



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:17 AM UTC

PDB ID : 9F2R / pdb_00009f2r
Title : Influenza A/H17N10 polymerase with bound promoter and 3' end of template in active site
Authors : Cusack, S.; Drncova, P.
Deposited on : 2024-04-23
Resolution : 1.96 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

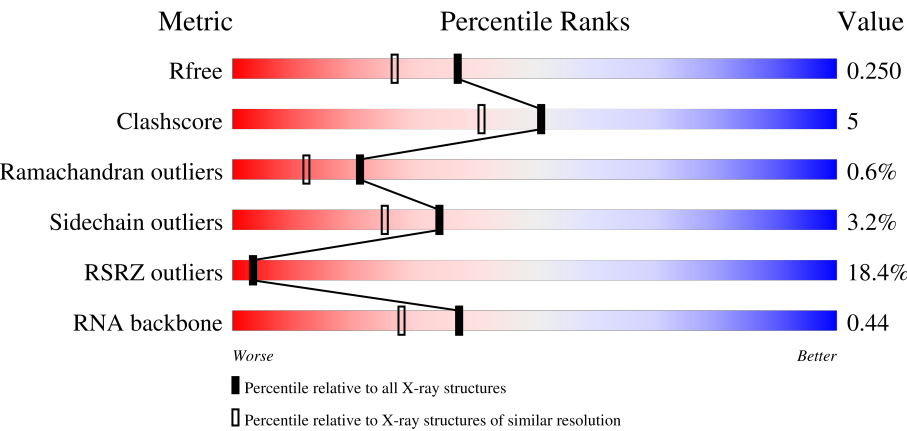
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)
RNA backbone	3983	1010 (2.32-1.60)

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	738	
2	B	776	
3	C	809	
4	R	21	

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Mol	Chain	Length	Quality of chain
5	V	16	6% 81% 12% 6%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 19393 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 Polymerase acidic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	708	Total	C	N	O	S	0	7	0
			5825	3696	985	1106	38			

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	GLY	-	expression tag	UNP H6QM92
A	-12	SER	-	expression tag	UNP H6QM92
A	-11	HIS	-	expression tag	UNP H6QM92
A	-10	HIS	-	expression tag	UNP H6QM92
A	-9	HIS	-	expression tag	UNP H6QM92
A	-8	HIS	-	expression tag	UNP H6QM92
A	-7	HIS	-	expression tag	UNP H6QM92
A	-6	HIS	-	expression tag	UNP H6QM92
A	-5	HIS	-	expression tag	UNP H6QM92
A	-4	HIS	-	expression tag	UNP H6QM92
A	-3	GLY	-	expression tag	UNP H6QM92
A	-2	SER	-	expression tag	UNP H6QM92
A	-1	GLY	-	expression tag	UNP H6QM92
A	0	SER	-	expression tag	UNP H6QM92
A	714	GLY	-	expression tag	UNP H6QM92
A	715	SER	-	expression tag	UNP H6QM92
A	716	GLY	-	expression tag	UNP H6QM92
A	717	SER	-	expression tag	UNP H6QM92
A	718	GLY	-	expression tag	UNP H6QM92
A	719	GLU	-	expression tag	UNP H6QM92
A	720	ASN	-	expression tag	UNP H6QM92
A	721	LEU	-	expression tag	UNP H6QM92
A	722	TYR	-	expression tag	UNP H6QM92
A	723	PHE	-	expression tag	UNP H6QM92
A	724	GLN	-	expression tag	UNP H6QM92

- Molecule 2 is a protein called RNA-directed RNA polymerase catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	737	Total	C	N	O	S	0	14	0
			5979	3759	1059	1121	40			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	GLY	-	expression tag	UNP H6QM91
B	-7	SER	-	expression tag	UNP H6QM91
B	-6	GLY	-	expression tag	UNP H6QM91
B	-5	SER	-	expression tag	UNP H6QM91
B	-4	GLY	-	expression tag	UNP H6QM91
B	-3	SER	-	expression tag	UNP H6QM91
B	-2	GLY	-	expression tag	UNP H6QM91
B	-1	SER	-	expression tag	UNP H6QM91
B	0	GLY	-	expression tag	UNP H6QM91
B	757	GLY	-	expression tag	UNP H6QM91
B	758	SER	-	expression tag	UNP H6QM91
B	759	GLY	-	expression tag	UNP H6QM91
B	760	SER	-	expression tag	UNP H6QM91
B	761	GLY	-	expression tag	UNP H6QM91
B	762	GLU	-	expression tag	UNP H6QM91
B	763	ASN	-	expression tag	UNP H6QM91
B	764	LEU	-	expression tag	UNP H6QM91
B	765	TYR	-	expression tag	UNP H6QM91
B	766	PHE	-	expression tag	UNP H6QM91
B	767	GLN	-	expression tag	UNP H6QM91

- Molecule 3 is a protein called Polymerase basic protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	731	Total	C	N	O	S	0	2	0
			5813	3665	1032	1084	32			

There are 49 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	GLY	-	expression tag	UNP H6QM90
C	-7	SER	-	expression tag	UNP H6QM90
C	-6	GLY	-	expression tag	UNP H6QM90
C	-5	SER	-	expression tag	UNP H6QM90
C	-4	GLY	-	expression tag	UNP H6QM90
C	-3	SER	-	expression tag	UNP H6QM90
C	-2	GLY	-	expression tag	UNP H6QM90

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	expression tag	UNP H6QM90
C	0	GLY	-	expression tag	UNP H6QM90
C	761	GLY	-	expression tag	UNP H6QM90
C	762	TRP	-	expression tag	UNP H6QM90
C	763	SER	-	expression tag	UNP H6QM90
C	764	HIS	-	expression tag	UNP H6QM90
C	765	PRO	-	expression tag	UNP H6QM90
C	766	GLN	-	expression tag	UNP H6QM90
C	767	PHE	-	expression tag	UNP H6QM90
C	768	GLU	-	expression tag	UNP H6QM90
C	769	LYS	-	expression tag	UNP H6QM90
C	770	GLY	-	expression tag	UNP H6QM90
C	771	GLY	-	expression tag	UNP H6QM90
C	772	GLY	-	expression tag	UNP H6QM90
C	773	SER	-	expression tag	UNP H6QM90
C	774	GLY	-	expression tag	UNP H6QM90
C	775	GLY	-	expression tag	UNP H6QM90
C	776	GLY	-	expression tag	UNP H6QM90
C	777	SER	-	expression tag	UNP H6QM90
C	778	GLY	-	expression tag	UNP H6QM90
C	779	GLY	-	expression tag	UNP H6QM90
C	780	SER	-	expression tag	UNP H6QM90
C	781	ALA	-	expression tag	UNP H6QM90
C	782	TRP	-	expression tag	UNP H6QM90
C	783	SER	-	expression tag	UNP H6QM90
C	784	HIS	-	expression tag	UNP H6QM90
C	785	PRO	-	expression tag	UNP H6QM90
C	786	GLN	-	expression tag	UNP H6QM90
C	787	PHE	-	expression tag	UNP H6QM90
C	788	GLU	-	expression tag	UNP H6QM90
C	789	LYS	-	expression tag	UNP H6QM90
C	790	GLY	-	expression tag	UNP H6QM90
C	791	ARG	-	expression tag	UNP H6QM90
C	792	SER	-	expression tag	UNP H6QM90
C	793	GLY	-	expression tag	UNP H6QM90
C	794	GLY	-	expression tag	UNP H6QM90
C	795	GLU	-	expression tag	UNP H6QM90
C	796	ASN	-	expression tag	UNP H6QM90
C	797	LEU	-	expression tag	UNP H6QM90
C	798	TYR	-	expression tag	UNP H6QM90
C	799	PHE	-	expression tag	UNP H6QM90
C	800	GLN	-	expression tag	UNP H6QM90

