



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 08:11 PM UTC

PDB ID : 3Q23 / pdb_00003q23
Title : X-ray crystal structure of the N4 mini-VRNAP and P2_7a promoter transcription initiation complex with GMPCPP and Manganese: sustrate complex II
Authors : Gleghorn, M.L.; Murakami, K.S.
Deposited on : 2010-12-19
Resolution : 1.80 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

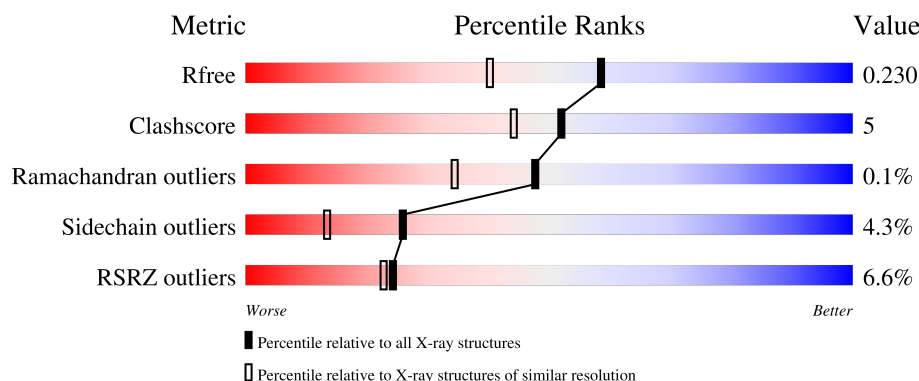
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 $\leq 5\%$. 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	1118	7% 86% 10% ..
1	B	1118	6% 86% 11% ..
2	C	36	50% 6% 44%
2	D	36	3% 56% 42%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20493 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			

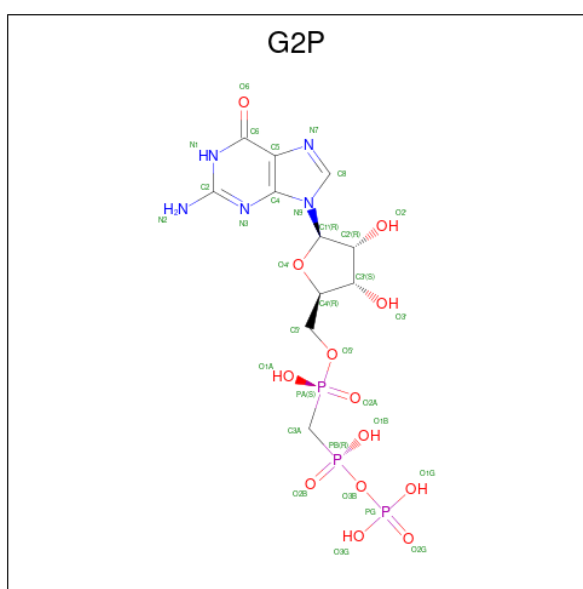
There are 24 discrepancies between the modelled and reference sequences:

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	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 PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: G2P) (formula: C₁₁H₁₈N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			32	11	5	13	3		
3	A	1	Total	C	N	O	P	0	0
			32	11	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			32	11	5	13	3		
3	B	1	Total	C	N	O	P	0	0
			32	11	5	13	3		

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

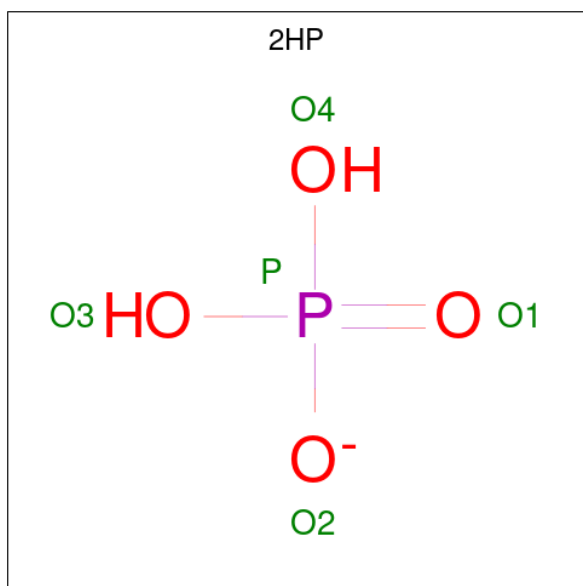
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mn	0	0
			2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Mn	0	0
			2	2		

- 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		

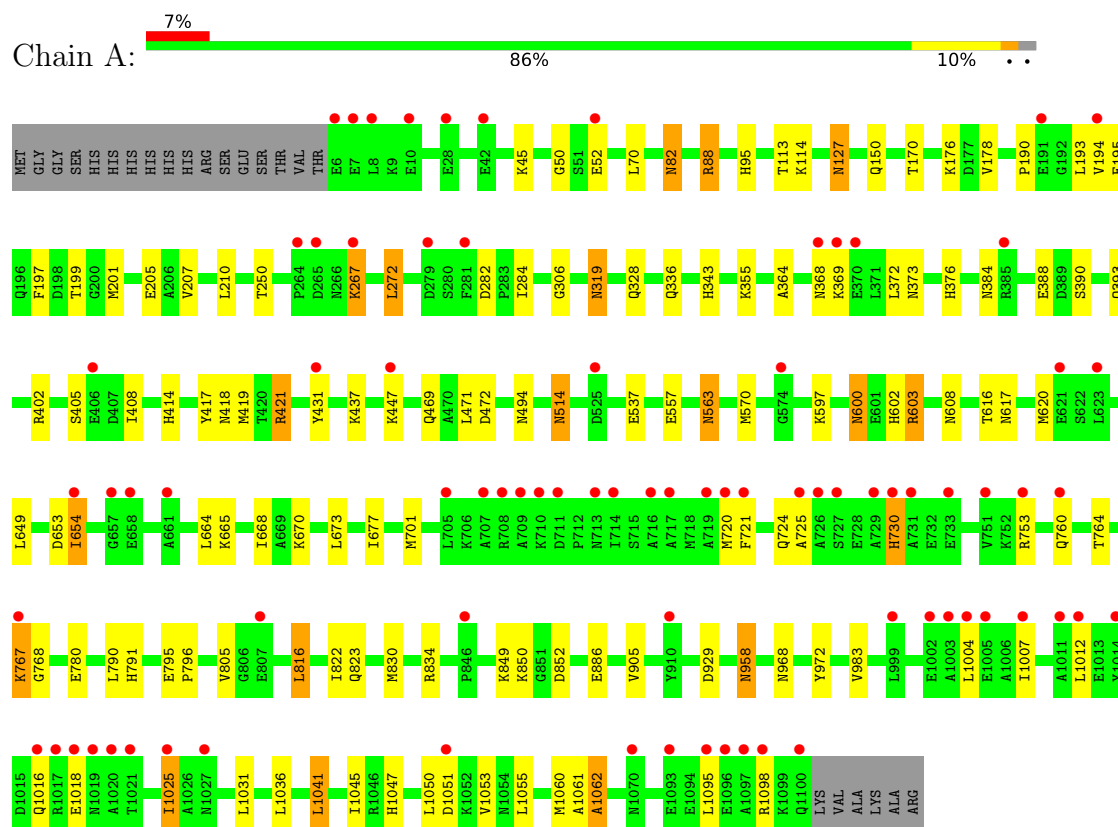
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1187	Total	O	0	0
			1187	1187		
6	C	92	Total	O	0	0
			92	92		
6	B	1240	Total	O	0	0
			1240	1240		
6	D	107	Total	O	0	0
			107	107		

