



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:59 AM UTC

PDB ID : 9GVU / pdb_00009gvu
Title : Human Rab27A in complex with cyclic peptide IMP-2660
Authors : Petracca, R.; Tersa, M.; De Vita, E.; Morgan, M.R.; Cota, E.; Tate, E.W.
Deposited on : 2024-09-25
Resolution : 2.10 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

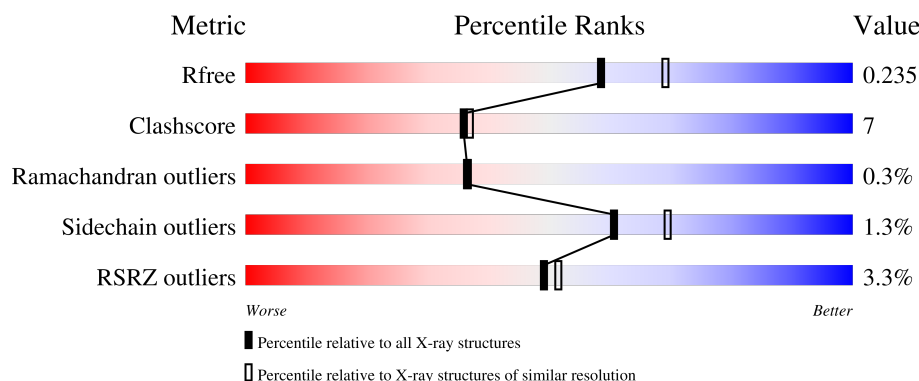
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	184	<div> <div>5%</div> <div> <div></div> <div>91%</div> <div>8%</div> <div>..</div> </div> </div>
1	B	184	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>13%</div> <div>..</div> </div> </div>
2	D	14	<div> <div>50%</div> <div>50%</div> </div>
2	F	14	<div> <div>93%</div> <div>7%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	206	-	X	-	-
4	GOL	F	101	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 3388 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 Ras-related protein Rab-27A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	184	Total	C	N	O	S	0	1	0
			1433	917	237	273	6			
1	B	183	Total	C	N	O	S	0	0	0
			1397	896	230	265	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	78	LEU	GLN	engineered mutation	UNP P51159
A	123	SER	CYS	engineered mutation	UNP P51159
A	188	SER	CYS	engineered mutation	UNP P51159
B	78	LEU	GLN	engineered mutation	UNP P51159
B	123	SER	CYS	engineered mutation	UNP P51159
B	188	SER	CYS	engineered mutation	UNP P51159

- Molecule 2 is a protein called Cyclic peptide IMP-2660.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	14	Total	C	N	O	S	0	0	0
			116	72	24	19	1			
2	F	14	Total	C	N	O	S	0	0	0
			117	73	24	19	1			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

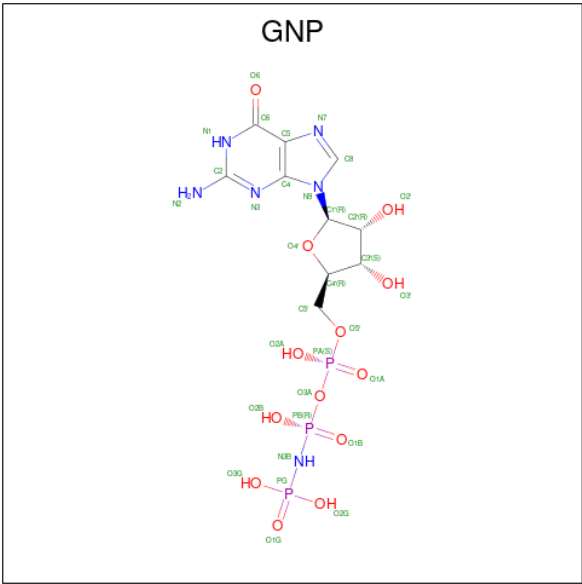
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
5	B	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

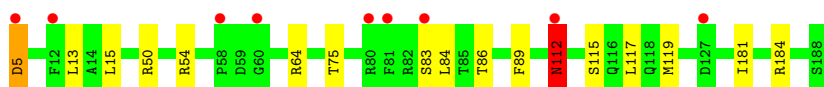
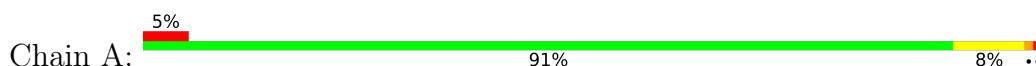
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	88	Total	O	0	0
			88	88		
6	B	71	Total	O	0	0
			71	71		
6	D	8	Total	O	0	0
			8	8		
6	F	8	Total	O	0	0
			8	8		