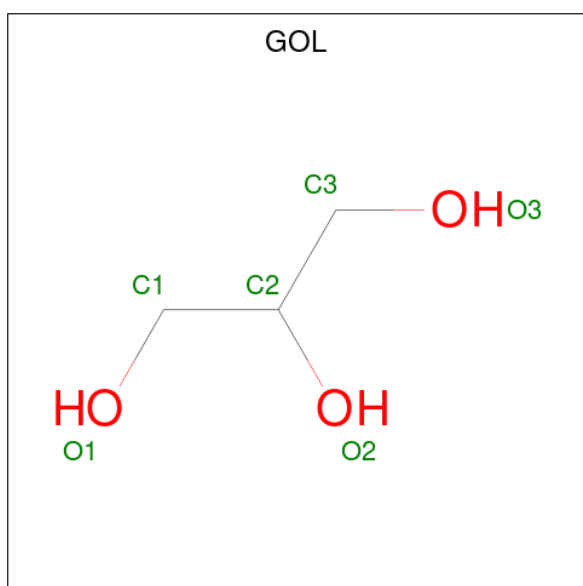
- Molecule 4 is a RNA chain called 3' end of the promoter vRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	R	15	Total	C	N	O	P	0	0	0
			289	129	43	103	14			

- Molecule 5 is a RNA chain called 5' end of the promoter vRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	V	16	Total	C	N	O	P	0	0	0
			342	152	67	107	16			

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

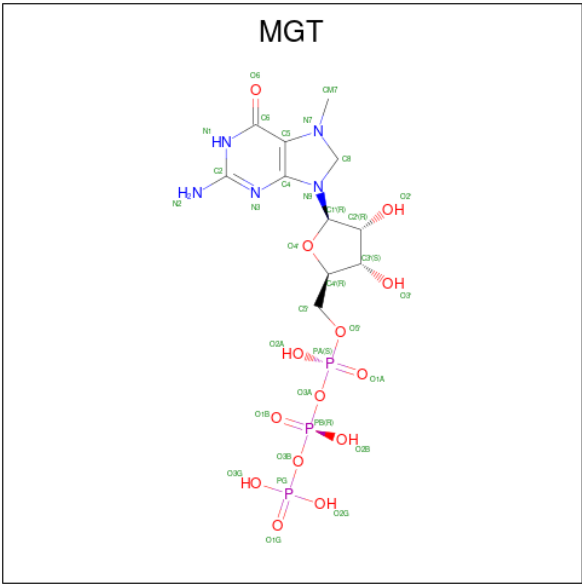


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Mg	0	0
			1	1		

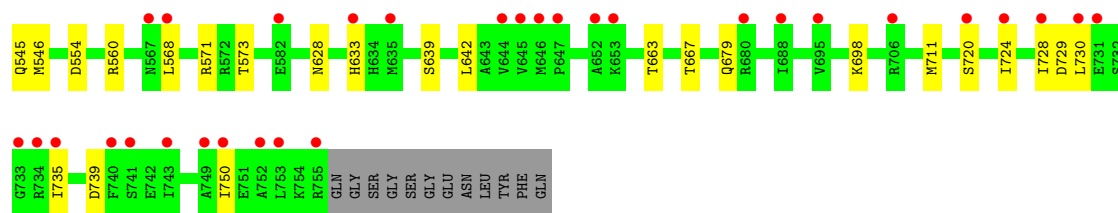
- Molecule 8 is 7N-METHYL-8-HYDROGUANOSINE-5'-TRIPHOSPHATE (CCD ID: MGT) (formula: C₁₁H₂₀N₅O₁₄P₃) (labeled as "Ligand of Interest" by depositor).



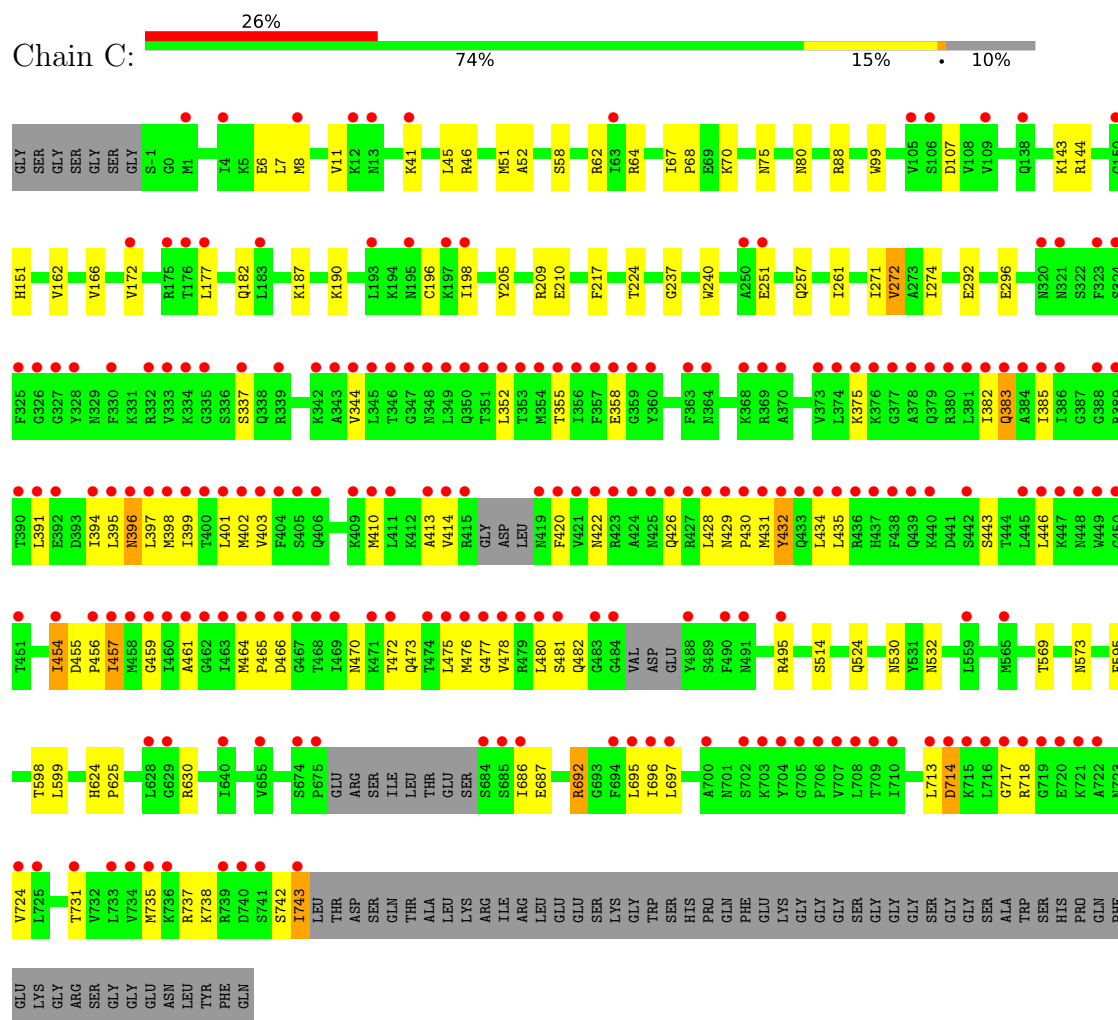
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	C	1	Total	C	N	O	P	0	0
			33	11	5	14	3		

- Molecule 9 is water.

