



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 04:41 PM UTC

PDB ID : 9O0Q / pdb_00009o0q
Title : Crystal structure of GMPPNP-bound mutant MRAS in complex with MRTX1133
Authors : Bonsor, D.A.; Simanshu, D.K.
Deposited on : 2025-04-03
Resolution : 1.90 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

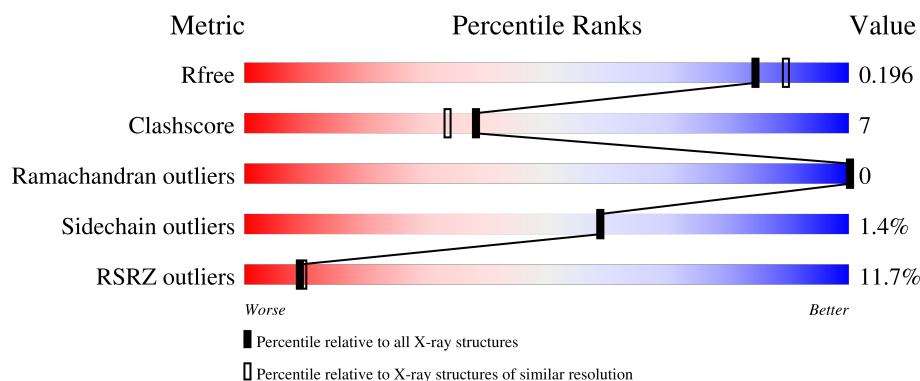
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	179	2% 86% 8% 6%
1	B	179	4% 85% 8% 6%
1	C	179	26% 73% 21% 6%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 4877 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.

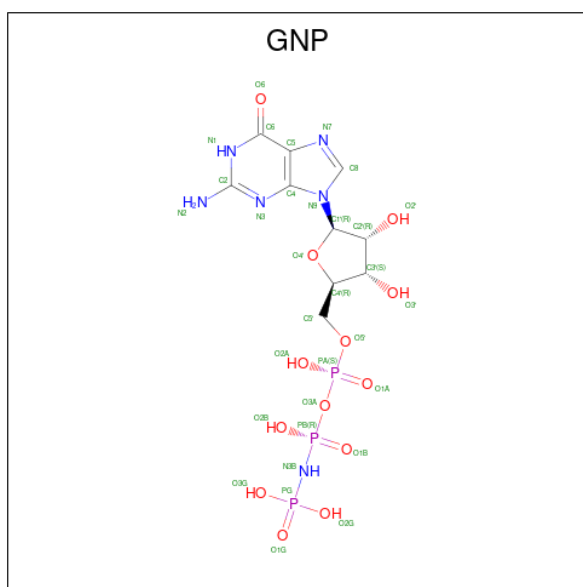
- Molecule 1 is a protein called Ras-related protein M-Ras.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	169	Total	C	N	O	S	0	0	0
			1375	876	234	260	5			
1	B	168	Total	C	N	O	S	0	1	0
			1378	878	234	261	5			
1	C	168	Total	C	N	O	S	0	0	0
			1326	843	227	252	4			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP O14807
A	74	TYR	PHE	engineered mutation	UNP O14807
A	105	HIS	ARG	engineered mutation	UNP O14807
A	106	TYR	PHE	engineered mutation	UNP O14807
A	109	GLN	LEU	engineered mutation	UNP O14807
B	0	GLY	-	expression tag	UNP O14807
B	74	TYR	PHE	engineered mutation	UNP O14807
B	105	HIS	ARG	engineered mutation	UNP O14807
B	106	TYR	PHE	engineered mutation	UNP O14807
B	109	GLN	LEU	engineered mutation	UNP O14807
C	0	GLY	-	expression tag	UNP O14807
C	74	TYR	PHE	engineered mutation	UNP O14807
C	105	HIS	ARG	engineered mutation	UNP O14807
C	106	TYR	PHE	engineered mutation	UNP O14807
C	109	GLN	LEU	engineered mutation	UNP O14807

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).