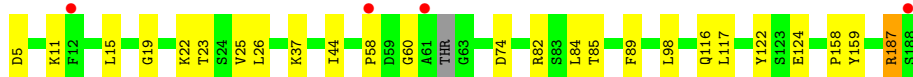
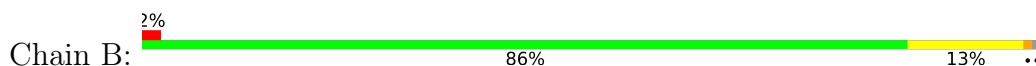
3 Residue-property plots [i](#)

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: Ras-related protein Rab-27A



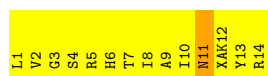
- Molecule 1: Ras-related protein Rab-27A



- Molecule 2: Cyclic peptide IMP-2660



- Molecule 2: Cyclic peptide IMP-2660



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.36Å 72.71Å 91.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.97 – 2.10 56.97 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (56.97-2.10) 99.8 (56.97-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.17.1_3660: ???)	Depositor
R, R_{free}	0.186 , 0.232 0.190 , 0.235	Depositor DCC
R_{free} test set	1410 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.029 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3388	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.68% 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: GNP, GOL, MG, DTY, XAK

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.40	1/1460 (0.1%)	0.52	0/1973
1	B	0.32	0/1423	0.51	0/1925
2	D	5.33	17/92 (18.5%)	2.17	4/121 (3.3%)
2	F	5.09	15/92 (16.3%)	2.20	3/121 (2.5%)
All	All	1.32	33/3067 (1.1%)	0.73	7/4140 (0.2%)

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	1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	14	ARG	NE-CZ	17.36	1.52	1.33
2	D	2	VAL	C-N	16.52	1.50	1.34
2	F	14	ARG	NE-CZ	16.12	1.50	1.33
2	D	5	ARG	NE-CZ	16.03	1.50	1.33
2	F	5	ARG	NE-CZ	15.42	1.50	1.33
2	F	9	ALA	C-N	13.90	1.51	1.33
2	D	9	ALA	C-N	13.81	1.50	1.33
2	D	8	ILE	C-N	13.33	1.52	1.33
2	F	2	VAL	C-N	13.15	1.49	1.33
2	F	8	ILE	C-N	12.99	1.51	1.33
2	D	6	HIS	C-N	12.74	1.50	1.33
2	F	7	THR	C-N	12.28	1.49	1.33
2	D	1	LEU	C-N	12.22	1.51	1.33
2	F	3	GLY	C-N	11.79	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	6	HIS	C-N	11.64	1.49	1.33
2	D	5	ARG	C-N	11.47	1.47	1.33
2	F	5	ARG	C-N	11.30	1.47	1.33
2	D	3	GLY	C-N	10.60	1.48	1.34
2	D	4	SER	C-N	10.14	1.47	1.33
2	F	10	ILE	C-N	9.75	1.47	1.33
2	D	10	ILE	C-N	9.40	1.46	1.33
2	D	7	THR	C-N	9.38	1.49	1.33
2	F	4	SER	C-N	9.19	1.47	1.33
2	F	1	LEU	C-N	8.82	1.50	1.33
2	D	3	GLY	N-CA	7.62	1.52	1.44
2	F	11	ASN	CG-ND2	7.56	1.49	1.33
2	D	11	ASN	CG-ND2	7.42	1.48	1.33
2	D	6	HIS	CB-CG	6.26	1.58	1.50
2	D	6	HIS	CG-CD2	6.02	1.42	1.35
2	F	6	HIS	CB-CG	6.00	1.58	1.50
2	F	3	GLY	N-CA	5.94	1.50	1.44
1	A	112	ASN	C-O	-5.48	1.17	1.24
2	D	2	VAL	C-O	-5.45	1.17	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	GLY	O-C-N	-6.70	117.46	123.29
2	D	9	ALA	CA-C-N	-6.23	115.02	123.12
2	D	9	ALA	C-N-CA	-6.23	115.02	123.12
2	F	11	ASN	CA-CB-CG	6.12	118.72	112.60
2	D	10	ILE	N-CA-C	-5.22	100.24	107.80
2	F	9	ALA	CA-C-N	-5.13	116.83	123.19
2	F	9	ALA	C-N-CA	-5.13	116.83	123.19

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	5	ASP	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	1433	0	1380	15	0
1	B	1397	0	1331	23	0
2	D	116	0	108	7	0
2	F	117	0	110	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	42	0	55	8	0
4	B	30	0	40	4	0
4	D	6	0	8	0	0
4	F	6	0	8	4	0
5	A	32	0	13	3	0
5	B	32	0	13	3	0
6	A	88	0	0	1	0
6	B	71	0	0	1	0
6	D	8	0	0	0	0
6	F	8	0	0	0	0
All	All	3388	0	3066	46	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 7.