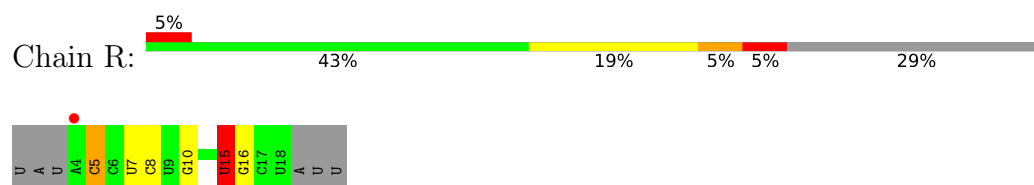
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	371	Total	O	0	0
			371	371		
9	B	409	Total	O	0	0
			409	409		
9	C	237	Total	O	0	0
			237	237		
9	R	22	Total	O	0	0
			22	22		
9	V	54	Total	O	0	0
			54	54		



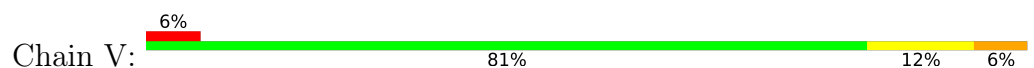
• Molecule 3: Polymerase basic protein 2

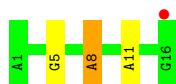


• Molecule 4: 3' end of the promoter vRNA



• Molecule 5: 5' end of the promoter vRNA





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.08Å 119.27Å 251.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	125.80 – 1.96 125.78 – 1.96	Depositor EDS
% Data completeness (in resolution range)	69.1 (125.80-1.96) 69.0 (125.78-1.96)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.189 , 0.245 0.197 , 0.250	Depositor DCC
R_{free} test set	6694 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 59.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19393	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.50	0/5947	0.99	4/8007 (0.0%)
2	B	0.53	0/6097	1.00	10/8236 (0.1%)
3	C	0.51	0/5911	0.97	5/7976 (0.1%)
4	R	0.53	0/319	1.12	2/494 (0.4%)
5	V	0.57	0/384	1.13	1/596 (0.2%)
All	All	0.52	0/18658	1.00	22/25309 (0.1%)

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	A	0	2
3	C	0	1
All	All	0	3

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	15	U	O3'-P-O5'	-7.14	93.29	104.00
2	B	185	PHE	CA-CB-CG	6.96	120.76	113.80
3	C	272	VAL	N-CA-CB	-6.93	100.44	112.08
1	A	332	THR	CA-CB-OG1	-6.54	99.79	109.60
2	B	554	ASP	CA-CB-CG	6.19	118.79	112.60
1	A	406	PHE	CA-CB-CG	-6.16	107.64	113.80
1	A	513	VAL	N-CA-CB	6.04	118.28	111.21
4	R	5	C	O3'-P-O5'	-6.00	95.00	104.00
2	B	216	ASN	CA-CB-CG	5.91	118.51	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	513	VAL	CB-CA-C	-5.86	102.96	110.98
2	B	135	ARG	CB-CA-C	-5.43	100.51	110.62
3	C	224	THR	CA-CB-OG1	-5.43	101.45	109.60
2	B	313	GLN	CB-CA-C	5.43	119.53	109.54
2	B	487	THR	CA-CB-OG1	-5.39	101.51	109.60
3	C	187	LYS	CB-CA-C	-5.34	102.74	110.96
3	C	187	LYS	N-CA-CB	5.31	117.67	109.91
3	C	598	THR	CA-CB-OG1	-5.28	101.69	109.60
2	B	96	ASP	CA-CB-CG	5.27	117.87	112.60
2	B	480	LYS	CB-CA-C	-5.26	100.56	110.67
5	V	8	A	O3'-P-O5'	-5.23	96.16	104.00
2	B	86	ASP	CA-CB-CG	5.15	117.75	112.60
2	B	169	ASP	CA-CB-CG	5.05	117.65	112.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	279	ARG	Sidechain
1	A	548	SER	Peptide
3	C	46	ARG	Sidechain