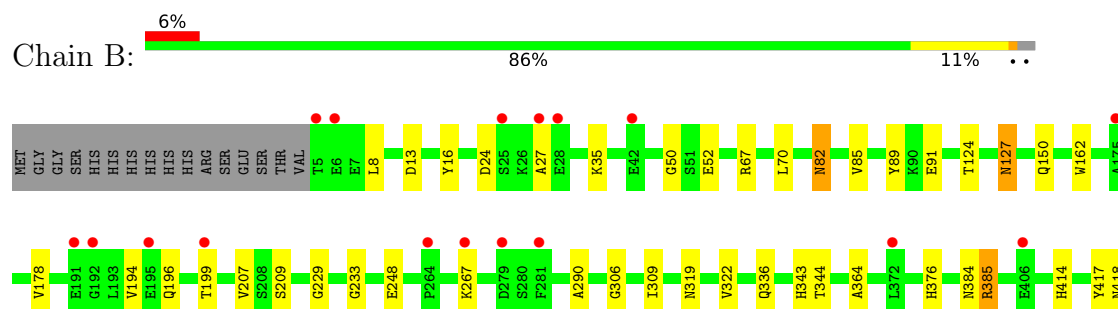
3 Residue-property plots [i](#)

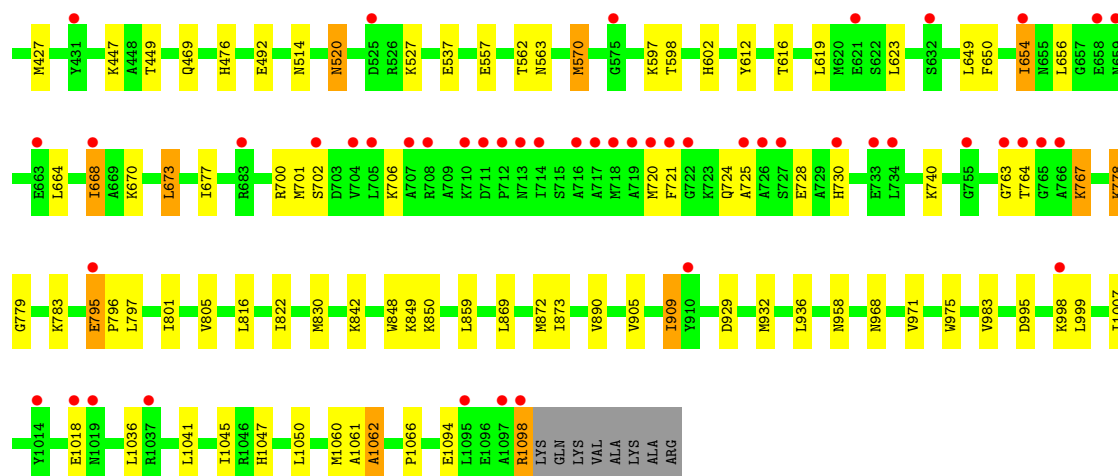
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



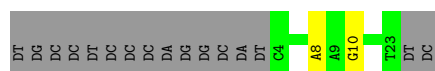
• Molecule 1: Virion RNA polymerase





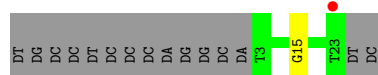
- Molecule 2: DNA (5'-D(*TP*GP*CP*CP*TP*CP*CP*CP*AP*GP*GP*CP*AP*TP*CP*CP*AP*AP*AP*AP*GP*AP*AP*GP*CP*GP*GP*AP*GP*CP*TP*TP*CP*TP*TP*C)-3')

Chain C: 50% 6% 44%



- 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: 3% 56% 42%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.83Å 111.86Å 276.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 50.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-1.80) 98.9 (50.00-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019, CNS	Depositor
R, R_{free}	0.200 , 0.231 0.198 , 0.230	Depositor DCC
R_{free} test set	11758 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20493	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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: MN, 2HP, G2P

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	0.45	0/8583	0.78	2/11609 (0.0%)
1	B	0.46	0/8572	0.79	0/11596
2	C	0.23	0/445	0.76	0/685
2	D	0.23	0/485	0.78	0/746
All	All	0.45	0/18085	0.78	2/24636 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	852	ASP	N-CA-C	-6.83	100.17	110.28
1	A	563	ASN	N-CA-C	5.02	116.44	110.97

There are no chirality outliers.

There are no planarity outliers.

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	90	0
1	B	8443	0	8465	86	0
2	C	396	0	211	2	0
2	D	432	0	236	1	0
3	A	64	0	27	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	64	0	27	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	5	0	0	0	0
5	B	5	0	0	1	0
6	A	1187	0	0	9	0
6	B	1240	0	0	13	0
6	C	92	0	0	2	0
6	D	107	0	0	1	0
All	All	20493	0	17445	179	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 5.