All (46) 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:187:ARG:HB3	2:D:13:DTY:HD1	1.59	0.84
1:A:54:ARG:HH12	4:A:207:GOL:H31	1.59	0.67
1:A:64:ARG:HA	4:A:206:GOL:H11	1.78	0.66
4:B:203:GOL:H31	5:B:207:GNP:H1'	1.79	0.65
1:A:83:SER:HB3	1:A:86:THR:HG23	1.80	0.63
1:B:159:TYR:H	4:B:205:GOL:H2	1.64	0.63
1:B:11:LYS:NZ	6:B:303:HOH:O	2.32	0.62
1:A:13:LEU:HD11	1:A:75:THR:HG23	1.85	0.57
1:A:5:ASP:N	1:A:50:ARG:HH22	2.04	0.55
1:A:15:LEU:CD1	1:A:117:LEU:HD21	2.37	0.55
1:B:19:GLY:H	5:B:207:GNP:HNB3	1.56	0.54
4:A:203:GOL:H12	5:A:209:GNP:N3	2.24	0.52
2:D:11:ASN:HD21	4:F:101:GOL:H31	1.74	0.52
1:B:89:PHE:HZ	1:B:117:LEU:HD23	1.76	0.51
1:A:115:SER:O	1:A:119:MET:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:TYR:CE2	2:D:1:LEU:HG	2.46	0.51
1:B:15:LEU:CD1	1:B:117:LEU:HD21	2.44	0.48
1:B:124:GLU:OE1	1:B:124:GLU:N	2.39	0.48
1:A:112:ASN:ND2	6:A:305:HOH:O	2.47	0.47
2:D:11:ASN:ND2	4:F:101:GOL:H31	2.30	0.46
2:D:12:XAK:C6	4:F:101:GOL:H32	2.45	0.46
1:A:13:LEU:HD11	1:A:75:THR:CG2	2.46	0.45
1:B:23:THR:OG1	1:B:74:ASP:OD2	2.34	0.45
1:B:5:ASP:N	1:B:5:ASP:OD1	2.48	0.45
1:B:44:ILE:HG13	1:B:74:ASP:O	2.17	0.45
1:B:15:LEU:HD11	1:B:117:LEU:HD21	1.99	0.44
1:B:37:LYS:O	4:B:204:GOL:O1	2.33	0.44
1:B:25:VAL:HG21	1:B:98:LEU:HD21	2.00	0.44
1:B:122:TYR:CD2	2:D:3:GLY:HA3	2.53	0.44
1:A:84:LEU:HD22	1:A:89:PHE:CE1	2.53	0.43
1:A:181:ILE:HD13	1:A:181:ILE:HA	1.78	0.43
1:A:184:ARG:O	4:A:208:GOL:H2	2.18	0.43
1:A:54:ARG:HH22	4:A:207:GOL:H31	1.84	0.43
1:B:84:LEU:CD1	1:B:116:GLN:HB3	2.50	0.42
1:B:82:ARG:O	1:B:85:THR:HG23	2.20	0.42
4:A:203:GOL:C1	5:A:209:GNP:H1'	2.50	0.41
1:B:22:LYS:NZ	5:B:207:GNP:O3G	2.47	0.41
1:B:58:PRO:C	1:B:60:GLY:H	2.28	0.41
1:B:26:LEU:HD12	1:B:74:ASP:HB2	2.03	0.41
1:B:158:PRO:HA	4:B:205:GOL:O2	2.21	0.41
1:B:124:GLU:H	1:B:124:GLU:CD	2.26	0.41
1:B:187:ARG:HG3	1:B:187:ARG:O	2.21	0.41
1:A:117:LEU:HD23	1:A:117:LEU:HA	1.86	0.41
1:A:54:ARG:NH1	4:A:207:GOL:H31	2.31	0.40
4:A:203:GOL:H11	5:A:209:GNP:H1'	2.04	0.40
2:D:11:ASN:HD21	4:F:101:GOL:C3	2.34	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	183/184 (100%)	179 (98%)	4 (2%)	0	100	100
1	B	179/184 (97%)	168 (94%)	10 (6%)	1 (1%)	21	18
2	D	10/14 (71%)	10 (100%)	0	0	100	100
2	F	10/14 (71%)	10 (100%)	0	0	100	100
All	All	382/396 (96%)	367 (96%)	14 (4%)	1 (0%)	36	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	187	ARG

