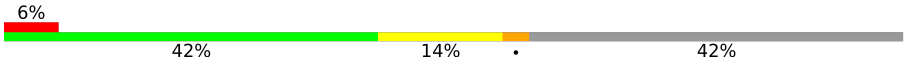
Chain B:

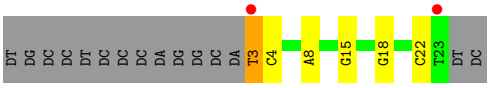




• Molecule 2: DNA (5'-D(*TP*GP*CP*CP*TP*CP*CP*CP*AP*GP*GP*CP*AP*TP*CP*CP*AP*AP*AP*AP*GP*AP*AP*GP*CP*GP*GP*AP*GP*CP*TP*TP*CP*TP*TP*C)-3')

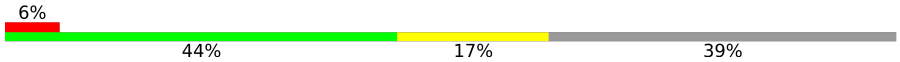
Chain C:

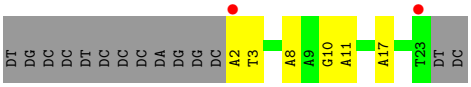




• Molecule 2: DNA (5'-D(*TP*GP*CP*CP*TP*CP*CP*CP*AP*GP*GP*CP*AP*TP*CP*CP*AP*AP*AP*AP*GP*AP*AP*GP*CP*GP*GP*AP*GP*CP*TP*TP*CP*TP*TP*C)-3')

Chain D:





4 Data and refinement statistics (i)

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) 98.9 (41.49-1.81)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.01%)	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 , 46.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, GTP, 2HP

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	0.38	0/8583	0.53	2/11609 (0.0%)
1	B	0.38	0/8572	0.54	0/11596
2	C	0.73	1/485 (0.2%)	1.29	3/746 (0.4%)
2	D	0.68	0/505	1.24	1/778 (0.1%)
All	All	0.40	1/18145 (0.0%)	0.60	6/24729 (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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	DT	C1'-N1	5.20	1.56	1.49

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	18	DG	O4'-C1'-N9	5.82	112.07	108.00
2	C	22	DC	O4'-C1'-N1	5.48	111.84	108.00
2	D	17	DA	O4'-C1'-N9	-5.33	104.27	108.00
1	A	540	ARG	NE-CZ-NH1	5.32	122.96	120.30
2	C	15	DG	P-O3'-C3'	5.12	125.85	119.70
1	A	540	ARG	NE-CZ-NH2	-5.02	117.79	120.30

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 (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	8454	0	8479	113	0
1	B	8443	0	8465	90	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	1	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	206	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 (206) 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: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:HA	1:A:701:MET:HE2	1.53	0.89
1:A:603:ARG:NH1	1:A:608:ASN:OD1	2.07	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:724:GLN:HA	1:B:724:GLN:OE1	1.88	0.72
1:A:364:ALA:H	1:A:384:ASN:ND2	1.89	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: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: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:A:1017:ARG:HH11	1:A:1017:ARG:CG	2.13	0.60
1:A:82:ASN:HD22	1:A:82:ASN:C	2.04	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:402:ARG:HA	1:A:408:ILE:HG22	1.86	0.57
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:82:ASN:C	1:B:82:ASN:HD22	2.10	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:1017:ARG:O	1:A:1018:GLU:C	2.45	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: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:A:597:LYS:HZ3	1:A:602:HIS:CD2	2.27	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: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: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
1:B:816:LEU:HD13	1:B:983:VAL:HG21	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:701:MET:HE2	1:A:701:MET:CA	2.35	0.48
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:771:ASN:C	1:A:771:ASN:HD22	2.16	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:B:722:GLY:O	1:B:723:LYS:C	2.52	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:721:PHE:HA	1:A:724:GLN:NE2	2.30	0.46
1:B:520:ASN:HD21	1:B:527:LYS:HZ3	1.63	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:863:GLN:CD	7:A:2137:HOH:O	2.53	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:52:GLU:H	1:A:52:GLU:CD	2.20	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:597:LYS:NZ	1:A:602:HIS:CD2	2.78	0.44
1:B:269:THR:O	2:D:11:DA:H5'	2.17	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: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:932:MET:HE2	7:B:1771:HOH:O	2.19	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: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
1:A:565:PRO:CG	1:A:673:LEU:HD12	2.50	0.42
1:A:951:ASP:OD2	4:A:1107:G:H5'	2.20	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:B:717:ALA:HB1	1:B:731:ALA:C	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:82:ASN:C	1:A:82:ASN:ND2	2.74	0.40
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:B:322:VAL:HG22	1:B:872:MET:CE	2.51	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
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 (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	1093/1117 (98%)	1067 (98%)	23 (2%)	3 (0%)	41	27
1	B	1092/1117 (98%)	1063 (97%)	23 (2%)	6 (0%)	29	15
All	All	2185/2234 (98%)	2130 (98%)	46 (2%)	9 (0%)	34	21