All (179) 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:385:ARG:HH11	1:B:385:ARG:HG2	1.14	1.12
1:B:469:GLN:HE22	1:B:557:GLU:H	1.10	1.00
1:A:469:GLN:HE22	1:A:557:GLU:H	1.13	0.97
1:A:603:ARG:NH1	1:A:608:ASN:OD1	2.06	0.89
1:B:322:VAL:HG22	1:B:872:MET:HE1	1.56	0.86
1:A:753:ARG:HG2	1:A:753:ARG:HH11	1.41	0.85
1:A:972:TYR:OH	1:A:1051:ASP:OD1	1.95	0.84
1:B:336:GLN:HE21	1:B:417:TYR:H	1.22	0.83
1:A:336:GLN:HE21	1:A:417:TYR:H	1.24	0.82
1:B:673:LEU:HD13	1:B:801:ILE:HG23	1.61	0.81
1:B:385:ARG:HG2	1:B:385:ARG:NH1	1.91	0.79
1:A:767:LYS:HE3	1:A:768:GLY:H	1.47	0.78
1:B:385:ARG:HH11	1:B:385:ARG:CG	1.95	0.77
1:B:932:MET:SD	6:B:2682:HOH:O	2.43	0.76
1:A:603:ARG:HB3	1:A:603:ARG:HH11	1.50	0.73
1:B:721:PHE:HA	1:B:724:GLN:HE21	1.54	0.72
1:A:968:ASN:HD21	1:A:1060:MET:H	1.37	0.72
1:B:654:ILE:HD11	1:B:668:ILE:HG21	1.72	0.71
1:A:701:MET:HA	1:A:701:MET:HE2	1.75	0.69
1:A:850:LYS:HB3	6:A:2255:HOH:O	1.93	0.68
1:B:449:THR:H	1:B:958:ASN:HD21	1.40	0.68
1:B:616:THR:HG23	1:B:664:LEU:HB2	1.75	0.68
1:A:178:VAL:HG21	1:A:194:VAL:HA	1.73	0.68
1:A:721:PHE:HA	1:A:724:GLN:HE21	1.59	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:ARG:HD2	6:C:29:HOH:O	1.93	0.67
1:A:753:ARG:HG2	1:A:753:ARG:NH1	2.08	0.66
1:A:958:ASN:H	1:A:958:ASN:HD22	1.43	0.66
1:B:968:ASN:HD21	1:B:1060:MET:H	1.44	0.66
1:B:995:ASP:OD2	1:B:998:LYS:HG2	1.95	0.65
1:A:82:ASN:HD22	1:A:82:ASN:C	2.05	0.65
1:A:418:ASN:HB2	6:A:1738:HOH:O	1.96	0.65
1:A:195:GLU:O	1:A:199:THR:HG23	1.95	0.65
1:A:364:ALA:H	1:A:384:ASN:ND2	1.96	0.64
1:A:402:ARG:HA	1:A:408:ILE:HG22	1.78	0.64
1:A:364:ALA:H	1:A:384:ASN:HD21	1.44	0.64
1:B:795:GLU:HB3	1:B:796:PRO:HD3	1.81	0.63
1:B:364:ALA:H	1:B:384:ASN:HD21	1.47	0.63
1:A:753:ARG:HH21	1:A:760:GLN:HE22	1.47	0.62
1:B:364:ALA:H	1:B:384:ASN:ND2	1.96	0.62
1:B:91:GLU:HG3	6:B:2109:HOH:O	2.00	0.62
1:A:830:MET:O	1:A:834:ARG:HG3	1.99	0.61
1:B:570:MET:HE3	1:B:975:TRP:HB3	1.82	0.61
1:A:617:ASN:HA	1:A:620:MET:HE3	1.83	0.61
1:B:127:ASN:HD22	1:B:127:ASN:H	1.48	0.61
1:A:45:LYS:HE3	6:A:1226:HOH:O	2.02	0.60
1:B:830:MET:HE3	1:B:999:LEU:HD23	1.82	0.60
1:B:650:PHE:HE2	1:B:700:ARG:HG3	1.67	0.60
1:A:603:ARG:NH1	1:A:603:ARG:HB3	2.17	0.60
1:A:968:ASN:ND2	1:A:1060:MET:H	1.99	0.60
1:A:207:VAL:HG11	1:A:905:VAL:HG21	1.82	0.59
1:A:670:LYS:NZ	3:A:1108:G2P:H3A1	2.17	0.59
1:B:196:GLN:O	1:B:199:THR:HG22	2.02	0.59
1:B:16:TYR:O	1:B:35:LYS:HE3	2.03	0.58
1:B:13:ASP:HA	1:B:35:LYS:HE2	1.86	0.58
1:A:886:GLU:O	2:C:8:DA:H4'	2.02	0.58
1:B:492:GLU:HG3	6:B:2683:HOH:O	2.03	0.58
1:B:476:HIS:ND1	5:B:1111:2HP:O2	2.32	0.57
1:B:816:LEU:HD13	1:B:983:VAL:HG21	1.86	0.57
1:A:616:THR:CG2	1:A:664:LEU:HB2	2.33	0.57
1:A:701:MET:HE1	1:A:720:MET:HE2	1.86	0.56
1:A:469:GLN:NE2	1:A:557:GLU:H	1.94	0.56
1:A:1012:LEU:HD11	1:A:1025:ILE:HG22	1.87	0.56
1:A:790:LEU:O	1:A:795:GLU:HG2	2.07	0.55
1:B:162:TRP:HE1	1:B:209:SER:HB2	1.70	0.55
1:A:597:LYS:NZ	1:A:602:HIS:HD2	2.05	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:597:LYS:NZ	1:B:602:HIS:HD2	2.05	0.54
1:A:52:GLU:H	1:A:52:GLU:CD	2.15	0.54
1:B:616:THR:CG2	1:B:664:LEU:HB2	2.38	0.54
1:A:653:ASP:HB2	1:A:668:ILE:HG23	1.89	0.54
1:A:795:GLU:HB2	1:A:796:PRO:HD3	1.89	0.54
1:B:848:TRP:CH2	1:B:850:LYS:HA	2.42	0.54
1:B:447:LYS:HE2	6:B:1947:HOH:O	2.06	0.54
1:B:701:MET:HE2	1:B:701:MET:HA	1.90	0.54
1:B:82:ASN:C	1:B:82:ASN:HD22	2.16	0.53
1:B:469:GLN:HE22	1:B:557:GLU:N	1.93	0.53
1:B:701:MET:HE1	1:B:720:MET:HE2	1.89	0.53
1:A:127:ASN:HD22	1:A:127:ASN:H	1.54	0.53
1:B:968:ASN:ND2	1:B:1060:MET:H	2.04	0.53
1:B:520:ASN:HD21	1:B:527:LYS:NZ	2.06	0.53
1:A:822:ILE:HG12	1:A:1007:ILE:HG23	1.91	0.52
1:B:207:VAL:HG11	1:B:905:VAL:HG21	1.92	0.52
1:B:1045:ILE:HD12	1:B:1094:GLU:HG3	1.91	0.52
1:B:995:ASP:CG	1:B:998:LYS:HG2	2.35	0.52
1:B:309:ILE:HB	6:B:2853:HOH:O	2.09	0.52
1:B:469:GLN:NE2	1:B:557:GLU:H	1.93	0.52
1:A:150:GLN:HG2	6:A:2213:HOH:O	2.09	0.51
1:A:469:GLN:HE22	1:A:557:GLU:N	1.95	0.51
1:A:343:HIS:HE1	1:A:537:GLU:OE2	1.92	0.51
1:A:570:MET:O	1:A:1047:HIS:HE1	1.94	0.51
1:A:816:LEU:HD13	1:A:983:VAL:HG21	1.91	0.51
1:B:178:VAL:HG21	1:B:194:VAL:HA	1.91	0.51
1:A:88:ARG:HD3	1:A:282:ASP:OD1	2.11	0.51
1:A:725:ALA:HB1	1:A:730:HIS:HB3	1.94	0.50
1:A:355:LYS:HD2	1:A:388:GLU:HG3	1.94	0.50
1:A:616:THR:HG22	1:A:620:MET:HE2	1.92	0.49
1:A:1047:HIS:HD2	6:A:1227:HOH:O	1.94	0.49
1:B:562:THR:HG22	1:B:612:TYR:CE1	2.47	0.49
1:B:229:GLY:O	1:B:233:GLY:HA3	2.13	0.49
3:B:1108:G2P:N7	6:B:1719:HOH:O	2.35	0.49
1:A:600:ASN:ND2	1:A:600:ASN:H	2.11	0.49
3:A:1111:G2P:N7	6:A:2285:HOH:O	2.35	0.48
1:A:563:ASN:HD21	1:A:929:ASP:HB3	1.78	0.48
1:B:725:ALA:HB1	1:B:730:HIS:HB3	1.95	0.48
1:B:849:LYS:HE3	6:B:2173:HOH:O	2.13	0.48
1:B:822:ILE:HG12	1:B:1007:ILE:HG23	1.97	0.47
6:A:1403:HOH:O	2:C:10:DG:H5'	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:GLN:HG2	1:A:431:TYR:HB2	1.97	0.47
1:B:343:HIS:HE1	1:B:537:GLU:OE2	1.97	0.47
1:B:50:GLY:H	1:B:150:GLN:NE2	2.13	0.46
1:A:849:LYS:HE3	6:A:1340:HOH:O	2.15	0.46
1:B:816:LEU:CD1	1:B:983:VAL:HG21	2.45	0.46
1:A:437:LYS:NZ	3:A:1111:G2P:O1A	2.46	0.46
1:A:1012:LEU:HB3	1:A:1016:GLN:HB2	1.97	0.46
1:A:50:GLY:H	1:A:150:GLN:NE2	2.13	0.46
1:B:344:THR:HG23	6:B:2334:HOH:O	2.16	0.46
1:B:673:LEU:CD1	1:B:801:ILE:HG23	2.39	0.46
1:B:1061:ALA:O	1:B:1062:ALA:HB2	2.16	0.46
1:A:670:LYS:HZ1	3:A:1108:G2P:H3A1	1.80	0.46
1:B:91:GLU:HG2	6:B:1977:HOH:O	2.15	0.46
1:B:1047:HIS:HD2	6:B:1777:HOH:O	1.98	0.46
1:A:1061:ALA:O	1:A:1062:ALA:HB2	2.17	0.45
1:A:170:THR:HG22	1:A:201:MET:HE3	1.99	0.45
1:A:328:GLN:HG2	1:A:419:MET:HE3	1.98	0.45
1:B:763:GLY:HA2	6:B:2238:HOH:O	2.16	0.45
2:D:15:DG:H5"	6:D:2496:HOH:O	2.16	0.45
1:A:958:ASN:HD22	1:A:958:ASN:N	2.13	0.45
1:B:764:THR:HG23	6:B:2337:HOH:O	2.16	0.45
1:A:654:ILE:CD1	1:A:668:ILE:HG21	2.47	0.45
1:B:778:LYS:HD3	1:B:779:GLY:H	1.82	0.45
1:A:665:LYS:O	1:A:668:ILE:HG13	2.17	0.44
1:B:449:THR:H	1:B:958:ASN:ND2	2.13	0.44
1:A:306:GLY:O	1:A:414:HIS:HE1	2.00	0.44
1:B:1094:GLU:O	1:B:1098:ARG:HG3	2.17	0.44
1:B:677:ILE:HD11	1:B:805:VAL:HG11	1.99	0.44
1:B:932:MET:HE2	1:B:971:VAL:HG22	1.99	0.44
1:A:654:ILE:HD11	1:A:668:ILE:HG21	1.98	0.44
1:B:24:ASP:HB3	1:B:27:ALA:HB2	2.00	0.44
1:A:319:ASN:OD1	1:A:421:ARG:HG2	2.18	0.44
1:B:418:ASN:HB2	6:B:2165:HOH:O	2.18	0.44
1:B:267:LYS:HA	1:B:267:LYS:HE2	1.99	0.43
1:A:384:ASN:HD22	1:A:384:ASN:HA	1.65	0.43
1:A:1012:LEU:HD22	1:A:1016:GLN:NE2	2.33	0.43
1:A:421:ARG:CD	6:C:29:HOH:O	2.60	0.43
1:B:842:LYS:HB3	1:B:848:TRP:CD2	2.53	0.43
1:B:890:VAL:HG11	1:B:909:ILE:HD11	1.99	0.43
1:B:563:ASN:HD21	1:B:929:ASP:HB3	1.83	0.43
1:A:603:ARG:NE	6:A:2211:HOH:O	2.42	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:616:THR:CG2	1:A:664:LEU:CB	2.96	0.43
1:B:570:MET:O	1:B:1047:HIS:HE1	2.02	0.43
1:B:619:LEU:HD22	1:B:797:LEU:HD13	1.99	0.43
1:A:267:LYS:HB2	1:A:267:LYS:HE2	1.76	0.43
1:A:306:GLY:O	1:A:414:HIS:CE1	2.72	0.43
1:B:50:GLY:H	1:B:150:GLN:HE22	1.66	0.42
1:B:598:THR:HG22	1:B:1066:PRO:HD3	2.01	0.42
1:B:89:TYR:CZ	1:B:290:ALA:HB3	2.54	0.42
1:B:306:GLY:O	1:B:414:HIS:CE1	2.73	0.42
1:B:376:HIS:HD2	1:B:702:SER:OG	2.02	0.42
1:A:373:ASN:HD22	1:A:376:HIS:H	1.67	0.42
1:A:514:ASN:HD22	1:A:514:ASN:H	1.67	0.42
1:A:190:PRO:HD2	1:A:193:LEU:HD22	2.02	0.42
1:A:201:MET:HE2	1:A:205:GLU:HG2	2.00	0.42
1:A:1041:LEU:O	1:A:1045:ILE:HG12	2.20	0.42
1:A:603:ARG:HH11	1:A:603:ARG:CB	2.25	0.42
1:A:319:ASN:HD22	1:A:319:ASN:HA	1.71	0.41
1:B:82:ASN:ND2	1:B:85:VAL:H	2.19	0.41
1:A:791:HIS:HA	1:A:795:GLU:HG3	2.03	0.41
1:B:650:PHE:CE2	1:B:700:ARG:HG3	2.51	0.41
1:B:767:LYS:O	1:B:767:LYS:HE2	2.20	0.41
1:A:600:ASN:H	1:A:600:ASN:HD22	1.68	0.41
1:A:197:PHE:HA	1:A:272:LEU:HD21	2.02	0.41
1:B:873:ILE:HD13	1:B:983:VAL:HG22	2.02	0.41
1:B:612:TYR:CE1	1:B:670:LYS:HG3	2.55	0.41
1:A:677:ILE:HD11	1:A:805:VAL:HG11	2.03	0.41
1:A:113:THR:HG22	1:A:114:LYS:HG3	2.02	0.40
1:A:267:LYS:HD3	1:A:267:LYS:N	2.37	0.40
1:A:95:HIS:HA	1:B:248:GLU:O	2.22	0.40
1:B:654:ILE:CD1	1:B:668:ILE:HG21	2.47	0.40
1:B:127:ASN:HD22	1:B:127:ASN:N	2.15	0.40
1:A:823:GLN:HE21	1:A:823:GLN:HB2	1.69	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	1093/1118 (98%)	1072 (98%)	20 (2%)	1 (0%)	48	34
1	B	1092/1118 (98%)	1074 (98%)	17 (2%)	1 (0%)	48	34
All	All	2185/2236 (98%)	2146 (98%)	37 (2%)	2 (0%)	48	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1062	ALA
1	A	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%)	872 (95%)	44 (5%)	23	11
1	B	915/935 (98%)	880 (96%)	35 (4%)	29	17
All	All	1831/1870 (98%)	1752 (96%)	79 (4%)	26	13