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	5825	0	5718	52	0
2	B	5979	0	5952	72	0
3	C	5813	0	5924	77	0
4	R	289	0	150	7	0
5	V	342	0	170	0	0
6	A	6	0	8	0	0
6	B	6	0	8	0	0
6	C	6	0	8	0	0
7	B	1	0	0	0	0
8	C	33	0	16	0	0
9	A	371	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	B	409	0	0	7	0
9	C	237	0	0	5	0
9	R	22	0	0	0	0
9	V	54	0	0	0	0
All	All	19393	0	17954	190	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 (190) 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:A:609[B]:ASN:O	1:A:609[B]:ASN:OD1	1.84	0.94
1:A:506:LEU:HD11	1:A:513:VAL:HG22	1.52	0.91
2:B:568:LEU:O	2:B:573:THR:HG21	1.71	0.89
2:B:491[A]:GLU:OE2	9:B:901:HOH:O	1.95	0.84
3:C:196:CYS:SG	3:C:198:ILE:HG22	2.23	0.78
2:B:41[B]:ASP:OD2	2:B:45:ARG:NH1	2.21	0.73
1:A:354:ASN:OD1	1:A:476[A]:GLN:HG2	1.92	0.70
2:B:216:ASN:HB3	9:B:1192:HOH:O	1.91	0.69
2:B:434:ARG:HH21	2:B:434:ARG:HG2	1.56	0.68
2:B:260:ARG:NH1	2:B:264:GLU:OE2	2.28	0.66
3:C:403:VAL:HA	3:C:410:MET:HE3	1.76	0.66
1:A:296:ALA:O	1:A:297:HIS:O	2.13	0.66
3:C:296:GLU:OE2	9:C:1001:HOH:O	2.13	0.66
1:A:506:LEU:HD11	1:A:513:VAL:CG2	2.26	0.65
2:B:216:ASN:ND2	2:B:398:GLU:OE1	2.29	0.65
3:C:530:ASN:ND2	3:C:532[A]:ASN:HD21	1.96	0.64
2:B:340:ALA:HB3	2:B:341:PRO:HD3	1.80	0.63
1:A:177:VAL:O	1:A:181:GLU:HG2	1.99	0.62
2:B:313:GLN:HG3	2:B:407:MET:HG3	1.83	0.61
2:B:148:GLU:HG3	9:B:1124:HOH:O	2.02	0.60
1:A:293:LEU:O	1:A:294:ASN:C	2.45	0.59
1:A:445:VAL:HG23	1:A:632[A]:CYS:SG	2.41	0.59
3:C:530:ASN:ND2	3:C:532[A]:ASN:ND2	2.50	0.59
3:C:64:ARG:NH1	3:C:80:ASN:OD1	2.33	0.59
3:C:456:PRO:O	3:C:457:ILE:C	2.45	0.59
1:A:262:PRO:HG2	1:A:713:MET:HE1	1.85	0.58
3:C:237:GLY:HA3	3:C:240:TRP:CE2	2.38	0.58
3:C:692:ARG:O	3:C:692:ARG:HG3	2.02	0.58
3:C:530:ASN:HD21	3:C:532[A]:ASN:HD21	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:633:HIS:HB3	2:B:667[A]:THR:HG21	1.88	0.56
2:B:244:PRO:HG3	2:B:411:MET:SD	2.45	0.56
3:C:697:LEU:HD11	3:C:735:MET:HB2	1.88	0.56
2:B:698:LYS:NZ	3:C:6:GLU:OE1	2.37	0.56
2:B:292:LYS:O	2:B:429:ARG:NH1	2.39	0.56
3:C:569:THR:O	3:C:573:ASN:ND2	2.38	0.56
2:B:326:THR:OG1	2:B:334:ARG:HD2	2.06	0.56
2:B:441:LEU:HD23	2:B:492:PHE:CZ	2.41	0.56
2:B:326:THR:O	2:B:334:ARG:HD3	2.05	0.56
2:B:750:ILE:HG13	3:C:8:MET:HE2	1.89	0.55
3:C:45:LEU:C	3:C:45:LEU:HD23	2.32	0.54
3:C:422:ASN:HD22	3:C:428:LEU:HD21	1.71	0.54
3:C:394:ILE:HD13	3:C:480:LEU:CD1	2.38	0.54
3:C:391:LEU:O	3:C:395:LEU:HG	2.08	0.54
1:A:158:ASP:O	1:A:159:ASP:C	2.50	0.54
2:B:735:ILE:HG12	2:B:739:ASP:HB2	1.90	0.54
3:C:41:LYS:HE3	4:R:15:U:C5	2.43	0.54
1:A:486:ASP:OD2	1:A:490:GLN:HB2	2.08	0.54
2:B:307:THR:HB	2:B:478:SER:HB2	1.90	0.54
2:B:336[B]:LEU:C	2:B:336[B]:LEU:HD23	2.33	0.54
2:B:350:ARG:NH1	2:B:371:GLU:OE2	2.40	0.53
3:C:530:ASN:HD21	3:C:532[A]:ASN:ND2	2.06	0.53
1:A:661:LEU:HD11	2:B:6:MET:HE1	1.90	0.53
3:C:352:LEU:HD13	3:C:420:PHE:CB	2.39	0.52
2:B:54[A]:ILE:HD11	9:B:1308:HOH:O	2.10	0.52
2:B:242:ALA:O	4:R:16:G:H1'	2.10	0.52
3:C:686:ILE:HA	3:C:696:ILE:O	2.10	0.52
1:A:90:ILE:HG12	2:B:724:ILE:HG12	1.91	0.52
2:B:434:ARG:HH21	2:B:434:ARG:CG	2.23	0.51
1:A:396[A]:ARG:NH1	1:A:533:GLU:OE1	2.44	0.51
2:B:720:SER:O	2:B:724:ILE:HD13	2.10	0.50
1:A:535:TYR:CD2	1:A:561:ARG:HG3	2.46	0.50
3:C:414:VAL:HG21	3:C:434:LEU:CD2	2.40	0.50
1:A:365:LEU:HG	1:A:516:ILE:HD11	1.93	0.50
3:C:383:GLN:NE2	3:C:385:ILE:HD11	2.26	0.50
3:C:495:ARG:HH11	3:C:495:ARG:HG3	1.76	0.50
3:C:151:HIS:HA	3:C:210:GLU:O	2.11	0.50
3:C:205:TYR:O	3:C:209:ARG:HG2	2.12	0.49
1:A:98:THR:OG1	1:A:100:ASN:HB2	2.13	0.49
3:C:687:GLU:HB2	3:C:696:ILE:HB	1.94	0.49
2:B:313:GLN:HB3	9:B:1033:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:PRO:HB3	2:B:54[B]:ILE:HD11	1.93	0.49
2:B:628:ASN:O	3:C:62:ARG:NH1	2.38	0.49
2:B:309:TRP:CG	2:B:445:ASP:HB3	2.47	0.49
1:A:475:TYR:HA	1:A:501:LYS:O	2.13	0.49
2:B:206:GLY:N	9:B:912:HOH:O	2.45	0.49
2:B:313:GLN:HG3	2:B:407:MET:CG	2.43	0.49
2:B:114:ILE:HD13	2:B:336[A]:LEU:HD23	1.94	0.49
4:R:10:G:N3	4:R:10:G:H2'	2.28	0.48
1:A:546:ARG:CB	1:A:551:THR:HG22	2.43	0.48
3:C:432:TYR:CD1	3:C:432:TYR:C	2.91	0.48
3:C:470:ASN:OD1	3:C:473:GLN:HB2	2.13	0.48
1:A:279:ARG:NH2	1:A:692:ASP:OD2	2.45	0.48
1:A:396[A]:ARG:HH12	1:A:533:GLU:CD	2.22	0.48
3:C:399:ILE:HD13	3:C:402:MET:CE	2.44	0.48
2:B:260:ARG:HA	2:B:414:MET:HG2	1.95	0.48
2:B:35:GLY:HA3	2:B:228:THR:HG22	1.96	0.48
2:B:396:MET:HA	2:B:400:THR:O	2.14	0.48
2:B:260:ARG:CA	2:B:414:MET:HG2	2.44	0.47
1:A:315:TRP:HA	9:A:1137:HOH:O	2.14	0.47
9:A:1141:HOH:O	2:B:711:MET:HG2	2.13	0.47
3:C:382:ILE:O	3:C:383:GLN:CB	2.63	0.47
3:C:454:ILE:O	3:C:472:THR:HB	2.15	0.47
3:C:385:ILE:CG2	3:C:481:SER:HB3	2.45	0.47
3:C:718:ARG:CZ	9:C:1009:HOH:O	2.61	0.47
2:B:571:ARG:NH1	3:C:52:ALA:O	2.47	0.47
1:A:711:LEU:HG	9:A:1145:HOH:O	2.14	0.46
3:C:257:GLN:NE2	3:C:261:ILE:HD11	2.30	0.46
3:C:7:LEU:O	3:C:11:VAL:HG23	2.15	0.46
3:C:375:LYS:HB2	3:C:382:ILE:HB	1.98	0.46
2:B:730:LEU:N	2:B:735:ILE:HG22	2.31	0.46
2:B:336[B]:LEU:HD23	2:B:336[B]:LEU:O	2.15	0.46
2:B:245:GLY:O	2:B:249:ARG:HG3	2.16	0.46
1:A:267:GLU:CD	1:A:707:LYS:HD3	2.41	0.46
3:C:271:ILE:HG12	9:C:1217:HOH:O	2.16	0.46
4:R:7:U:H2'	4:R:8:C:C6	2.51	0.46
3:C:624:HIS:O	3:C:625:PRO:C	2.58	0.45
1:A:293:LEU:HD13	1:A:492:ARG:NH2	2.31	0.45
3:C:429:ASN:CG	3:C:432:TYR:HB3	2.41	0.45
3:C:481:SER:OG	3:C:482:GLN:N	2.49	0.45
1:A:568:ILE:HG12	2:B:30:TYR:CE1	2.51	0.45
2:B:344:PHE:CE1	2:B:409:MET:HE3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:VAL:HG22	1:A:636:LEU:HD22	1.99	0.45
2:B:489:THR:HG22	2:B:498:ARG:HA	1.98	0.45
3:C:403:VAL:HG21	3:C:435:LEU:HA	1.99	0.45
3:C:352:LEU:HD13	3:C:420:PHE:HB2	1.98	0.45
3:C:713:LEU:O	3:C:714:ASP:C	2.59	0.45
3:C:70:LYS:HA	3:C:75:ASN:O	2.17	0.45
3:C:352:LEU:HD13	3:C:420:PHE:HB3	1.99	0.45
2:B:259:ALA:HB3	2:B:414:MET:HB3	1.99	0.45
1:A:51:PHE:HB3	1:A:63:LYS:O	2.17	0.44
1:A:374:MET:HE2	1:A:378:ASP:HB2	1.99	0.44
3:C:397:LEU:O	3:C:401:LEU:HG	2.16	0.44
3:C:395:LEU:O	3:C:398:MET:HB3	2.18	0.44
1:A:263:ARG:HG3	1:A:713:MET:HE2	2.00	0.44
2:B:227:MET:HG3	4:R:15:U:H5'	1.99	0.44
2:B:663:THR:HG21	3:C:99:TRP:CD1	2.53	0.44
3:C:383:GLN:HA	3:C:477:GLY:O	2.18	0.44
1:A:258[B]:GLU:CD	9:A:1094:HOH:O	2.61	0.44
1:A:167:SER:HA	1:A:170:ARG:CZ	2.47	0.44
1:A:609[B]:ASN:O	1:A:609[B]:ASN:CG	2.59	0.44
1:A:711:LEU:HD12	9:A:1221:HOH:O	2.17	0.44
3:C:595:PHE:CE2	3:C:599:LEU:HD11	2.52	0.44
2:B:730:LEU:HA	2:B:735:ILE:HG22	2.00	0.43
3:C:695:LEU:HD13	3:C:737:ARG:CG	2.48	0.43
1:A:90:ILE:HG23	2:B:724:ILE:HG12	2.01	0.43
2:B:356:MET:HE2	2:B:356:MET:HB2	1.93	0.43
3:C:478:VAL:HG21	9:C:1237:HOH:O	2.17	0.43
2:B:560[A]:ARG:HH21	3:C:51:MET:CB	2.32	0.43
1:A:604:GLU:HB2	1:A:605:PRO:HD3	2.01	0.43
2:B:633:HIS:CB	2:B:667[A]:THR:HG21	2.49	0.43
1:A:415:SER:O	1:A:447:GLN:HA	2.18	0.42
1:A:707:LYS:HA	1:A:707:LYS:HE2	2.01	0.42
1:A:124:ARG:HB3	1:A:192:ARG:HG3	2.01	0.42
3:C:257:GLN:NE2	3:C:261:ILE:CD1	2.82	0.42
3:C:395:LEU:HA	3:C:398:MET:HE2	2.01	0.42
1:A:391:GLU:HB3	1:A:392:PRO:HD2	2.01	0.42
3:C:713:LEU:HD21	3:C:724:VAL:HG22	2.02	0.42
1:A:53:PHE:CZ	1:A:66:ASP:HA	2.54	0.42
3:C:718:ARG:HB3	3:C:738:LYS:HA	2.02	0.42
1:A:582:GLN:HB2	2:B:509:LEU:HD11	2.02	0.42
3:C:717:GLY:O	3:C:718:ARG:C	2.61	0.42
1:A:87:ALA:O	1:A:91:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:162:ARG:HG3	2:B:165:ASP:OD2	2.19	0.42
3:C:58:SER:O	3:C:88:ARG:NH1	2.52	0.42
3:C:177:LEU:HD13	3:C:182:GLN:HB3	2.01	0.42
1:A:442:THR:HG22	9:A:924:HOH:O	2.20	0.42
2:B:394[A]:HIS:CE1	9:B:1155:HOH:O	2.71	0.42
1:A:614:TRP:CD1	2:B:8[A]:ILE:HD11	2.55	0.42
2:B:8[A]:ILE:HD12	2:B:8[A]:ILE:HA	1.89	0.42
3:C:383:GLN:HE21	3:C:385:ILE:HD11	1.84	0.42
1:A:89:THR:O	1:A:93:SER:OG	2.36	0.41
3:C:402:MET:HE1	3:C:446:LEU:HD21	2.00	0.41
2:B:256:GLU:OE1	2:B:414:MET:HB2	2.20	0.41
2:B:430:GLU:CD	2:B:430:GLU:H	2.28	0.41
3:C:67:ILE:HB	3:C:68:PRO:HD2	2.02	0.41
3:C:464:MET:O	3:C:466:ASP:N	2.50	0.41
1:A:705:PHE:CZ	1:A:709:VAL:HG21	2.55	0.41
3:C:426:GLN:HG2	9:C:1197:HOH:O	2.20	0.41
3:C:724:VAL:O	3:C:731:THR:HA	2.21	0.41
4:R:15:U:O5'	4:R:15:U:H2'	2.19	0.41
2:B:38:TYR:O	2:B:41[A]:ASP:HB2	2.20	0.41
2:B:730:LEU:CA	2:B:735:ILE:HG22	2.50	0.41
3:C:143:LYS:HE3	3:C:524:GLN:OE1	2.21	0.41
3:C:395:LEU:O	3:C:396:ASN:C	2.63	0.41
3:C:630:ARG:O	3:C:692:ARG:NH1	2.54	0.41
3:C:475:LEU:HB2	3:C:478:VAL:HB	2.03	0.41
1:A:438:ARG:HD3	2:B:546[B]:MET:HG3	2.03	0.41
2:B:434:ARG:CG	2:B:434:ARG:NH2	2.83	0.41
2:B:35:GLY:CA	2:B:228:THR:HG22	2.51	0.41
3:C:162:VAL:O	3:C:166:VAL:HG23	2.21	0.41
3:C:742:SER:O	3:C:743:ILE:HD12	2.21	0.40
1:A:1:MET:HG2	1:A:187:LEU:HD22	2.03	0.40
2:B:729:ASP:C	2:B:735:ILE:HG22	2.47	0.40
1:A:423:LEU:HD11	2:B:545:GLN:HB3	2.03	0.40
2:B:183:THR:HG22	2:B:184:HIS:N	2.36	0.40
1:A:263:ARG:HG3	1:A:713:MET:CE	2.51	0.40
2:B:344:PHE:CD1	2:B:409:MET:HE3	2.57	0.40
2:B:639:SER:HA	2:B:642:LEU:HD12	2.04	0.40
3:C:337:SER:HB2	3:C:358:GLU:C	2.47	0.40
4:R:15:U:O5'	4:R:15:U:C2'	2.70	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	709/738 (96%)	663 (94%)	42 (6%)	4 (1%)	21	12
2	B	747/776 (96%)	724 (97%)	23 (3%)	0	100	100
3	C	725/809 (90%)	683 (94%)	32 (4%)	10 (1%)	9	3
All	All	2181/2323 (94%)	2070 (95%)	97 (4%)	14 (1%)	21	12