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	147/157 (94%)	146 (99%)	1 (1%)	76	83
1	B	141/157 (90%)	141 (100%)	0	100	100
2	D	10/10 (100%)	8 (80%)	2 (20%)	1	0
2	F	10/10 (100%)	9 (90%)	1 (10%)	7	5
All	All	308/334 (92%)	304 (99%)	4 (1%)	61	69

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	ASN
2	D	5	ARG
2	D	14	ARG
2	F	11	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	105	GLN
2	F	6	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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$
2	XAK	D	12	2	10,10,14	4.10	3 (30%)	9,11,17	2.75	3 (33%)
2	XAK	F	12	2	11,11,14	2.56	3 (27%)	9,12,17	0.91	0
2	DTY	D	13	2	11,12,13	1.40	2 (18%)	10,15,17	0.56	0
2	DTY	F	13	2	11,12,13	1.56	2 (18%)	10,15,17	0.87	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
2	XAK	D	12	2	-	4/10/11/15	-
2	XAK	F	12	2	-	3/11/12/15	-
2	DTY	D	13	2	-	0/5/6/8	0/1/1/1
2	DTY	F	13	2	-	0/5/6/8	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	12	XAK	C3-N5	12.05	1.50	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	12	XAK	C3-N5	7.19	1.50	1.33
2	D	13	DTY	CB-CG	3.19	1.58	1.51
2	F	13	DTY	CB-CG	3.13	1.58	1.51
2	F	13	DTY	OH-CZ	3.08	1.43	1.37
2	D	12	XAK	O4-C3	-3.05	1.17	1.23
2	D	13	DTY	OH-CZ	2.77	1.43	1.37
2	F	12	XAK	C4-C	2.68	1.62	1.47
2	D	12	XAK	C4-C	2.38	1.60	1.47
2	F	12	XAK	O4-C3	-2.35	1.18	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	12	XAK	C1-C3-N5	6.44	124.69	116.18
2	D	12	XAK	C6-N5-C3	-3.40	116.29	122.21
2	D	12	XAK	O4-C3-N5	-2.93	118.24	123.13

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	12	XAK	C2-C1-C3-O4
2	F	12	XAK	N-C1-C2-S3
2	F	12	XAK	C2-C1-C3-N5
2	D	12	XAK	C2-C1-C3-O4
2	D	12	XAK	N-C1-C3-O4
2	D	12	XAK	N-C1-C2-S3
2	D	12	XAK	C2-C1-C3-N5