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 (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	916/934 (98%)	877 (96%)	39 (4%)	29	14
1	B	915/934 (98%)	882 (96%)	33 (4%)	35	19
All	All	1831/1868 (98%)	1759 (96%)	72 (4%)	32	17

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	GLU
1	A	70	LEU
1	A	82	ASN
1	A	88	ARG
1	A	127	ASN
1	A	163	ARG
1	A	250	THR
1	A	261	GLU
1	A	267	LYS
1	A	272	LEU
1	A	319	ASN
1	A	368	ASN
1	A	372	LEU
1	A	405	SER
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	771	ASN
1	A	778	LYS
1	A	817	GLN
1	A	958	ASN
1	A	1004	LEU
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	A	1096	GLU
1	B	52	GLU
1	B	70	LEU
1	B	82	ASN

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Mol	Chain	Res	Type
1	B	124	THR
1	B	127	ASN
1	B	163	ARG
1	B	213	LYS
1	B	319	ASN
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	623	LEU
1	B	649	LEU
1	B	683	ARG
1	B	706	LYS
1	B	715	SER
1	B	724	GLN
1	B	727	SER
1	B	733	GLU
1	B	783	LYS
1	B	795	GLU
1	B	817	GLN
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 (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	A	127	ASN
1	A	150	GLN
1	A	316	GLN
1	A	319	ASN
1	A	324	ASN
1	A	336	GLN
1	A	343	HIS

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Mol	Chain	Res	Type
1	A	348	GLN
1	A	368	ASN
1	A	373	ASN
1	A	375	ASN
1	A	384	ASN
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	563	ASN
1	A	600	ASN
1	A	602	HIS
1	A	613	GLN
1	A	629	ASN
1	A	639	GLN
1	A	724	GLN
1	A	760	GLN
1	A	771	ASN
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	878	GLN
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
1	B	127	ASN
1	B	140	GLN
1	B	150	GLN
1	B	186	GLN
1	B	196	GLN
1	B	314	ASN
1	B	316	GLN

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Mol	Chain	Res	Type
1	B	319	ASN
1	B	324	ASN
1	B	336	GLN
1	B	343	HIS
1	B	348	GLN
1	B	375	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	781	GLN
1	B	786	GLN
1	B	817	GLN
1	B	833	GLN
1	B	878	GLN
1	B	893	GLN
1	B	914	GLN
1	B	958	ASN
1	B	968	ASN
1	B	1047	HIS
1	B	1059	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
5	2HP	A	1108	-	4,4,4	5.64	2 (50%)	6,6,6	0.79	0
3	GTP	A	1106	4	26,34,34	1.08	2 (7%)	32,54,54	1.47	5 (15%)
6	POP	B	1107	-	6,8,8	0.72	0	13,13,13	1.25	1 (7%)
6	POP	A	1109	-	6,8,8	0.80	0	13,13,13	1.30	1 (7%)
5	2HP	B	1106	-	4,4,4	5.64	2 (50%)	6,6,6	0.95	0
4	G	A	1107	3	18,25,26	1.03	2 (11%)	19,37,40	0.94	1 (5%)