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	ARG
1	A	297	HIS
3	C	443	SER
3	C	457	ILE
1	A	159	ASP
3	C	383	GLN
3	C	714	ASP
3	C	413	ALA
3	C	476	MET
3	C	461	ALA
1	A	610	ARG
3	C	459	GLY
3	C	465	PRO
3	C	430	PRO

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	639/657 (97%)	616 (96%)	23 (4%)	31	21
2	B	657/676 (97%)	637 (97%)	20 (3%)	36	27
3	C	647/706 (92%)	628 (97%)	19 (3%)	37	29
All	All	1943/2039 (95%)	1881 (97%)	62 (3%)	34	25

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	24	TYR
1	A	29	GLN
1	A	61	ILE
1	A	71	MET
1	A	72	LEU
1	A	124	ARG
1	A	142	ASN
1	A	151	ASP
1	A	157	THR
1	A	170	ARG
1	A	179	ARG
1	A	237	LYS
1	A	332	THR
1	A	380	LYS
1	A	445	VAL
1	A	487	THR
1	A	513	VAL
1	A	542	ASP
1	A	553	MET
1	A	561	ARG
1	A	613[A]	ASP
1	A	613[B]	ASP
2	B	1	MET
2	B	19	SER
2	B	32	HIS
2	B	80	SER
2	B	118	ARG
2	B	122	LEU
2	B	162	ARG
2	B	163	LEU
2	B	185	PHE
2	B	207	LYS
2	B	228	THR