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	12	XAK	1	0
2	D	13	DTY	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 2 are monoatomic - leaving 16 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
4	GOL	A	202	-	5,5,5	0.91	0	5,5,5	1.11	0
4	GOL	A	204	-	5,5,5	0.92	0	5,5,5	1.08	0
4	GOL	B	203	-	5,5,5	0.88	0	5,5,5	1.01	0
4	GOL	B	205	-	5,5,5	1.02	0	5,5,5	0.88	0
4	GOL	A	207	-	5,5,5	0.80	0	5,5,5	1.14	0
4	GOL	D	101	-	5,5,5	0.99	0	5,5,5	0.96	0
4	GOL	A	208	-	5,5,5	0.77	0	5,5,5	1.20	0
4	GOL	A	205	-	5,5,5	1.02	0	5,5,5	1.11	1 (20%)
5	GNP	B	207	3	34,34,34	1.20	4 (11%)	47,54,54	0.81	2 (4%)
4	GOL	B	206	-	5,5,5	1.18	1 (20%)	5,5,5	1.06	0
5	GNP	A	209	3	34,34,34	1.25	5 (14%)	47,54,54	0.98	1 (2%)
4	GOL	B	204	-	5,5,5	0.84	0	5,5,5	1.25	1 (20%)
4	GOL	A	203	-	5,5,5	0.96	0	5,5,5	1.16	1 (20%)
4	GOL	B	202	-	5,5,5	0.73	0	5,5,5	1.19	1 (20%)
4	GOL	A	206	-	5,5,5	1.28	1 (20%)	5,5,5	1.21	1 (20%)
4	GOL	F	101	-	5,5,5	1.00	0	5,5,5	0.86	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
4	GOL	A	202	-	-	3/4/4/4	-
4	GOL	A	204	-	-	3/4/4/4	-
4	GOL	B	203	-	-	0/4/4/4	-
4	GOL	B	205	-	-	1/4/4/4	-
4	GOL	A	207	-	-	2/4/4/4	-
4	GOL	D	101	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	208	-	-	2/4/4/4	-
4	GOL	A	205	-	-	1/4/4/4	-
5	GNP	B	207	3	-	2/18/38/38	0/3/3/3
4	GOL	B	206	-	-	0/4/4/4	-
5	GNP	A	209	3	-	3/18/38/38	0/3/3/3
4	GOL	B	204	-	-	4/4/4/4	-
4	GOL	A	203	-	-	2/4/4/4	-
4	GOL	B	202	-	-	3/4/4/4	-
4	GOL	A	206	-	-	4/4/4/4	-
4	GOL	F	101	-	-	4/4/4/4	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	207	GNP	PB-O3A	4.54	1.64	1.59
5	A	209	GNP	PB-O3A	3.38	1.63	1.59
5	A	209	GNP	PB-O1B	3.03	1.50	1.46
5	A	209	GNP	PG-O1G	2.87	1.50	1.46
5	B	207	GNP	PB-O1B	2.75	1.50	1.46
4	A	206	GOL	O2-C2	-2.67	1.35	1.43
5	A	209	GNP	PG-N3B	2.66	1.70	1.63
5	A	209	GNP	PB-O2B	-2.65	1.49	1.56
5	B	207	GNP	PG-O1G	2.54	1.50	1.46
5	B	207	GNP	PG-N3B	2.36	1.69	1.63
4	B	206	GOL	C3-C2	2.04	1.59	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	209	GNP	O1G-PG-N3B	-5.36	103.88	111.77
5	B	207	GNP	O1G-PG-N3B	-3.77	106.21	111.77
4	B	204	GOL	C3-C2-C1	-2.19	103.78	111.80
4	A	203	GOL	C3-C2-C1	-2.12	104.02	111.80
4	B	202	GOL	C3-C2-C1	-2.07	104.21	111.80
5	B	207	GNP	O2G-PG-O1G	-2.04	108.33	113.45
4	A	205	GOL	C3-C2-C1	-2.03	104.36	111.80
4	A	206	GOL	C3-C2-C1	-2.01	104.44	111.80

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	206	GOL	O1-C1-C2-C3
4	A	207	GOL	C1-C2-C3-O3
4	A	207	GOL	O2-C2-C3-O3
4	B	202	GOL	C1-C2-C3-O3
4	D	101	GOL	C1-C2-C3-O3
4	F	101	GOL	O1-C1-C2-O2
4	F	101	GOL	O1-C1-C2-C3
4	F	101	GOL	C1-C2-C3-O3
5	A	209	GNP	PG-N3B-PB-O1B
5	B	207	GNP	PA-O3A-PB-O1B
5	B	207	GNP	PA-O3A-PB-O2B
4	A	203	GOL	O1-C1-C2-O2
4	A	206	GOL	O1-C1-C2-O2
4	D	101	GOL	O2-C2-C3-O3
4	A	202	GOL	C1-C2-C3-O3
4	A	203	GOL	O1-C1-C2-C3
4	A	204	GOL	C1-C2-C3-O3
4	A	206	GOL	C1-C2-C3-O3
4	B	204	GOL	O1-C1-C2-C3
4	B	204	GOL	C1-C2-C3-O3
4	B	204	GOL	O1-C1-C2-O2
4	F	101	GOL	O2-C2-C3-O3
4	A	206	GOL	O2-C2-C3-O3
4	B	202	GOL	O2-C2-C3-O3
4	A	204	GOL	O2-C2-C3-O3
4	B	202	GOL	O1-C1-C2-O2
4	B	205	GOL	O2-C2-C3-O3
4	A	202	GOL	O2-C2-C3-O3
4	A	204	GOL	O1-C1-C2-O2
4	A	205	GOL	O1-C1-C2-O2
4	A	202	GOL	O1-C1-C2-O2
4	A	208	GOL	O2-C2-C3-O3
4	A	208	GOL	C1-C2-C3-O3
5	A	209	GNP	PA-O3A-PB-O2B
4	B	204	GOL	O2-C2-C3-O3
5	A	209	GNP	PA-O3A-PB-O1B

There are no ring outliers.