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	B	1107	-	-	0/6/6/6	-
6	POP	A	1109	-	-	2/6/6/6	-
3	GTP	A	1106	4	-	4/18/38/38	0/3/3/3
4	G	A	1107	3	-	0/3/25/26	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1108	2HP	P-O3	8.01	1.78	1.54
5	B	1106	2HP	P-O3	7.99	1.78	1.54
5	B	1106	2HP	P-O4	7.89	1.78	1.54
5	A	1108	2HP	P-O4	7.87	1.78	1.54
3	A	1106	GTP	C5-C6	-3.71	1.39	1.47
4	A	1107	G	C5-C6	-2.41	1.42	1.47
4	A	1107	G	C8-N7	-2.33	1.31	1.35
3	A	1106	GTP	C2-N3	2.18	1.38	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1106	GTP	PB-O3B-PG	-4.00	119.11	132.83
6	A	1109	POP	P2-O-P1	-3.20	121.86	132.83
3	A	1106	GTP	C5-C6-N1	3.14	119.50	113.95
6	B	1107	POP	P2-O-P1	-3.03	122.42	132.83
3	A	1106	GTP	C8-N7-C5	3.01	108.72	102.99
3	A	1106	GTP	C2-N1-C6	-2.63	120.25	125.10
4	A	1107	G	O6-C6-C5	2.09	128.46	124.37
3	A	1106	GTP	O6-C6-C5	-2.02	120.43	124.37

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

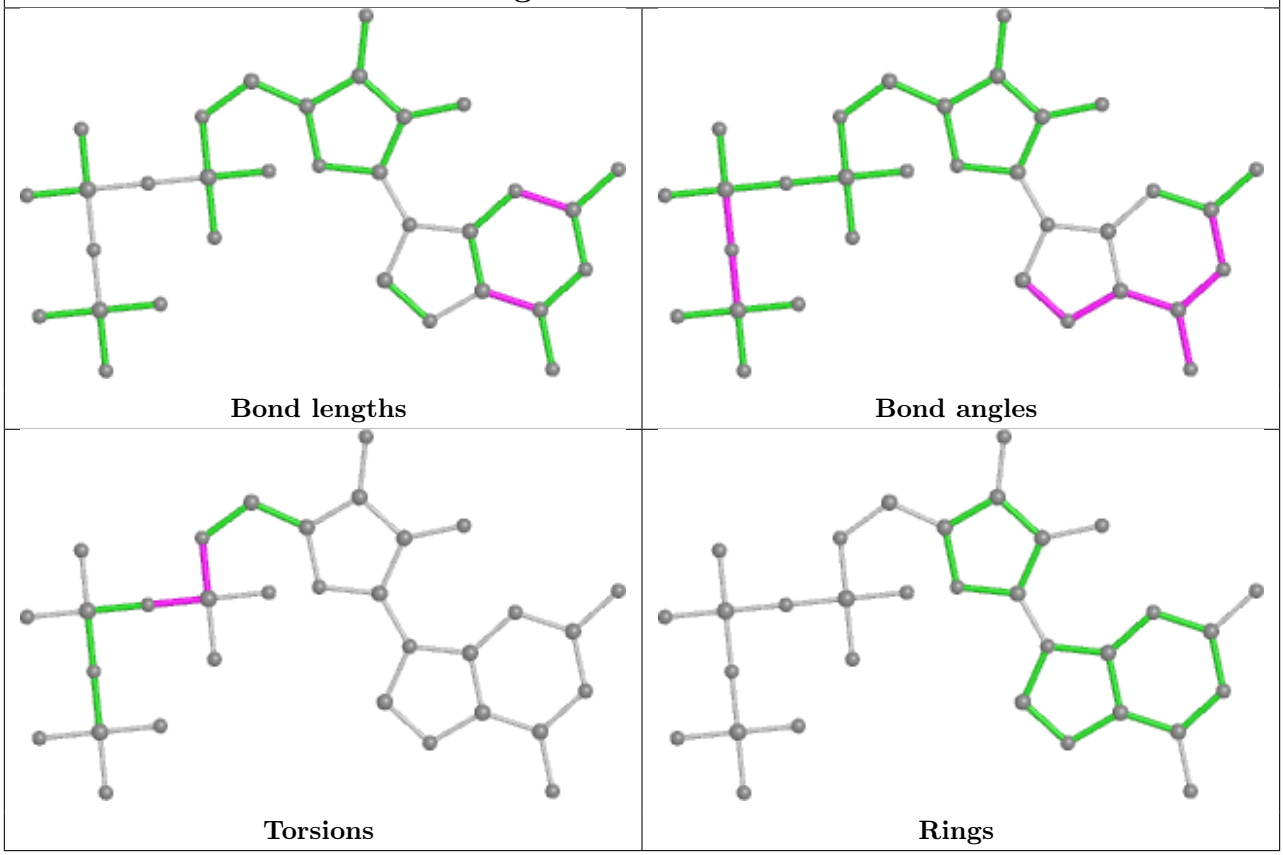
There are no ring outliers.