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Mol	Chain	Res	Type
2	B	296	GLU
2	B	337	LEU
2	B	356	MET
2	B	409	MET
2	B	430	GLU
2	B	441	LEU
2	B	485	ASN
2	B	679	GLN
2	B	728	ILE
3	C	107	ASP
3	C	144	ARG
3	C	172	VAL
3	C	190	LYS
3	C	217	PHE
3	C	251	GLU
3	C	272	VAL
3	C	274	ILE
3	C	292	GLU
3	C	344	VAL
3	C	355	THR
3	C	396	ASN
3	C	431	MET
3	C	432	TYR
3	C	454	ILE
3	C	455	ASP
3	C	514	SER
3	C	692	ARG
3	C	743	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	30	ASN
1	A	82	GLN
1	A	294	ASN
1	A	466	ASN
1	A	582	GLN
2	B	99	HIS
2	B	127	GLN
2	B	329	GLN
2	B	461	GLN

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Mol	Chain	Res	Type
3	C	13	ASN
3	C	243	GLN
3	C	285	HIS
3	C	379	GLN
3	C	383	GLN
3	C	396	ASN
3	C	422	ASN
3	C	548	ASN
3	C	556	ASN
3	C	573	ASN
3	C	601	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	R	13/21 (61%)	2 (15%)	0
5	V	15/16 (93%)	2 (13%)	1 (6%)
All	All	28/37 (75%)	4 (14%)	1 (3%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	R	5	C
4	R	15	U
5	V	8	A
5	V	11	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	V	5	G

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

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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
6	GOL	C	902	-	5,5,5	0.21	0	5,5,5	0.39	0
8	MGT	C	901	-	34,35,35	0.90	1 (2%)	45,56,56	0.86	0
6	GOL	B	801	-	5,5,5	0.14	0	5,5,5	0.44	0
6	GOL	A	801	-	5,5,5	0.13	0	5,5,5	0.37	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	GOL	C	902	-	-	4/4/4/4	-
8	MGT	C	901	-	-	5/22/50/50	0/3/3/3
6	GOL	B	801	-	-	0/4/4/4	-
6	GOL	A	801	-	-	1/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	901	MGT	C5-N7	4.09	1.40	1.35

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	902	GOL	O1-C1-C2-C3
6	C	902	GOL	C1-C2-C3-O3
8	C	901	MGT	PB-O3B-PG-O3G

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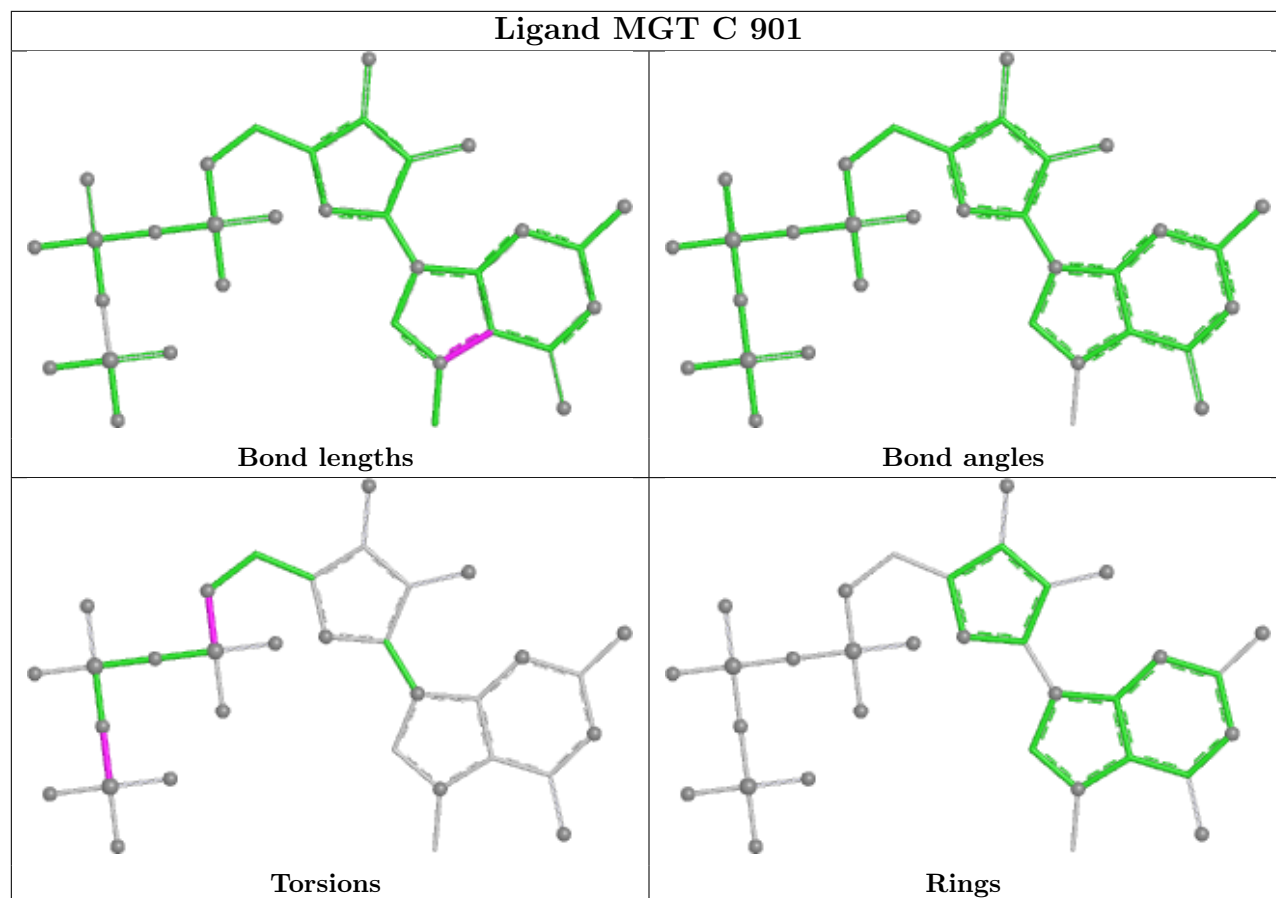
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Mol	Chain	Res	Type	Atoms
8	C	901	MGT	C5'-O5'-PA-O3A
8	C	901	MGT	C5'-O5'-PA-O2A
6	C	902	GOL	O2-C2-C3-O3
6	C	902	GOL	O1-C1-C2-O2
8	C	901	MGT	PB-O3B-PG-O1G
6	A	801	GOL	O1-C1-C2-O2
8	C	901	MGT	C5'-O5'-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

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	708/738 (95%)	0.92	152 (21%) 2 2	13, 39, 117, 154	7 (0%)
2	B	737/776 (94%)	0.24	46 (6%) 26 31	11, 31, 68, 118	14 (1%)
3	C	731/809 (90%)	1.35	207 (28%) 1 1	13, 47, 113, 154	2 (0%)
4	R	15/21 (71%)	0.17	1 (6%) 24 27	29, 49, 78, 97	0
5	V	16/16 (100%)	-0.38	1 (6%) 26 30	21, 26, 65, 94	0
All	All	2207/2360 (93%)	0.82	407 (18%) 3 3	11, 38, 109, 154	23 (1%)

All (407) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	420	PHE	8.0
3	C	480	LEU	7.2
3	C	457	ILE	7.1
3	C	349	LEU	7.0
3	C	352	LEU	6.7
3	C	446	LEU	6.7
3	C	463	ILE	6.4
3	C	628	LEU	6.3
3	C	460	ILE	6.3
3	C	347	GLY	6.2
3	C	421	VAL	6.0
3	C	325	PHE	5.7
1	A	293	LEU	5.7
3	C	478	VAL	5.7
1	A	315	TRP	5.6
3	C	348	ASN	5.6
3	C	432	TYR	5.6
1	A	72	LEU	5.5
1	A	187	LEU	5.5
3	C	449	TRP	5.5