10 monomers are involved in 18 short contacts:

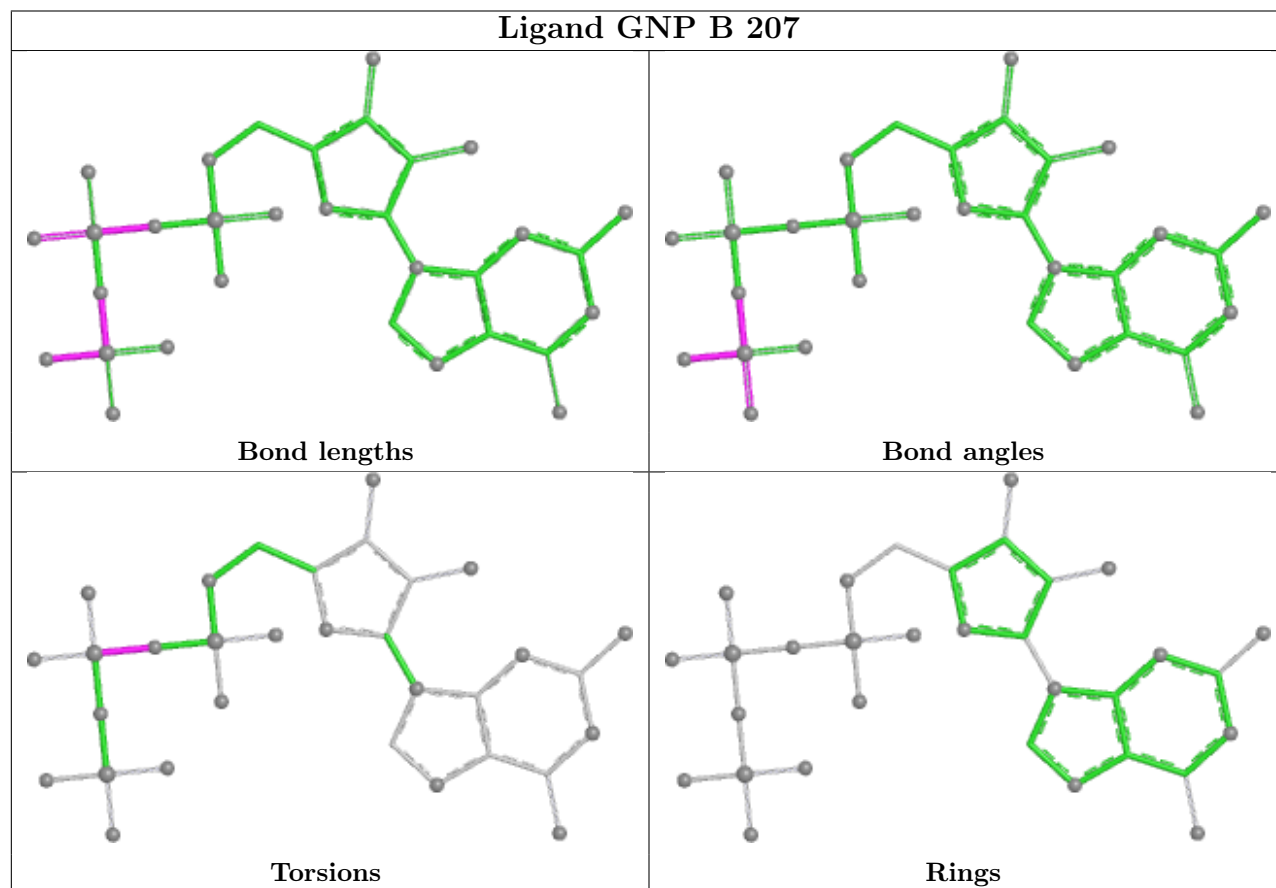
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	203	GOL	1	0
4	B	205	GOL	2	0