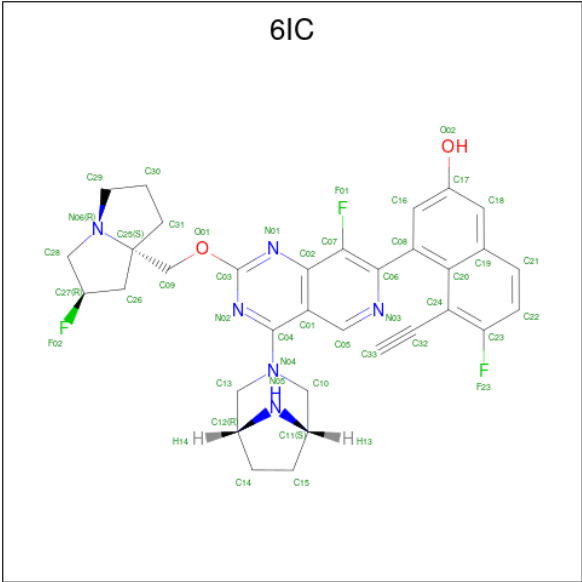


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
2	B	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
2	C	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

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

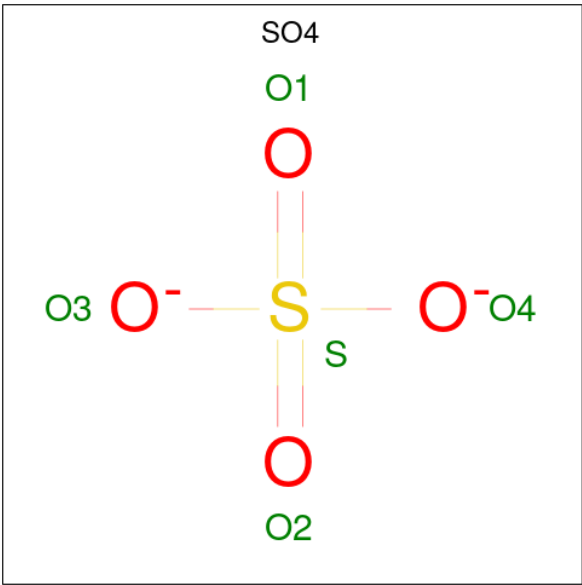
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 4-(4-[(1R,5S)-3,8-diazabicyclo[3.2.1]octan-3-yl]-8-fluoro-2-[[[(2R,4R,7aS)-2-fluorotetrahydro-1H-pyrrolizin-7a(5H)-yl]methoxy}pyrido[4,3-d]pyrimidin-7-yl)-5-ethynyl-6-fluoronaphthalen-2-ol (CCD ID: 6IC) (formula: C₃₃H₃₁F₃N₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			44	33	3	6	2		
4	B	1	Total	C	F	N	O	0	0
			44	33	3	6	2		
4	C	1	Total	C	F	N	O	0	0
			44	33	3	6	2		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



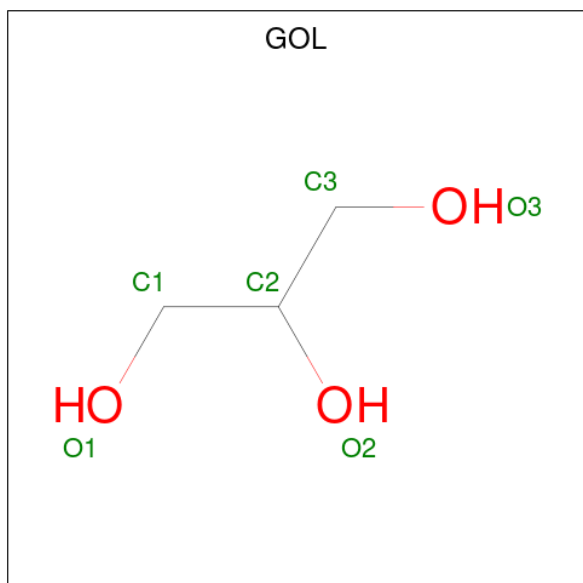
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		

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

- 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		

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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	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cl	0	0
			1	1		
7	C	1	Total	Cl	0	0
			1	1		