All (79) 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	176	LYS
1	A	210	LEU
1	A	250	THR
1	A	267	LYS
1	A	272	LEU
1	A	284	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	319	ASN
1	A	368	ASN
1	A	369	LYS
1	A	372	LEU
1	A	390	SER
1	A	405	SER
1	A	421	ARG
1	A	447	LYS
1	A	471	LEU
1	A	472	ASP
1	A	494	ASN
1	A	514	ASN
1	A	600	ASN
1	A	603	ARG
1	A	649	LEU
1	A	654	ILE
1	A	673	LEU
1	A	730	HIS
1	A	764	THR
1	A	767	LYS
1	A	780	GLU
1	A	816	LEU
1	A	958	ASN
1	A	1004	LEU
1	A	1018	GLU
1	A	1025	ILE
1	A	1031	LEU
1	A	1036	LEU
1	A	1041	LEU
1	A	1050	LEU
1	A	1053	VAL
1	A	1055	LEU
1	A	1095	LEU
1	A	1098	ARG
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	319	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	385	ARG
1	B	427	MET
1	B	514	ASN
1	B	520	ASN
1	B	570	MET
1	B	623	LEU
1	B	649	LEU
1	B	654	ILE
1	B	656	LEU
1	B	668	ILE
1	B	673	LEU
1	B	706	LYS
1	B	728	GLU
1	B	740	LYS
1	B	767	LYS
1	B	778	LYS
1	B	783	LYS
1	B	795	GLU
1	B	859	LEU
1	B	869	LEU
1	B	909	ILE
1	B	936	LEU
1	B	1018	GLU
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 (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	A	127	ASN
1	A	150	GLN
1	A	169	ASN
1	A	186	GLN
1	A	324	ASN
1	A	336	GLN
1	A	343	HIS
1	A	348	GLN
1	A	368	ASN
1	A	373	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	375	ASN
1	A	384	ASN
1	A	404	GLN
1	A	414	HIS
1	A	455	GLN
1	A	456	ASN
1	A	457	ASN
1	A	464	GLN
1	A	469	GLN
1	A	494	ASN
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	760	GLN
1	A	781	GLN
1	A	803	GLN
1	A	815	GLN
1	A	823	GLN
1	A	833	GLN
1	A	856	GLN
1	A	863	GLN
1	A	893	GLN
1	A	954	ASN
1	A	958	ASN
1	A	968	ASN
1	A	982	ASN
1	A	1035	ASN
1	A	1038	ASN
1	A	1047	HIS
1	A	1059	GLN
1	B	82	ASN
1	B	127	ASN
1	B	140	GLN
1	B	150	GLN
1	B	196	GLN
1	B	225	ASN
1	B	255	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	376	HIS
1	B	384	ASN
1	B	393	GLN
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	724	GLN
1	B	760	GLN
1	B	786	GLN
1	B	833	GLN
1	B	856	GLN
1	B	892	ASN
1	B	914	GLN
1	B	954	ASN
1	B	958	ASN
1	B	968	ASN
1	B	1047	HIS
1	B	1059	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 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	G2P	B	1109	4	30,34,34	1.27	4 (13%)	46,54,54	1.77	14 (30%)
5	2HP	B	1111	-	4,4,4	5.84	2 (50%)	6,6,6	0.93	0
3	G2P	A	1108	4	30,34,34	1.13	2 (6%)	46,54,54	1.71	11 (23%)
3	G2P	B	1108	4	30,34,34	1.12	3 (10%)	46,54,54	1.69	10 (21%)
5	2HP	A	1110	-	4,4,4	5.77	2 (50%)	6,6,6	0.81	0
3	G2P	A	1111	4	30,34,34	1.13	3 (10%)	46,54,54	1.72	11 (23%)