3 monomers are involved in 4 short contacts:

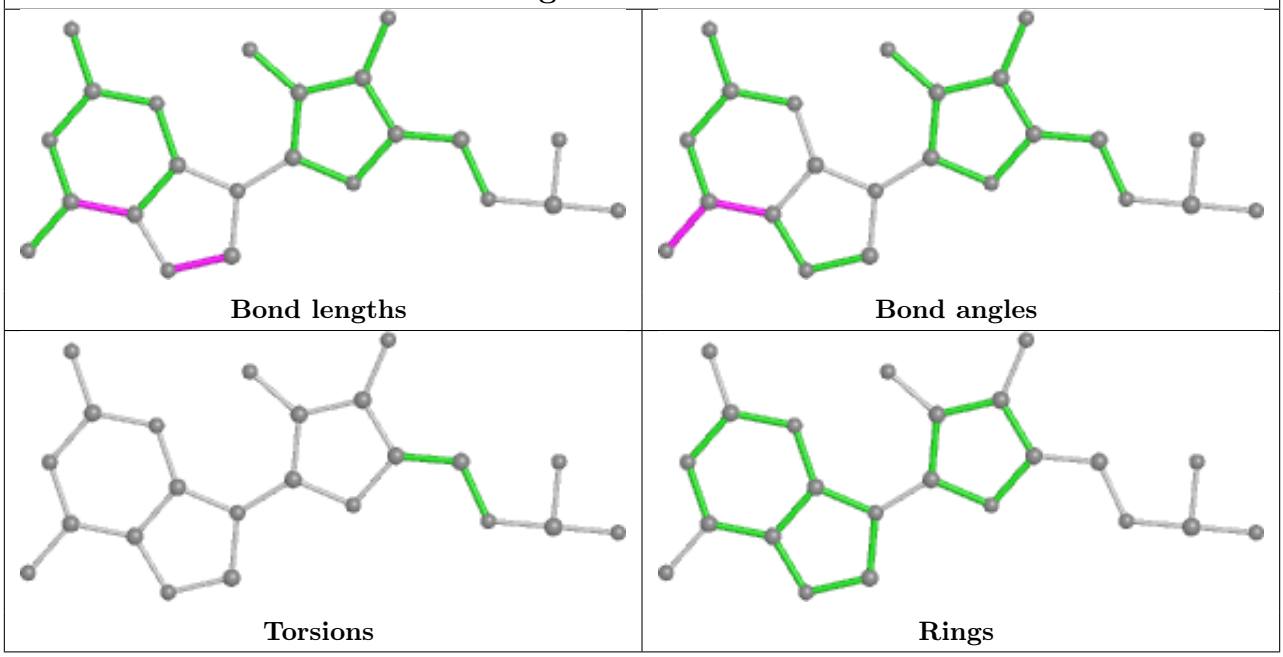
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1109	POP	2	0
5	B	1106	2HP	1	0
4	A	1107	G	1	0

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 then 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.