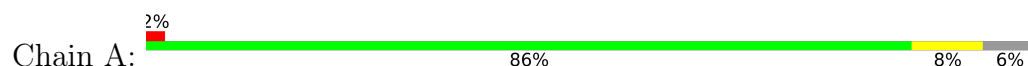
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	237	Total	O	0	0
			237	237		
8	B	180	Total	O	0	0
			180	180		
8	C	69	Total	O	0	0
			69	69		

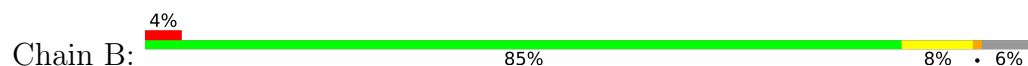
3 Residue-property plots [i](#)

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.

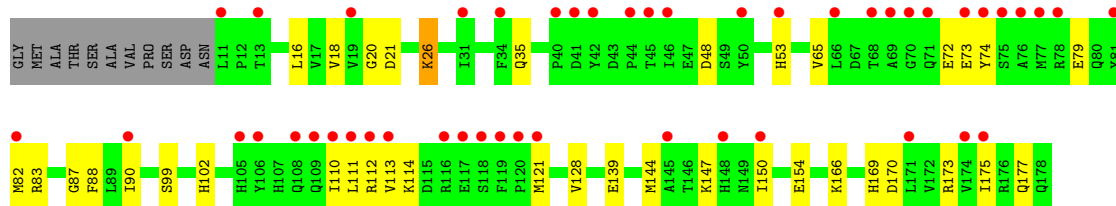
- Molecule 1: Ras-related protein M-Ras



- Molecule 1: Ras-related protein M-Ras



- Molecule 1: Ras-related protein M-Ras



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	82.06Å 110.88Å 194.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.70 – 1.90 44.70 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (44.70-1.90) 99.6 (44.70-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 1.90Å)	Xtriage
Refinement program	PHENIX 1.21_5207	Depositor
R, R_{free}	0.177 , 0.207 (Not available) , 0.196	Depositor DCC
R_{free} test set	3561 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.532	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 59.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4877	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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: MG, GOL, 6IC, SO4, GNP, CL

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	0.88	1/1405 (0.1%)	0.88	0/1901
1	B	0.71	0/1408	0.90	1/1904 (0.1%)
1	C	0.55	0/1353	0.69	0/1834
All	All	0.73	1/4166 (0.0%)	0.83	1/5639 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	138	ARG	C-N	7.88	1.44	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	41	ASP	CA-CB-CG	7.35	119.95	112.60