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	G2P	B	1109	4	-	6/19/38/38	0/3/3/3
3	G2P	A	1108	4	-	5/19/38/38	0/3/3/3
3	G2P	B	1108	4	-	5/19/38/38	0/3/3/3
3	G2P	A	1111	4	-	2/19/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1111	2HP	P-O4	8.26	1.78	1.54
5	B	1111	2HP	P-O3	8.17	1.78	1.54
5	A	1110	2HP	P-O3	8.12	1.78	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1110	2HP	P-O4	8.10	1.78	1.54
3	B	1109	G2P	PB-O3B	3.30	1.62	1.58
3	A	1108	G2P	PB-O3B	3.24	1.62	1.58
3	A	1111	G2P	PB-O3B	3.04	1.61	1.58
3	B	1108	G2P	PB-O3B	2.94	1.61	1.58
3	B	1109	G2P	C5'-C4'	2.82	1.60	1.51
3	B	1109	G2P	PA-O1A	-2.23	1.50	1.56
3	B	1108	G2P	PA-O1A	-2.12	1.51	1.56
3	A	1108	G2P	PA-O1A	-2.09	1.51	1.56
3	B	1109	G2P	PB-O1B	-2.05	1.51	1.56
3	A	1111	G2P	PA-O1A	-2.05	1.51	1.56
3	A	1111	G2P	PB-O1B	-2.01	1.51	1.56
3	B	1108	G2P	PB-O1B	-2.00	1.51	1.56

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1111	G2P	C5-C4-N3	-5.64	119.41	128.39
3	B	1108	G2P	C5-C4-N3	-5.38	119.82	128.39
3	B	1109	G2P	C5-C4-N3	-5.21	120.10	128.39
3	A	1111	G2P	C2-N3-C4	4.77	120.52	112.30
3	A	1108	G2P	C5-C4-N3	-4.71	120.89	128.39
3	B	1108	G2P	C2-N3-C4	4.69	120.37	112.30
3	B	1109	G2P	C2-N3-C4	4.57	120.18	112.30
3	A	1108	G2P	C2-N3-C4	4.35	119.78	112.30
3	B	1109	G2P	C2'-C1'-N9	-3.44	103.69	113.25
3	A	1108	G2P	C2'-C1'-N9	-3.30	104.08	113.25
3	A	1111	G2P	N9-C4-N3	3.27	132.49	125.95
3	B	1108	G2P	N9-C4-N3	3.13	132.22	125.95
3	B	1109	G2P	N9-C4-N3	2.77	131.50	125.95
3	A	1111	G2P	O1A-PA-O2A	2.71	118.76	109.95
3	A	1108	G2P	N9-C4-N3	2.66	131.28	125.95
3	B	1109	G2P	O1A-PA-O2A	2.64	118.56	109.95
3	A	1111	G2P	O1B-PB-O2B	2.59	118.38	109.95
3	B	1108	G2P	O1B-PB-O2B	2.50	118.07	109.95
3	A	1111	G2P	C2-N1-C6	-2.43	120.70	125.11
3	B	1109	G2P	C4-C5-N7	-2.43	106.82	110.67
3	B	1108	G2P	N9-C8-N7	-2.37	109.00	113.40
3	A	1108	G2P	N9-C8-N7	-2.37	109.01	113.40
3	B	1108	G2P	O6-C6-C5	-2.35	120.33	126.53
3	A	1108	G2P	C6-C5-N7	2.33	134.54	130.29
3	B	1108	G2P	C2-N1-C6	-2.33	120.88	125.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1111	G2P	C4-C5-N7	-2.32	106.99	110.67
3	B	1109	G2P	C2-N1-C6	-2.30	120.94	125.11
3	A	1111	G2P	C5-C6-N1	2.29	119.09	113.25
3	A	1108	G2P	C5-C6-N1	2.29	119.09	113.25
3	A	1111	G2P	O6-C6-C5	-2.28	120.52	126.53
3	B	1108	G2P	C4-C5-N7	-2.28	107.06	110.67
3	A	1108	G2P	PB-O3B-PG	-2.27	124.33	132.45
3	B	1109	G2P	PB-O3B-PG	-2.26	124.35	132.45
3	B	1108	G2P	C5-C6-N1	2.25	118.98	113.25
3	B	1108	G2P	O1A-PA-O2A	2.25	117.27	109.95
3	A	1111	G2P	N9-C8-N7	-2.23	109.27	113.40
3	B	1109	G2P	C5-C6-N1	2.18	118.81	113.25
3	B	1109	G2P	N9-C8-N7	-2.18	109.36	113.40
3	A	1108	G2P	C4-C5-N7	-2.15	107.27	110.67
3	A	1108	G2P	O1B-PB-O2B	2.11	116.81	109.95
3	B	1109	G2P	O1B-PB-O2B	2.07	116.69	109.95
3	A	1108	G2P	O1A-PA-O2A	2.05	116.62	109.95
3	B	1109	G2P	C6-C5-N7	2.04	134.00	130.29
3	A	1111	G2P	C8-N7-C5	2.03	107.88	104.26
3	B	1109	G2P	N2-C2-N1	2.03	121.04	116.76
3	B	1109	G2P	O6-C6-C5	-2.03	121.19	126.53

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1108	G2P	PB-O3B-PG-O1G
3	A	1108	G2P	PB-O3B-PG-O3G
3	A	1108	G2P	PA-C3A-PB-O3B
3	A	1108	G2P	PA-C3A-PB-O2B
3	A	1111	G2P	C5'-O5'-PA-O2A
3	B	1108	G2P	PB-C3A-PA-O1A
3	B	1108	G2P	PB-C3A-PA-O5'
3	B	1108	G2P	C5'-O5'-PA-O2A
3	B	1109	G2P	PB-O3B-PG-O1G
3	B	1109	G2P	PB-O3B-PG-O3G
3	B	1109	G2P	PA-C3A-PB-O3B
3	B	1109	G2P	PA-C3A-PB-O1B
3	B	1109	G2P	PA-C3A-PB-O2B
3	A	1108	G2P	PA-C3A-PB-O1B
3	A	1111	G2P	PB-C3A-PA-O1A
3	B	1108	G2P	PB-C3A-PA-O2A

Continued on next page...

Continued from previous page...