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Mol	Chain	Res	Type	RSRZ
3	C	411	LEU	5.4
3	C	399	ILE	5.3
3	C	434	LEU	5.3
1	A	24	TYR	5.3
3	C	454	ILE	5.2
3	C	404	PHE	5.2
3	C	414	VAL	5.2
1	A	549	ILE	5.2
3	C	469	ILE	5.1
1	A	149	SER	5.1
3	C	428	LEU	5.1
3	C	459	GLY	5.0
3	C	384	ALA	5.0
3	C	722	ALA	5.0
3	C	431	MET	5.0
1	A	150	PHE	5.0
3	C	374	LEU	4.9
1	A	144	TYR	4.9
3	C	484	GLY	4.8
3	C	413	ALA	4.8
3	C	177	LEU	4.8
3	C	461	ALA	4.8
3	C	465	PRO	4.8
3	C	356	ILE	4.8
3	C	456	PRO	4.7
3	C	403	VAL	4.7
2	B	735	ILE	4.7
3	C	381	LEU	4.7
1	A	152	GLY	4.6
3	C	354	MET	4.6
3	C	391	LEU	4.6
3	C	445	LEU	4.6
3	C	708	LEU	4.6
1	A	70	ALA	4.6
3	C	475	LEU	4.6
1	A	201	LEU	4.6
3	C	435	LEU	4.6
3	C	430	PRO	4.6
3	C	438	PHE	4.5
3	C	716	LEU	4.5
2	B	185	PHE	4.5
3	C	429	ASN	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	35	PHE	4.5
1	A	62	VAL	4.5
1	A	56	LEU	4.5
3	C	467	GLY	4.5
1	A	156	ALA	4.4
1	A	14	LEU	4.4
1	A	73	LYS	4.4
2	B	724	ILE	4.3
1	A	28	PRO	4.3
1	A	190	SER	4.3
3	C	357	PHE	4.3
3	C	326	GLY	4.3
1	A	4	PHE	4.2
1	A	148	PHE	4.2
3	C	345	LEU	4.2
3	C	395	LEU	4.2
3	C	458	MET	4.2
3	C	376	LYS	4.2
3	C	333	VAL	4.2
3	C	377	GLY	4.2
3	C	410	MET	4.2
1	A	60	THR	4.2
3	C	725	LEU	4.2
1	A	127	VAL	4.2
1	A	441	PHE	4.1
3	C	397	LEU	4.1
1	A	176	PHE	4.1
3	C	373	VAL	4.1
1	A	117	PHE	4.1
3	C	360	TYR	4.1
1	A	162	ILE	4.0
3	C	344	VAL	4.0
3	C	451	THR	4.0
3	C	401	LEU	4.0
1	A	54	ILE	4.0
1	A	714	GLY	4.0
1	A	13	ILE	4.0
3	C	450	GLY	4.0
3	C	675	PRO	4.0
3	C	713	LEU	3.9
1	A	507	ARG	3.9
1	A	20	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	178	LEU	3.9
1	A	51	PHE	3.8
1	A	112	TYR	3.8
1	A	147	ILE	3.8
3	C	12	LYS	3.8
2	B	734	ARG	3.8
1	A	102	LYS	3.8
3	C	686	ILE	3.8
3	C	488	TYR	3.7
1	A	25	GLY	3.7
3	C	419	ASN	3.7
1	A	163	LEU	3.7
1	A	5	VAL	3.7
2	B	183	THR	3.7
3	C	559	LEU	3.6
1	A	161	TYR	3.6
3	C	464	MET	3.6
3	C	704	TYR	3.6
1	A	143	VAL	3.6
1	A	145	ILE	3.6
3	C	382	ILE	3.6
1	A	182	LEU	3.6
3	C	422	ASN	3.5
1	A	48	TYR	3.5
3	C	743	ILE	3.5
3	C	433	GLN	3.5
1	A	155	MET	3.5
3	C	476	MET	3.5
3	C	477	GLY	3.5
3	C	351	THR	3.5
3	C	195	ASN	3.5
1	A	46	PHE	3.5
3	C	330	PHE	3.5
1	A	545	ILE	3.4
1	A	191	PHE	3.4
1	A	151	ASP	3.4
2	B	186	GLN	3.4
1	A	295	PRO	3.4
1	A	22	LYS	3.4
1	A	548	SER	3.4
1	A	157	THR	3.4
1	A	61	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
3	C	466	ASP	3.4
1	A	45	CYS	3.3
3	C	707	VAL	3.3
3	C	343	ALA	3.3
1	A	11	PRO	3.3
1	A	299	GLY	3.3
1	A	130	TYR	3.3
3	C	479	ARG	3.3
1	A	71	MET	3.3
2	B	206	GLY	3.3
3	C	327	GLY	3.3
3	C	468	THR	3.3
1	A	131	TYR	3.2
1	A	132	TYR	3.2
1	A	547	THR	3.2
1	A	105	PHE	3.2
1	A	137	LYS	3.2
3	C	409	LYS	3.2
1	A	171	ILE	3.2
3	C	655	VAL	3.2
3	C	385	ILE	3.2
1	A	175	LEU	3.2
3	C	402	MET	3.2
3	C	700	ALA	3.1
3	C	324	SER	3.1
5	V	16	G	3.1
3	C	490	PHE	3.1
3	C	721	LYS	3.1
3	C	406	GLN	3.1
1	A	135	ALA	3.1
3	C	394	ILE	3.1
1	A	63	LYS	3.1
2	B	635	MET	3.1
3	C	355	THR	3.1
3	C	474	THR	3.1
3	C	439	GLN	3.1
1	A	53	PHE	3.1
3	C	398	MET	3.1
3	C	346	THR	3.1
3	C	437	HIS	3.1
1	A	121	GLY	3.1
2	B	652	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	645	VAL	3.0
3	C	363	PHE	3.0
3	C	447	LYS	3.0
3	C	710	ILE	3.0
1	A	508	ASN	3.0
1	A	76	PHE	3.0
1	A	37	ALA	3.0
3	C	378	ALA	3.0
3	C	358	GLU	3.0
3	C	328	TYR	3.0
3	C	342	LYS	3.0
3	C	353	THR	3.0
3	C	375	LYS	3.0
3	C	462	GLY	3.0
3	C	198	ILE	3.0
3	C	105	VAL	2.9
3	C	734	VAL	2.9
3	C	440	LYS	2.9
2	B	730	LEU	2.9
3	C	193	LEU	2.9
3	C	350	GLN	2.9
3	C	724	VAL	2.9
1	A	40	THR	2.9
1	A	146	HIS	2.9
3	C	389	ARG	2.9
2	B	743	ILE	2.9
1	A	7	THR	2.9
1	A	12	MET	2.9
3	C	565	MET	2.9
1	A	38	ILE	2.9
3	C	696	ILE	2.9
3	C	733	LEU	2.9
3	C	719	GLY	2.9
1	A	414	ASN	2.8
3	C	379	GLN	2.8
1	A	94	ILE	2.8
1	A	120	ILE	2.8
3	C	321	ASN	2.8
3	C	472	THR	2.8
1	A	66	ASP	2.8
1	A	58	GLY	2.8
3	C	427	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	176	THR	2.8
2	B	740	PHE	2.8
1	A	301	GLY	2.8
3	C	150	GLY	2.8
1	A	106	LEU	2.8
3	C	386	ILE	2.8
3	C	731	THR	2.8
1	A	188	TRP	2.8
1	A	177	VAL	2.8
1	A	39	SER	2.7
1	A	134	LYS	2.7
3	C	368	LYS	2.7
3	C	720	GLU	2.7
3	C	396	ASN	2.7
1	A	52	HIS	2.7
3	C	735	MET	2.7
2	B	753	LEU	2.7
1	A	79	ILE	2.7
1	A	6	ARG	2.7
3	C	423	ARG	2.7
3	C	736	LYS	2.7
3	C	109	VAL	2.7
1	A	183	ALA	2.7
3	C	629	GLY	2.7
3	C	380	ARG	2.7
1	A	138	LEU	2.7
2	B	568	LEU	2.7
1	A	18	GLU	2.7
2	B	184	HIS	2.7
3	C	415	ARG	2.6
3	C	495	ARG	2.6
3	C	334	LYS	2.6
1	A	294	ASN	2.6
1	A	122	VAL	2.6
3	C	703	LYS	2.6
2	B	309	TRP	2.6
1	A	297	HIS	2.6
1	A	418	ILE	2.6
2	B	688	ILE	2.6
3	C	1	MET	2.6
1	A	17	ALA	2.6
1	A	445	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	207	LYS	2.6
1	A	21	MET	2.6
2	B	646	MET	2.6
3	C	8	MET	2.6
1	A	486	ASP	2.6
2	B	0	GLY	2.6
2	B	285	VAL	2.6
1	A	184	THR	2.6
2	B	633	HIS	2.5
3	C	706	PRO	2.5
3	C	323	PHE	2.5
1	A	67	ASP	2.5
4	R	4	A	2.5
1	A	33	ASN	2.5
1	A	292	VAL	2.5
1	A	551	THR	2.5
3	C	175	ARG	2.5
3	C	717	GLY	2.5
1	A	75	ARG	2.5
2	B	454[A]	HIS	2.5
3	C	442	SER	2.5
3	C	685	SER	2.5
3	C	400	THR	2.5
1	A	158	ASP	2.5
3	C	335	GLY	2.5
2	B	567	ASN	2.5
1	A	118	ILE	2.5
3	C	106	SER	2.5
3	C	337	SER	2.5
2	B	752	ALA	2.5
2	B	755	ARG	2.4
1	A	3	ASN	2.4
1	A	114	THR	2.4
2	B	741	SER	2.4
3	C	695	LEU	2.4
1	A	9	PHE	2.4
3	C	714	ASP	2.4
2	B	680	ARG	2.4
1	A	317	TRP	2.4
2	B	582	GLU	2.4
3	C	251	GLU	2.4
1	A	346	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	388	TYR	2.4
1	A	552	ILE	2.4
1	A	44	VAL	2.4
3	C	741	SER	2.4
1	A	19	LYS	2.4
1	A	546	ARG	2.3
2	B	228	THR	2.3
3	C	138	GLN	2.3
2	B	750	ILE	2.3
1	A	32	GLY	2.3
3	C	740	ASP	2.3
3	C	383	GLN	2.3
1	A	36	ALA	2.3
3	C	250	ALA	2.3
3	C	370	ALA	2.3
3	C	424	ALA	2.3
1	A	78	ILE	2.3
2	B	360	LYS	2.3
2	B	733	GLY	2.3
1	A	57	GLU	2.3
2	B	731	GLU	2.3
3	C	183	LEU	2.3
1	A	16	ARG	2.3
3	C	339	ARG	2.3
3	C	674	SER	2.3
1	A	180	GLN	2.3
1	A	89	THR	2.3
3	C	197	LYS	2.3
3	C	709	THR	2.3
3	C	684	SER	2.2
1	A	86	ILE	2.2
3	C	640	ILE	2.2
2	B	644	VAL	2.2
3	C	172	VAL	2.2
1	A	42	MET	2.2
3	C	392	GLU	2.2
3	C	702	SER	2.2
1	A	505	HIS	2.2
2	B	208	LYS	2.2
1	A	492	ARG	2.2
3	C	369	ARG	2.2
2	B	695	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	697	LEU	2.2
1	A	186	GLY	2.2
2	B	720	SER	2.2
3	C	359	GLY	2.2
1	A	185	ALA	2.2
2	B	706	ARG	2.2
3	C	13	ASN	2.2
3	C	471	LYS	2.2
3	C	436	ARG	2.2
1	A	313	THR	2.2
2	B	653	LYS	2.2
1	A	1	MET	2.1
3	C	364	ASN	2.1
3	C	491	ASN	2.1
1	A	499	ILE	2.1
1	A	129	ASP	2.1
3	C	390	THR	2.1
3	C	405	SER	2.1
3	C	388	GLY	2.1
1	A	95	CYS	2.1
3	C	739	ARG	2.1
2	B	280	ALA	2.1
1	A	352	PHE	2.1
3	C	694	PHE	2.1
1	A	90	ILE	2.1
1	A	345	ILE	2.1
2	B	728	ILE	2.1
3	C	41	LYS	2.1
1	A	195	GLU	2.1
2	B	290	MET	2.1
3	C	715	LYS	2.1
3	C	483	GLY	2.1
1	A	96	ASN	2.1
3	C	320	ASN	2.1
2	B	647	PRO	2.1
3	C	426	GLN	2.1
1	A	296	ALA	2.1
3	C	332	ARG	2.1
1	A	101	SER	2.0
3	C	63	ILE	2.0
3	C	705	GLY	2.0
3	C	425	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
3	C	448	ASN	2.0
1	A	711	LEU	2.0
2	B	749	ALA	2.0
1	A	15	GLU	2.0
3	C	481	SER	2.0
3	C	4	ILE	2.0
1	A	100	ASN	2.0
1	A	103	PRO	2.0
3	C	718	ARG	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](#)