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	1375	0	1353	10	0
1	B	1378	0	1359	11	0
1	C	1326	0	1286	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	32	0	13	0	0
2	B	32	0	13	0	0
2	C	32	0	13	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	44	0	0	2	0
4	B	44	0	0	2	0
4	C	44	0	0	6	0
5	A	20	0	0	0	0
5	B	30	0	0	0	0
5	C	5	0	0	1	0
6	A	12	0	16	2	0
6	B	12	0	16	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	237	0	0	7	0
8	B	180	0	0	2	0
8	C	69	0	0	1	0
All	All	4877	0	4069	58	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 (58) 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:C:20:GLY:O	1:C:26:LYS:HE2	1.92	0.69
1:C:26:LYS:NZ	2:C:201:GNP:O1G	2.26	0.69
1:C:139:GLU:H	1:C:139:GLU:CD	2.01	0.67
1:C:173:ARG:O	1:C:177:GLN:HG2	1.99	0.62
4:B:203:6IC:C32	4:B:203:6IC:C06	2.78	0.61
4:A:203:6IC:C32	4:A:203:6IC:C06	2.79	0.60
1:A:69:ALA:HA	8:A:337:HOH:O	2.00	0.59
1:B:46:ILE:HD13	1:B:48:ASP:HB2	1.84	0.59
1:C:121:MET:HG3	1:C:150:ILE:HG21	1.85	0.58
1:A:71:GLN:NE2	8:A:303:HOH:O	2.39	0.56
1:C:128:VAL:HG11	1:C:154:GLU:HB3	1.88	0.55
6:A:208:GOL:H32	8:A:380:HOH:O	2.09	0.53
1:B:49:SER:HA	1:B:65:VAL:O	2.09	0.53
1:C:21:ASP:OD2	1:C:102:HIS:ND1	2.31	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:ASP:O	1:A:116:ARG:HD3	2.09	0.51
1:C:110:ILE:HG13	4:C:203:6IC:F23	2.00	0.51
1:B:35:GLN:HG3	1:C:35:GLN:HG3	1.93	0.50
1:C:87:GLY:HA3	1:C:175:ILE:HD11	1.94	0.49
1:C:82:MET:HG3	4:C:203:6IC:C19	2.42	0.49
1:A:143:GLU:OE2	8:A:301:HOH:O	2.20	0.48
1:B:51:LEU:HD11	1:C:53:HIS:CD2	2.49	0.48
1:C:169:HIS:ND1	5:C:204:SO4:O1	2.44	0.47
6:A:208:GOL:H12	8:A:466:HOH:O	2.14	0.47
1:C:18:VAL:HG12	1:C:26:LYS:HG2	1.95	0.47
1:C:83:ARG:O	1:C:114:LYS:NZ	2.41	0.47
1:C:88:PHE:O	1:C:121:MET:HA	2.15	0.47
4:C:203:6IC:C32	4:C:203:6IC:C06	2.93	0.47
1:A:46:ILE:O	1:A:46:ILE:HD12	2.15	0.47
1:C:21:ASP:OD2	1:C:99:SER:HA	2.15	0.46
4:B:203:6IC:C32	4:B:203:6IC:C07	2.94	0.46
1:C:121:MET:CG	1:C:150:ILE:HG21	2.46	0.46
1:C:82:MET:CE	1:C:88:PHE:HE2	2.29	0.46
1:B:15:LYS:HE2	1:B:15:LYS:HB2	1.78	0.45
1:C:79:GLU:O	1:C:83:ARG:HG3	2.17	0.44
1:B:142:LYS:HE2	8:B:312:HOH:O	2.16	0.44
1:C:90:ILE:CD1	1:C:121:MET:HE2	2.47	0.44
1:C:16:LEU:HB2	1:C:65:VAL:HG22	2.00	0.44
1:C:170:ASP:OD1	1:C:173:ARG:NH1	2.50	0.43
1:A:139:GLU:HG3	8:A:424:HOH:O	2.19	0.43
1:A:178:GLN:NE2	8:A:307:HOH:O	2.48	0.43
1:A:42:TYR:CZ	1:A:44:PRO:HG3	2.53	0.43
1:A:145:ALA:HB1	1:A:150:ILE:O	2.18	0.43
1:B:35:GLN:HE21	1:C:35:GLN:CG	2.32	0.42
1:C:74:TYR:CD2	1:C:112:ARG:NH2	2.88	0.42
1:C:74:TYR:HA	4:C:203:6IC:O02	2.19	0.42
1:C:166:LYS:NZ	1:C:170:ASP:OD2	2.51	0.42
1:C:72:GLU:HG3	4:C:203:6IC:C02	2.49	0.42
1:B:34:PHE:CE2	1:B:52:LYS:HB3	2.55	0.42
1:B:69:ALA:HA	8:B:309:HOH:O	2.21	0.41
4:A:203:6IC:C32	4:A:203:6IC:C07	2.99	0.41
1:C:139:GLU:CD	1:C:139:GLU:N	2.76	0.41
1:A:46:ILE:HD13	1:A:48:ASP:HB2	2.02	0.41
1:B:158:LYS:HB3	1:B:158:LYS:HE3	1.64	0.41
1:C:72:GLU:OE1	8:C:302:HOH:O	2.22	0.40
1:B:17:VAL:HG12	1:B:19:VAL:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:ILE:HG22	1:C:111:LEU:HD23	2.04	0.40
1:C:113:VAL:HG21	4:C:203:6IC:C18	2.52	0.40
1:C:144:MET:SD	1:C:147:LYS:HE2	2.61	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	167/179 (93%)	165 (99%)	2 (1%)	0	100	100
1	B	167/179 (93%)	164 (98%)	3 (2%)	0	100	100
1	C	166/179 (93%)	161 (97%)	5 (3%)	0	100	100
All	All	500/537 (93%)	490 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	151/159 (95%)	150 (99%)	1 (1%)	76	78
1	B	152/159 (96%)	150 (99%)	2 (1%)	61	61
1	C	141/159 (89%)	138 (98%)	3 (2%)	47	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	444/477 (93%)	438 (99%)	6 (1%)	59 59