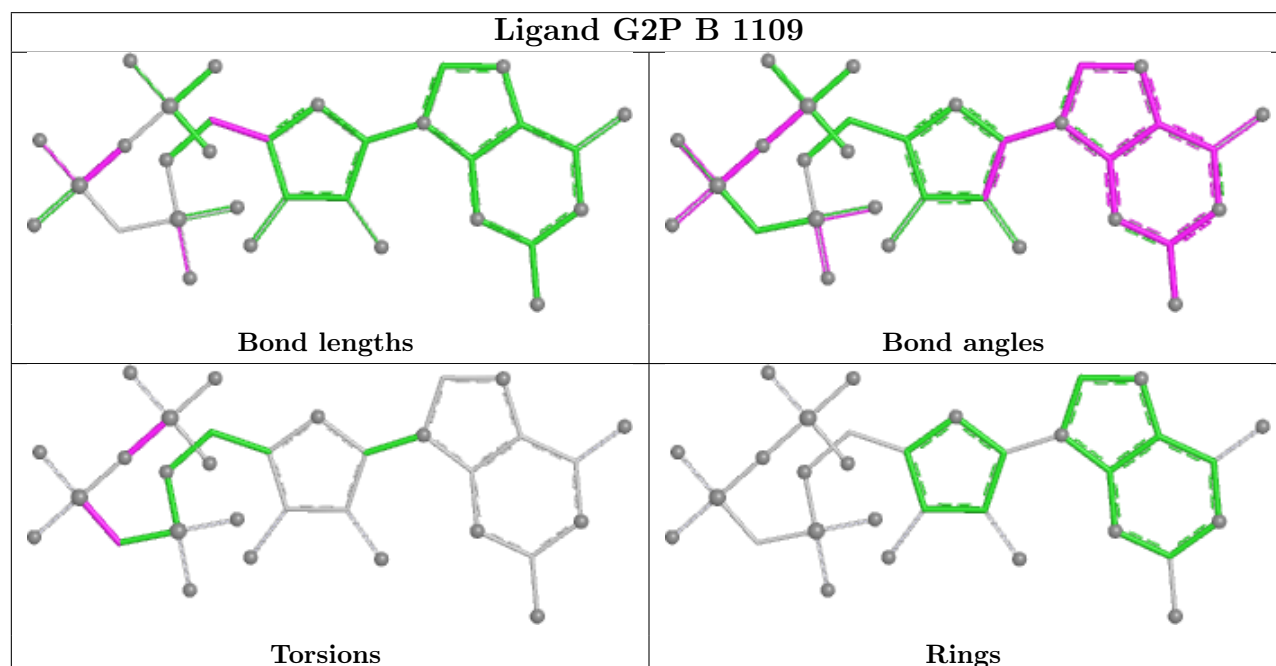
Mol	Chain	Res	Type	Atoms
3	B	1108	G2P	C5'-O5'-PA-O1A
3	B	1109	G2P	PB-O3B-PG-O2G

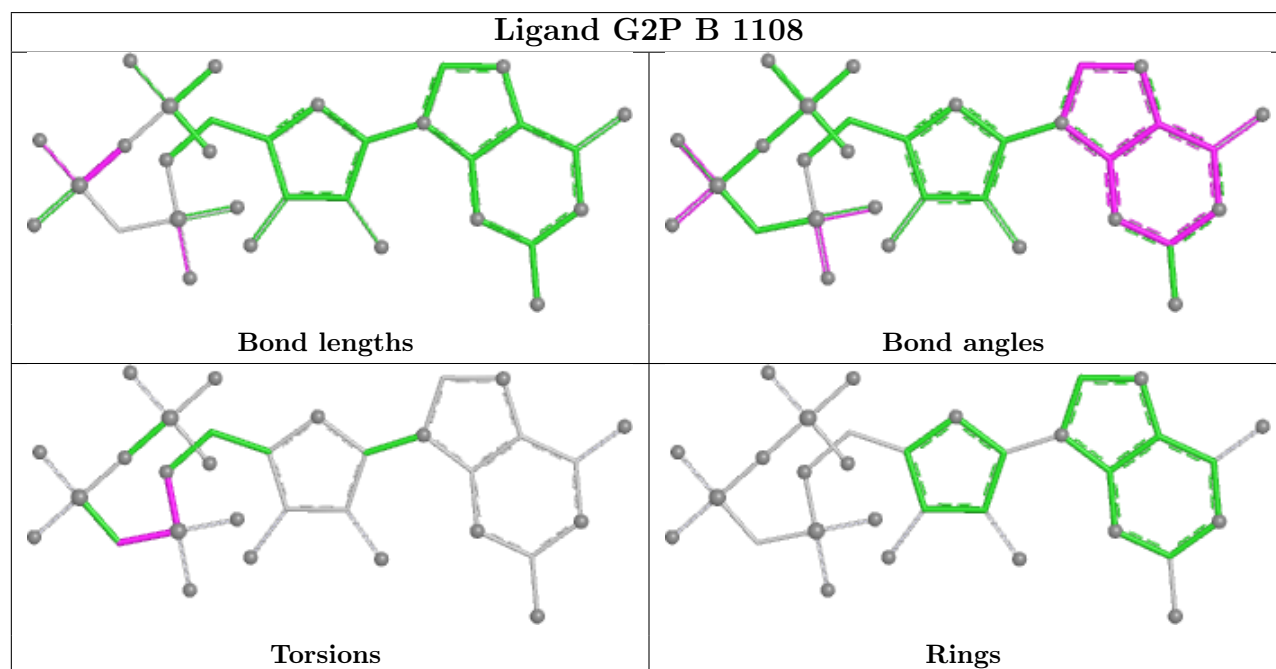
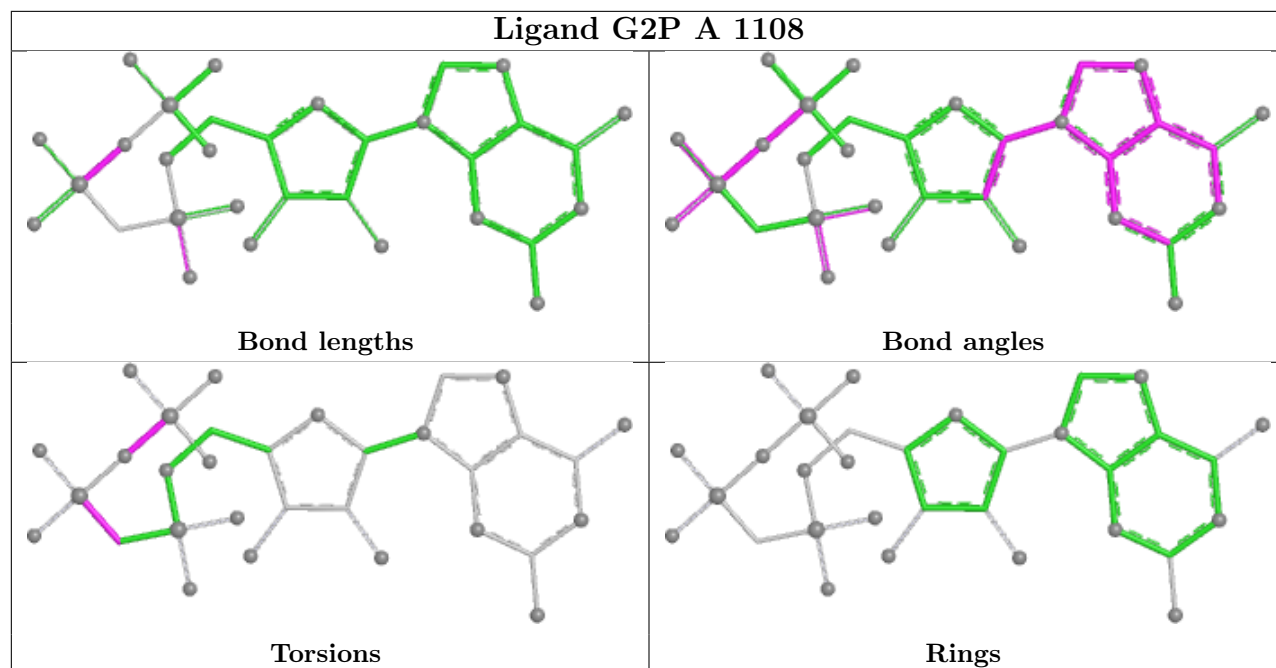
There are no ring outliers.