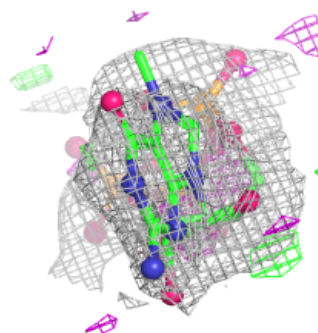
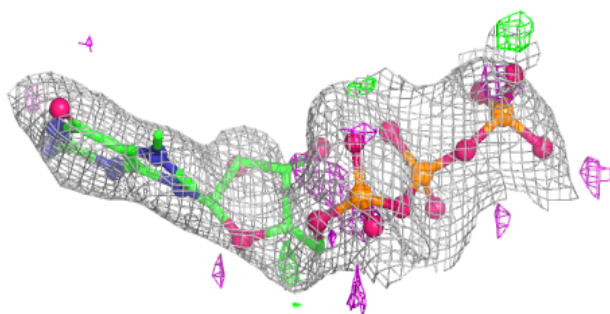
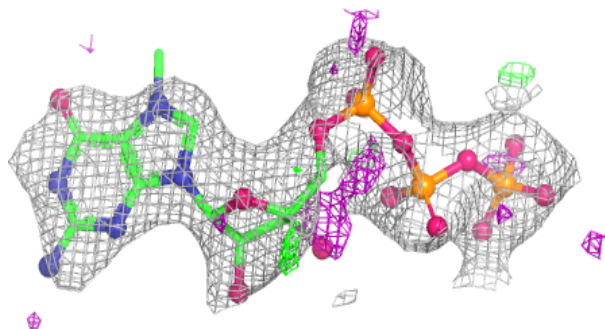
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	MGT	C	901	33/33	0.81	0.13	69,77,93,99	0
7	MG	B	802	1/1	0.84	0.11	50,50,50,50	0
6	GOL	C	902	6/6	0.84	0.15	43,51,52,54	0
6	GOL	A	801	6/6	0.92	0.10	28,35,37,42	0
6	GOL	B	801	6/6	0.95	0.10	38,46,48,49	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 MGT C 901:

$2mF_o-DF_c$ (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.