Ligand GTP A 1106



Ligand G A 1107



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(Å^2)	Q<0.9
1	A	1095/1117 (98%)	0.22	56 (5%)	28	22	16, 29, 53, 79	0
1	B	1094/1117 (97%)	0.26	70 (6%)	19	15	17, 27, 54, 84	0
2	C	21/36 (58%)	0.02	2 (9%)	8	6	29, 33, 59, 102	0
2	D	22/36 (61%)	0.07	2 (9%)	9	7	24, 38, 60, 88	0
All	All	2232/2306 (96%)	0.24	130 (5%)	23	18	16, 28, 54, 102	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	23	DT	8.2
1	B	723	LYS	6.3
1	A	1018	GLU	6.2
1	B	727	SER	6.1
1	A	726	ALA	5.8
1	B	677	ILE	5.6
1	B	768	GLY	5.6
1	B	1014	TYR	5.2
1	A	264	PRO	5.1
1	A	1014	TYR	5.0
1	B	725	ALA	4.9
1	B	264	PRO	4.9
1	A	1015	ASP	4.9
2	D	23	DT	4.8
1	B	708	ARG	4.8
1	B	713	ASN	4.6
1	B	714	ILE	4.5
1	B	724	GLN	4.4
1	A	910	TYR	4.4
1	B	729	ALA	4.2
1	A	729	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	1099	LYS	3.9
1	B	704	VAL	3.8
1	A	7	GLU	3.7
1	A	28	GLU	3.6
1	B	5	THR	3.6
1	B	726	ALA	3.5
1	B	767	LYS	3.5
1	A	727	SER	3.4
1	A	711	ASP	3.4
1	B	711	ASP	3.4
1	A	754	LYS	3.3
1	A	767	LYS	3.3
1	B	769	LYS	3.3
1	B	770	ILE	3.3
1	A	265	ASP	3.3
1	A	725	ALA	3.2
1	B	706	LYS	3.2
1	A	768	GLY	3.2
1	B	678	TYR	3.2
1	A	188	LEU	3.2
1	B	1018	GLU	3.2
1	B	718	MET	3.2
1	B	730	HIS	3.1
1	A	707	ALA	3.1
1	A	8	LEU	3.1
1	A	713	ASN	3.1
1	A	658	GLU	3.0
1	B	70	LEU	3.0
1	B	910	TYR	3.0
1	A	708	ARG	3.0
1	B	734	LEU	3.0
1	B	764	THR	2.9
2	D	2	DA	2.9
1	B	707	ALA	2.9
1	B	192	GLY	2.9
1	B	715	SER	2.9
1	A	710	LYS	2.9
1	B	42	GLU	2.8
1	B	710	LYS	2.8
1	A	712	PRO	2.8
1	B	1015	ASP	2.7
1	A	10	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	42	GLU	2.7
1	B	6	GLU	2.7
1	B	406	GLU	2.7
1	B	705	LEU	2.7
1	B	8	LEU	2.7
1	A	1034	ARG	2.7
1	A	719	ALA	2.6
1	B	899	LEU	2.6
1	A	723	LYS	2.6
1	B	712	PRO	2.6
1	A	1098	ARG	2.6
1	A	657	GLY	2.6
1	B	1016	GLN	2.6
1	A	753	ARG	2.6
1	B	719	ALA	2.5
1	A	1100	GLN	2.5
1	A	406	GLU	2.5
1	A	730	HIS	2.5
1	A	267	LYS	2.5
1	B	370	GLU	2.5
1	B	754	LYS	2.5
1	B	191	GLU	2.4
1	B	260	SER	2.4
1	B	102	ILE	2.4
1	B	265	ASP	2.4
1	A	714	ILE	2.4
1	A	1025	ILE	2.4
1	B	1096	GLU	2.3
1	B	1019	ASN	2.3
1	B	371	LEU	2.3
1	B	765	GLY	2.2
1	B	262	ILE	2.2
1	A	43	GLU	2.2
1	B	281	PHE	2.2
1	B	28	GLU	2.2
1	B	722	GLY	2.2
1	A	1031	LEU	2.2
1	B	763	GLY	2.2
2	C	3	DT	2.2
1	A	26	LYS	2.2
1	B	74	LYS	2.2
1	B	772	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	75	GLU	2.1
1	A	1017	ARG	2.1
1	A	932	MET	2.1
1	A	262	ILE	2.1
1	B	1070	ASN	2.1
1	B	7	GLU	2.1
1	B	242	ILE	2.1
1	A	371	LEU	2.1
1	B	766	ALA	2.1
1	B	932	MET	2.1
1	B	240	ALA	2.1
1	A	75	GLU	2.1
1	A	1096	GLU	2.1
1	B	323	ARG	2.1
1	A	70	LEU	2.1
1	A	706	LYS	2.1
1	B	261	GLU	2.0
1	A	752	LYS	2.0
1	A	281	PHE	2.0
1	A	733	GLU	2.0
1	A	770	ILE	2.0
1	A	718	MET	2.0
1	B	1098	ARG	2.0
1	A	1002	GLU	2.0
1	B	728	GLU	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 monosaccharides in this entry.