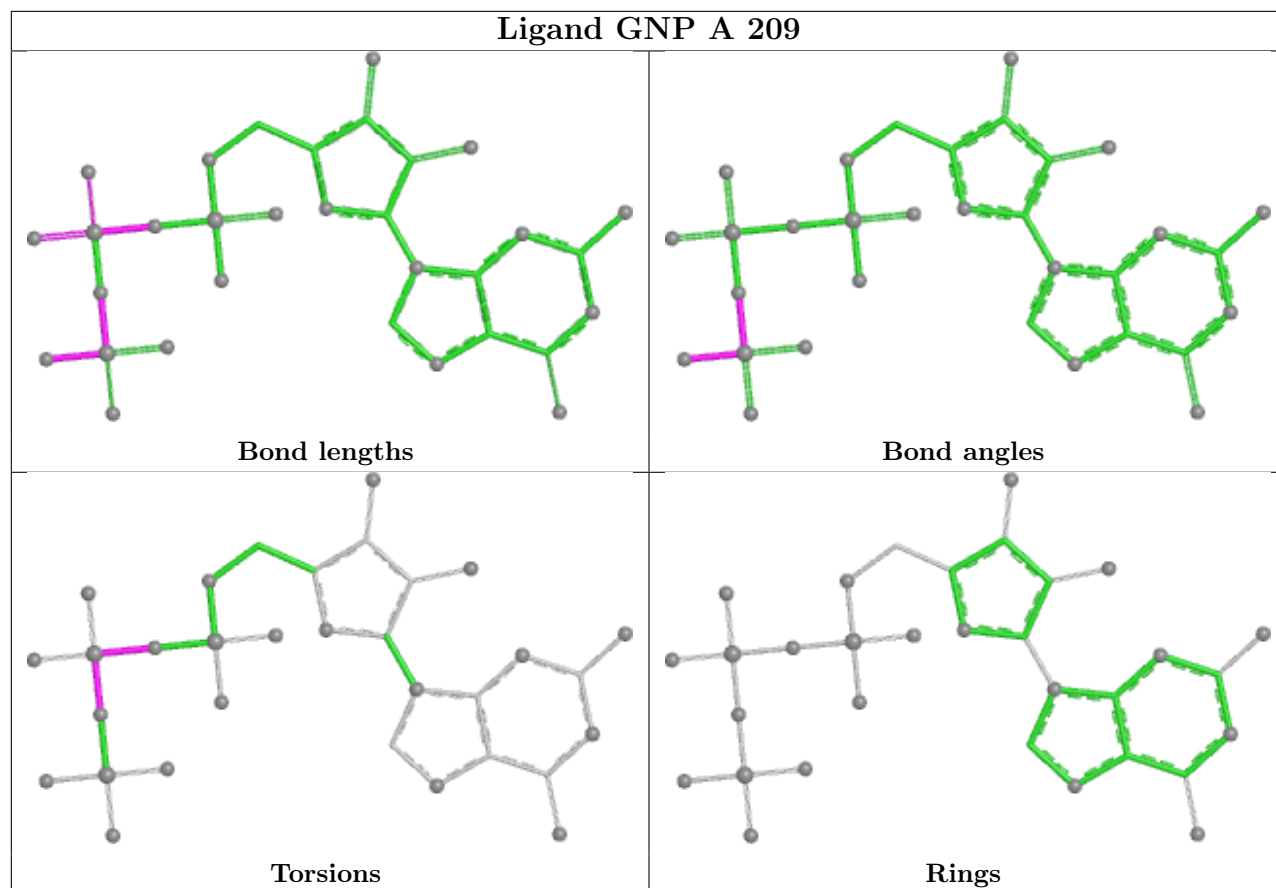
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	207	GOL	3	0
4	A	208	GOL	1	0
5	B	207	GNP	3	0
5	A	209	GNP	3	0
4	B	204	GOL	1	0
4	A	203	GOL	3	0
4	A	206	GOL	1	0
4	F	101	GOL	4	0

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 [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	184/184 (100%)	0.08	9 (4%)	35	37	23, 40, 68, 87	5 (2%)
1	B	183/184 (99%)	0.13	4 (2%)	62	65	29, 44, 75, 96	3 (1%)
2	D	12/14 (85%)	0.50	0	100	100	37, 40, 47, 49	0
2	F	12/14 (85%)	-0.14	0	100	100	36, 39, 46, 48	0
All	All	391/396 (98%)	0.11	13 (3%)	49	51	23, 42, 71, 96	8 (2%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	61	ALA	4.2
1	B	188	SER	3.5
1	B	58	PRO	3.3
1	A	12	PHE	3.0
1	A	5	ASP	2.8
1	A	81	PHE	2.6
1	A	60	GLY	2.6
1	A	83	SER	2.4
1	A	58	PRO	2.2
1	B	12	PHE	2.2
1	A	80	ARG	2.2
1	A	112	ASN	2.1
1	A	127	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(\AA^2)	Q<0.9
2	XAK	D	12	11/15	0.76	0.14	50,55,63,76	0
2	XAK	F	12	12/15	0.82	0.14	49,58,70,78	0
2	DTY	F	13	12/13	0.91	0.11	39,47,51,59	0
2	DTY	D	13	12/13	0.93	0.10	44,54,61,66	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