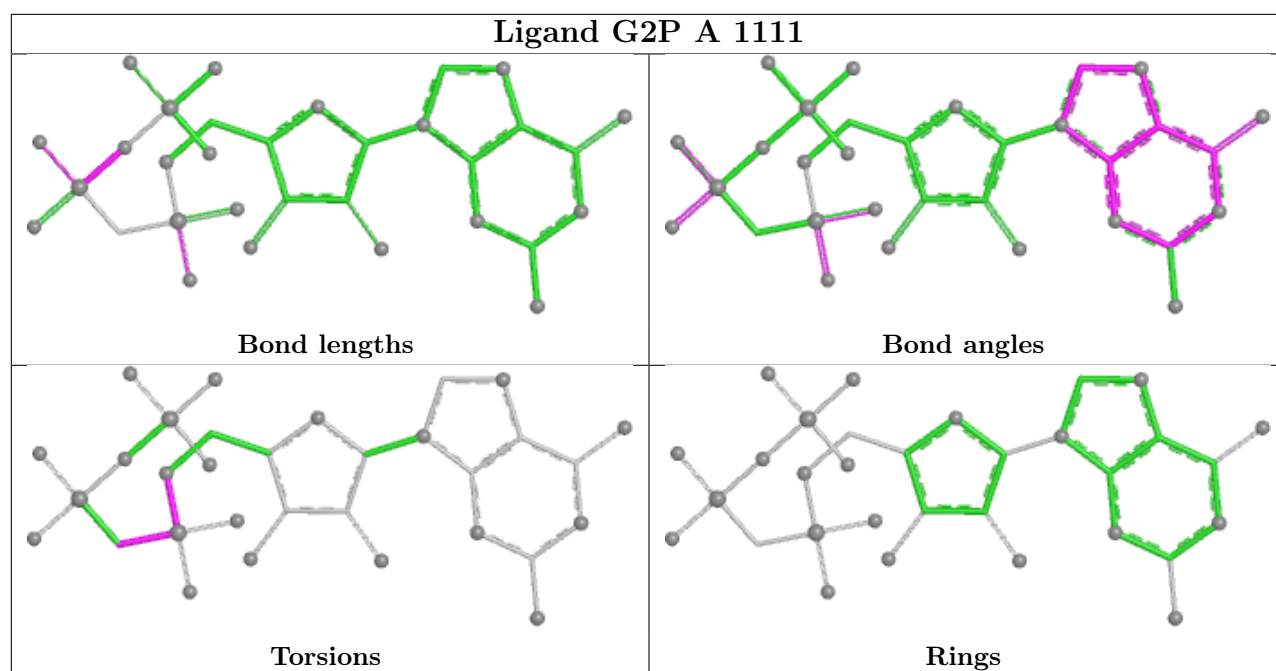
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1111	2HP	1	0
3	A	1108	G2P	2	0
3	B	1108	G2P	1	0
3	A	1111	G2P	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 [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

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%)	0.38	81 (7%) 20 19	13, 25, 47, 75	0
1	B	1094/1118 (97%)	0.34	66 (6%) 27 26	14, 23, 44, 71	0
2	C	20/36 (55%)	-0.22	0 100 100	19, 29, 50, 55	0
2	D	21/36 (58%)	-0.12	1 (4%) 35 34	21, 25, 43, 75	0
All	All	2230/2308 (96%)	0.35	148 (6%) 24 23	13, 24, 46, 75	0

All (148) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1016	GLN	5.7
1	A	1020	ALA	5.4
1	B	725	ALA	5.2
1	B	726	ALA	5.2
1	A	1019	ASN	5.0
1	A	910	TYR	4.4
1	B	730	HIS	4.1
1	A	1097	ALA	4.0
1	A	1018	GLU	3.9
1	B	910	TYR	3.9
1	B	707	ALA	3.7
1	B	191	GLU	3.6
1	A	1025	ILE	3.6
1	A	1014	TYR	3.6
1	A	8	LEU	3.6
1	A	1095	LEU	3.6
1	B	654	ILE	3.5
1	A	726	ALA	3.5
1	B	281	PHE	3.4
1	A	1012	LEU	3.4
1	B	719	ALA	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	766	ALA	3.3
1	A	1017	ARG	3.3
1	B	755	GLY	3.3
1	B	717	ALA	3.2
1	B	264	PRO	3.2
1	B	28	GLU	3.2
1	B	720	MET	3.2
1	B	765	GLY	3.1
1	B	659	ASN	3.1
1	A	1011	ALA	3.1
1	A	714	ILE	3.1
1	B	721	PHE	3.1
1	B	763	GLY	3.1
1	B	705	LEU	3.1
1	B	764	THR	3.1
1	A	1004	LEU	3.0
1	A	1098	ARG	3.0
1	A	447	LYS	3.0
1	A	710	LYS	3.0
1	A	717	ALA	3.0
1	B	714	ILE	3.0
1	B	708	ARG	2.9
1	A	281	PHE	2.9
1	B	42	GLU	2.9
1	A	1027	ASN	2.9
1	A	729	ALA	2.9
1	B	5	THR	2.9
1	B	192	GLY	2.9
1	A	28	GLU	2.9
1	A	713	ASN	2.9
1	A	1051	ASP	2.8
1	B	710	LYS	2.8
1	A	1096	GLU	2.8
1	B	1097	ALA	2.8
1	B	195	GLU	2.8
1	B	525	ASP	2.8
1	A	654	ILE	2.7
1	A	368	ASN	2.7
1	A	719	ALA	2.7
1	B	722	GLY	2.7
2	D	23	DT	2.7
1	B	406	GLU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	661	ALA	2.7
1	B	734	LEU	2.7
1	A	730	HIS	2.7
1	A	707	ALA	2.6
1	B	199	THR	2.6
1	A	10	GLU	2.6
1	B	6	GLU	2.6
1	A	657	GLY	2.6
1	B	711	ASP	2.6
1	B	716	ALA	2.6
1	A	807	GLU	2.6
1	B	632	SER	2.6
1	B	712	PRO	2.6
1	A	406	GLU	2.6
1	A	1002	GLU	2.6
1	A	1021	THR	2.6
1	A	6	GLU	2.5
1	A	191	GLU	2.5
1	A	431	TYR	2.5
1	A	267	LYS	2.5
1	A	760	GLN	2.5
1	A	7	GLU	2.5
1	B	1014	TYR	2.5
1	B	702	SER	2.5
1	B	727	SER	2.5
1	A	52	GLU	2.4
1	A	1100	GLN	2.4
1	B	27	ALA	2.4
1	A	194	VAL	2.4
1	B	733	GLU	2.4
1	A	1007	ILE	2.4
1	A	727	SER	2.4
1	B	372	LEU	2.4
1	A	716	ALA	2.4
1	A	731	ALA	2.4
1	A	767	LYS	2.4
1	B	683	ARG	2.3
1	B	1095	LEU	2.3
1	A	733	GLU	2.3
1	B	998	LYS	2.3
1	A	753	ARG	2.3
1	A	42	GLU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	621	GLU	2.3
1	A	709	ALA	2.3
1	A	1003	ALA	2.3
1	A	265	ASP	2.3
1	A	264	PRO	2.2
1	A	721	PHE	2.2
1	B	431	TYR	2.2
1	B	663	GLU	2.2
1	A	279	ASP	2.2
1	B	1019	ASN	2.2
1	A	708	ARG	2.2
1	B	1018	GLU	2.2
1	A	370	GLU	2.2
1	A	711	ASP	2.2
1	B	575	GLY	2.2
1	A	846	PRO	2.2
1	A	621	GLU	2.2
1	A	658	GLU	2.2
1	A	574	GLY	2.2
1	A	369	LYS	2.2
1	A	1005	GLU	2.1
1	B	279	ASP	2.1
1	B	704	VAL	2.1
1	A	623	LEU	2.1
1	A	705	LEU	2.1
1	B	1098	ARG	2.1
1	B	658	GLU	2.1
1	B	718	MET	2.1
1	A	525	ASP	2.1
1	B	795	GLU	2.1
1	A	720	MET	2.1
1	A	999	LEU	2.1
1	A	1070	ASN	2.1
1	A	725	ALA	2.1
1	B	175	ALA	2.1
1	B	25	SER	2.1
1	A	1093	GLU	2.1
1	A	385	ARG	2.1
1	B	1037	ARG	2.1
1	B	668	ILE	2.0
1	B	713	ASN	2.0
1	B	267	LYS	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	751	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](#)