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	GLU
1	B	122	ILE
1	B	158	LYS
1	C	26	LYS
1	C	48	ASP
1	C	73	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	HIS
1	A	178	GLN
1	B	35	GLN
1	B	59	GLN
1	C	35	GLN
1	C	53	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 5 are monoatomic - leaving 21 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$
5	SO4	B	209	-	4,4,4	0.81	0	6,6,6	0.40	0
6	GOL	A	208	-	5,5,5	0.56	0	5,5,5	1.29	1 (20%)
5	SO4	B	205	-	4,4,4	0.74	0	6,6,6	0.31	0
5	SO4	A	206	-	4,4,4	0.82	0	6,6,6	0.27	0
4	6IC	B	203	-	49,51,51	1.00	5 (10%)	57,78,78	1.22	3 (5%)
2	GNP	B	201	3	34,34,34	2.58	9 (26%)	47,54,54	1.92	9 (19%)
5	SO4	A	204	-	4,4,4	0.72	0	6,6,6	0.70	0
5	SO4	B	208	-	4,4,4	0.73	0	6,6,6	0.39	0
4	6IC	A	203	-	49,51,51	0.93	2 (4%)	57,78,78	1.44	4 (7%)
6	GOL	B	210	-	5,5,5	0.41	0	5,5,5	0.89	0
5	SO4	B	204	-	4,4,4	0.76	0	6,6,6	0.47	0
2	GNP	A	201	3	34,34,34	1.11	5 (14%)	47,54,54	0.84	2 (4%)
6	GOL	B	211	-	5,5,5	0.29	0	5,5,5	0.59	0
5	SO4	A	205	-	4,4,4	0.82	0	6,6,6	0.32	0
4	6IC	C	203	-	49,51,51	0.59	0	57,78,78	1.49	8 (14%)
5	SO4	B	206	-	4,4,4	0.75	0	6,6,6	0.19	0
2	GNP	C	201	3	34,34,34	2.04	6 (17%)	47,54,54	1.89	7 (14%)
5	SO4	A	207	-	4,4,4	0.82	0	6,6,6	0.49	0
6	GOL	A	209	-	5,5,5	0.51	0	5,5,5	0.91	0
5	SO4	C	204	-	4,4,4	0.77	0	6,6,6	0.19	0
5	SO4	B	207	-	4,4,4	0.81	0	6,6,6	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	A	209	-	-	4/4/4/4	-
2	GNP	A	201	3	-	3/18/38/38	0/3/3/3
6	GOL	B	211	-	-	0/4/4/4	-
4	6IC	A	203	-	-	1/14/55/55	0/8/8/8
6	GOL	A	208	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	B	210	-	-	4/4/4/4	-
4	6IC	C	203	-	-	2/14/55/55	0/8/8/8
2	GNP	C	201	3	-	3/18/38/38	0/3/3/3
4	6IC	B	203	-	-	1/14/55/55	0/8/8/8
2	GNP	B	201	3	-	2/18/38/38	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	GNP	PB-O3A	8.66	1.69	1.59
2	C	201	GNP	PG-N3B	6.77	1.81	1.63
2	B	201	GNP	PG-N3B	6.08	1.79	1.63
2	C	201	GNP	PG-O1G	5.55	1.54	1.46
2	B	201	GNP	PA-O3A	5.07	1.65	1.59
2	B	201	GNP	PG-O1G	4.91	1.53	1.46
2	C	201	GNP	PB-O3A	4.60	1.64	1.59
2	B	201	GNP	C6-N1	4.35	1.47	1.38
2	C	201	GNP	PB-O1B	4.11	1.52	1.46
2	A	201	GNP	PG-O3G	-3.34	1.47	1.56
4	A	203	6IC	C05-C01	3.20	1.45	1.42
4	B	203	6IC	C05-C01	2.94	1.45	1.42
2	B	201	GNP	PB-O1B	2.83	1.50	1.46
4	B	203	6IC	C13-C12	2.82	1.56	1.52
2	B	201	GNP	PG-O3G	-2.79	1.49	1.56
2	A	201	GNP	PG-O2G	-2.66	1.49	1.56
2	A	201	GNP	PB-O1B	2.65	1.50	1.46
4	B	203	6IC	C24-C20	2.58	1.47	1.43
2	C	201	GNP	C6-N1	2.55	1.43	1.38
2	A	201	GNP	PB-O2B	-2.51	1.50	1.56
4	B	203	6IC	C04-N02	2.46	1.35	1.32
2	B	201	GNP	C5'-C4'	2.21	1.58	1.51
2	A	201	GNP	PG-O1G	2.21	1.49	1.46
2	B	201	GNP	C2-N2	2.18	1.39	1.34
4	B	203	6IC	C10-C11	2.10	1.55	1.52
4	A	203	6IC	C10-C11	2.08	1.55	1.52
2	C	201	GNP	PA-O5'	2.07	1.67	1.59