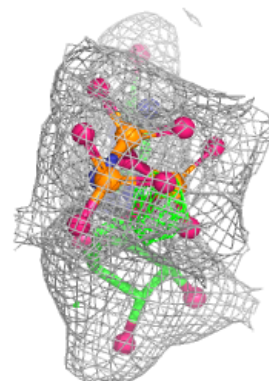
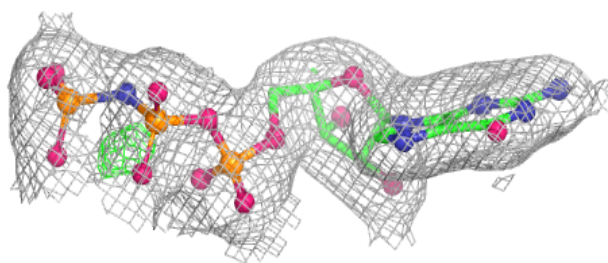
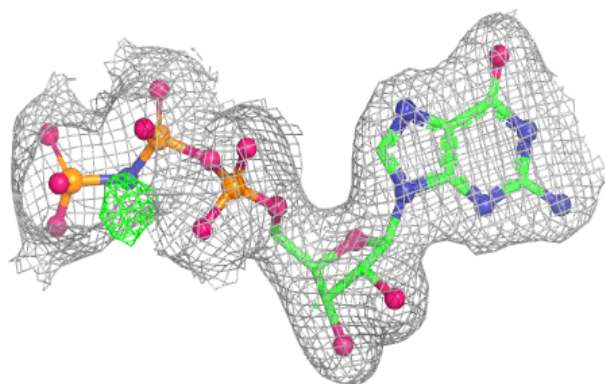
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	B	205	6/6	0.76	0.14	56,59,63,65	0
4	GOL	A	207	6/6	0.81	0.10	59,66,69,73	0
4	GOL	D	101	6/6	0.83	0.12	58,62,64,67	0
4	GOL	F	101	6/6	0.83	0.12	45,57,59,68	0
4	GOL	B	204	6/6	0.84	0.13	49,50,54,57	0
4	GOL	B	206	6/6	0.84	0.12	57,58,60,61	0
4	GOL	A	205	6/6	0.88	0.10	49,53,61,66	0
4	GOL	A	206	6/6	0.88	0.13	51,56,66,72	0
4	GOL	A	202	6/6	0.90	0.13	45,54,57,64	0
4	GOL	B	202	6/6	0.91	0.10	46,50,53,60	0
4	GOL	A	204	6/6	0.92	0.09	43,45,49,49	0
4	GOL	A	208	6/6	0.92	0.10	43,48,58,62	0
4	GOL	B	203	6/6	0.93	0.08	44,46,54,60	0
4	GOL	A	203	6/6	0.94	0.07	40,47,50,50	0
5	GNP	A	209	32/32	0.98	0.05	30,33,39,41	0
5	GNP	B	207	32/32	0.98	0.04	30,35,38,39	0
3	MG	A	201	1/1	1.00	0.08	32,32,32,32	0
3	MG	B	201	1/1	1.00	0.01	33,33,33,33	0

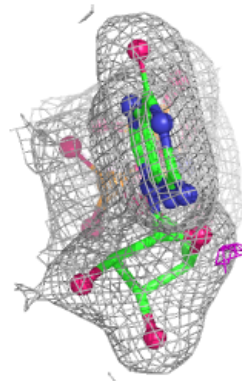
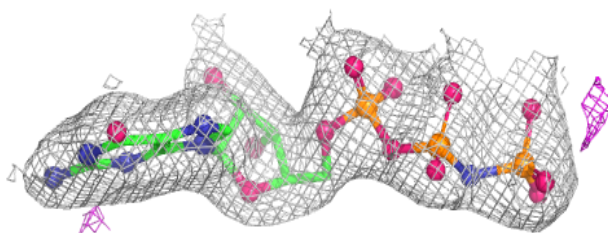
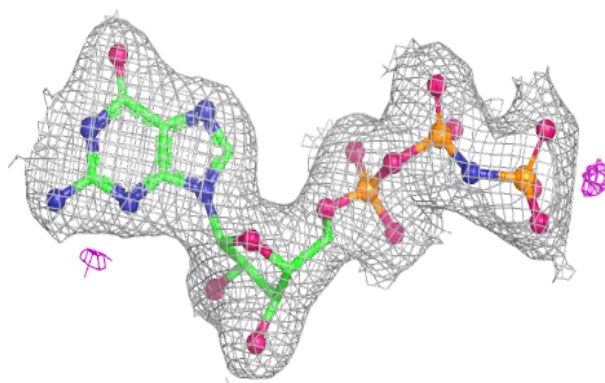
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GNP A 209:

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

**Electron density around GNP B 207:**

$2mF_o-DF_c$ (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.