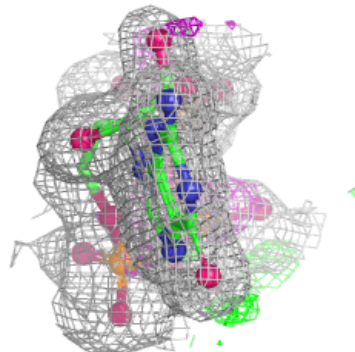
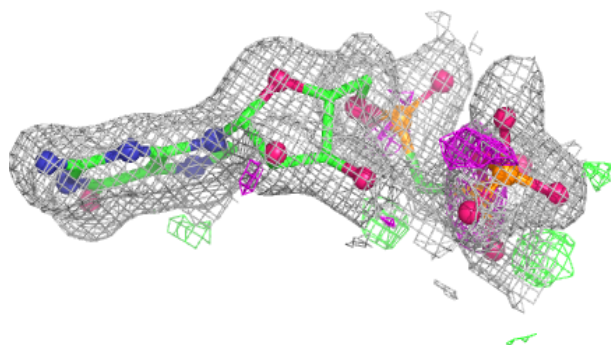
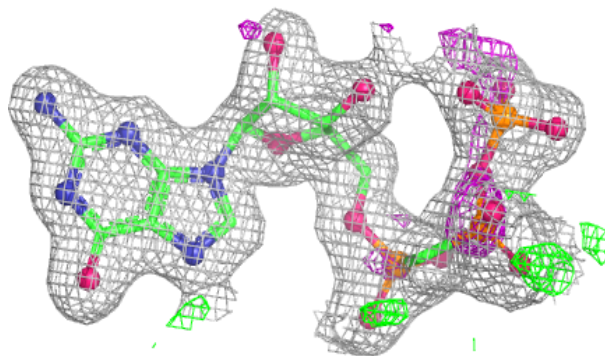
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	G2P	B	1108	32/32	0.92	0.09	21,24,34,34	0
5	2HP	B	1111	5/5	0.93	0.15	33,33,34,34	0
5	2HP	A	1110	5/5	0.94	0.13	30,30,31,31	0
3	G2P	A	1111	32/32	0.95	0.08	18,20,27,28	0
3	G2P	A	1108	32/32	0.97	0.06	15,17,18,19	0
3	G2P	B	1109	32/32	0.97	0.06	17,19,22,22	0
4	MN	B	1107	1/1	1.00	0.04	20,20,20,20	0
4	MN	B	1110	1/1	1.00	0.04	19,19,19,19	0
4	MN	A	1107	1/1	1.00	0.04	16,16,16,16	0
4	MN	A	1109	1/1	1.00	0.03	17,17,17,17	0

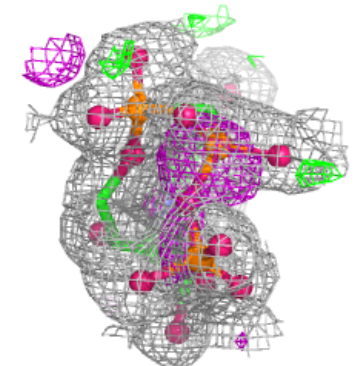
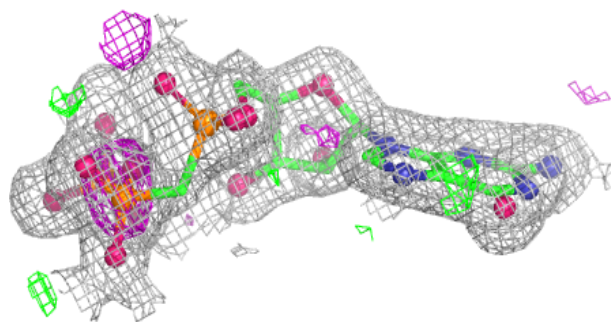
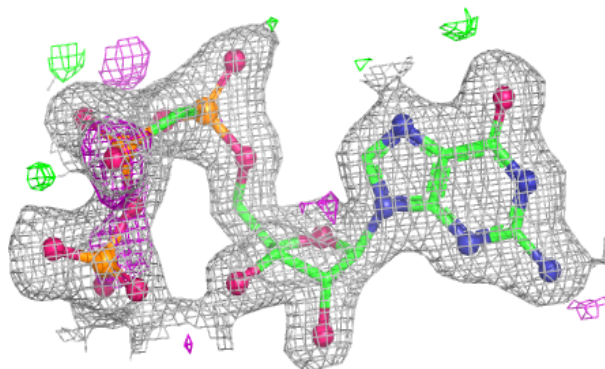
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around G2P B 1108:

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

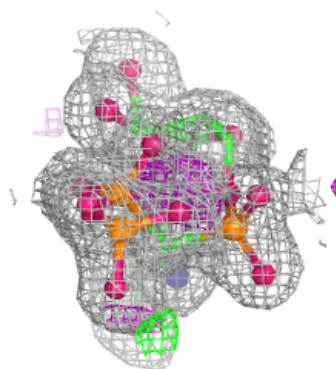
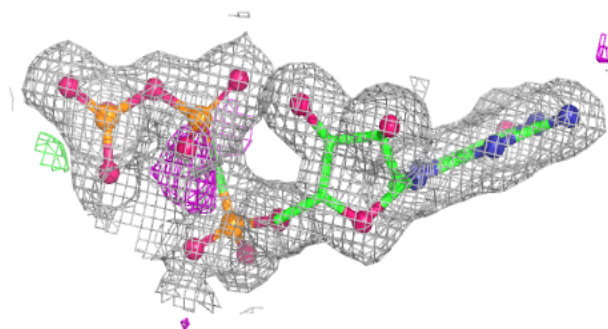
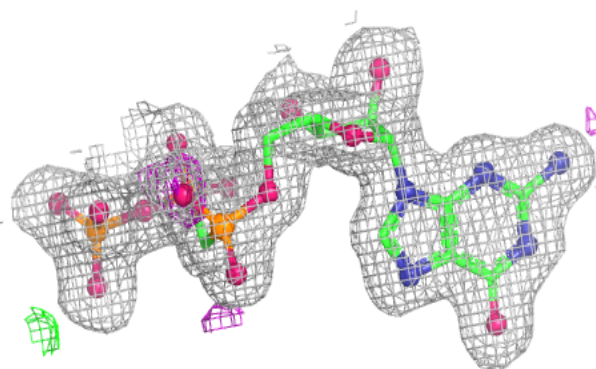
**Electron density around G2P A 1111:**

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

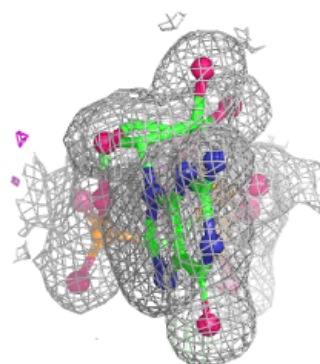
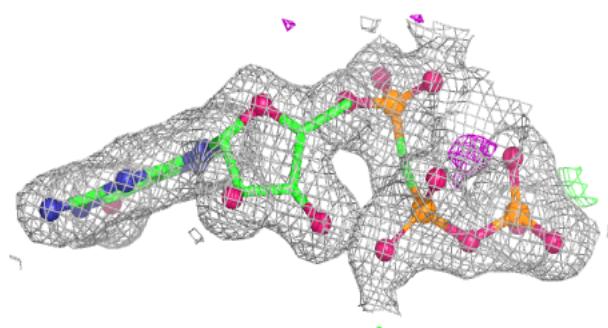
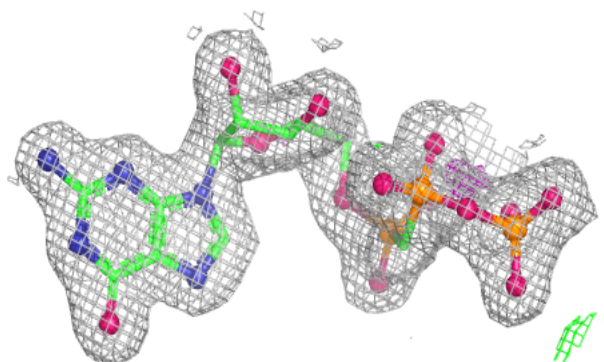


Electron density around G2P A 1108:

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

**Electron density around G2P B 1109:**

$2mF_o-DF_c$ (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.