6.4 Ligands (i)

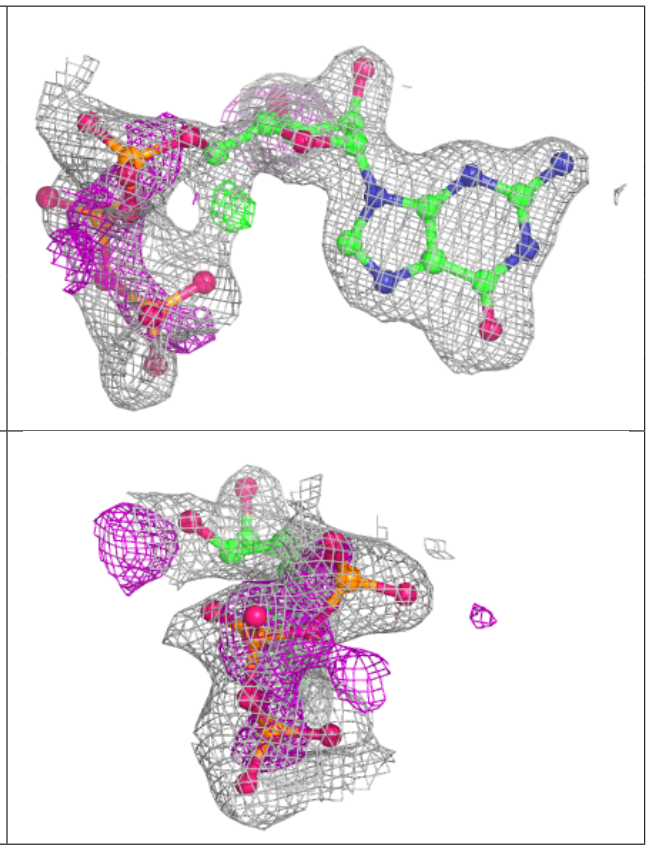
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	POP	A	1109	9/9	0.69	0.32	95,95,95,95	0
6	POP	B	1107	9/9	0.73	0.28	72,72,73,73	0
3	GTP	A	1106	32/32	0.78	0.18	44,51,72,73	0
4	G	A	1107	23/24	0.78	0.17	36,39,48,49	0
5	2HP	B	1106	5/5	0.88	0.23	42,43,43,43	0
5	2HP	A	1108	5/5	0.96	0.08	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.

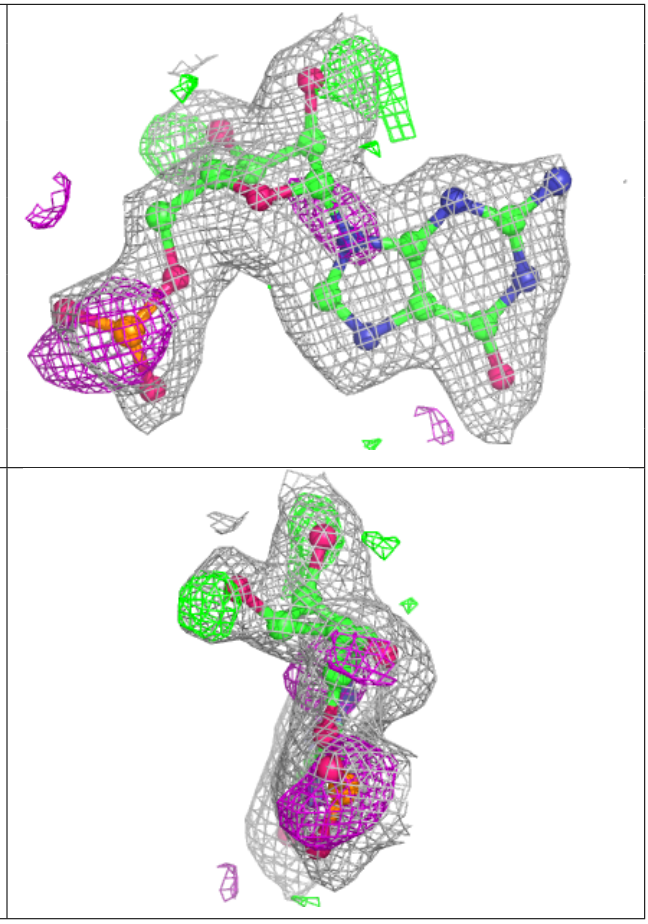
Electron density around GTP A 1106:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



Electron density around G A 1107:

$2mF_o$-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.