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	201	GNP	O1G-PG-N3B	-8.48	99.28	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	201	GNP	O1B-PB-N3B	7.60	122.96	111.77
4	A	203	6IC	C15-C11-C10	7.09	118.38	111.70
2	C	201	GNP	O2A-PA-O3A	5.03	120.87	107.27
4	C	203	6IC	C29-N06-C28	4.84	123.57	114.48
2	B	201	GNP	O2B-PB-O1B	4.68	119.90	109.87
2	C	201	GNP	O1G-PG-N3B	-4.52	105.11	111.77
4	B	203	6IC	C15-C11-C10	4.51	115.95	111.70
2	A	201	GNP	O2B-PB-O1B	4.14	118.74	109.87
4	C	203	6IC	C11-C10-N04	-3.95	107.08	110.19
4	C	203	6IC	C16-C08-C06	-3.78	113.45	119.16
2	C	201	GNP	O3G-PG-O1G	3.52	122.28	113.45
2	C	201	GNP	O3A-PA-O1A	-3.43	100.37	110.70
4	B	203	6IC	C08-C06-N03	3.28	121.53	115.27
2	B	201	GNP	O2G-PG-O3G	3.24	116.31	107.59
4	A	203	6IC	C08-C06-N03	3.17	121.32	115.27
4	C	203	6IC	C26-C25-C31	3.09	118.74	113.58
2	B	201	GNP	O3'-C3'-C2'	-2.97	102.29	111.82
2	C	201	GNP	O2A-PA-O1A	2.83	125.63	112.44
2	C	201	GNP	O3A-PB-N3B	-2.75	98.96	106.59
2	B	201	GNP	O2A-PA-O1A	2.65	124.79	112.44
2	B	201	GNP	C2-N3-C4	2.60	116.77	112.30
4	A	203	6IC	O01-C09-C25	-2.51	102.95	106.59
2	B	201	GNP	O5'-C5'-C4'	-2.47	100.59	108.99
4	C	203	6IC	C10-N04-C04	2.46	127.34	118.91
4	B	203	6IC	O02-C17-C16	-2.38	113.63	119.85
4	C	203	6IC	C31-C30-C29	-2.29	99.93	104.20
2	A	201	GNP	O3G-PG-O1G	-2.13	108.10	113.45
6	A	208	GOL	C3-C2-C1	2.12	119.59	111.80
2	B	201	GNP	C4'-O4'-C1'	2.10	114.10	109.47
4	A	203	6IC	C30-C31-C25	-2.10	101.87	104.62
2	B	201	GNP	C2'-C3'-C4'	2.09	106.66	102.61
4	C	203	6IC	C20-C24-C32	-2.05	120.12	123.78
4	C	203	6IC	C01-C04-N04	2.02	124.64	121.18

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	GNP	PB-N3B-PG-O1G
2	A	201	GNP	PG-N3B-PB-O1B
2	B	201	GNP	PB-N3B-PG-O1G
2	B	201	GNP	PG-N3B-PB-O1B

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Mol	Chain	Res	Type	Atoms
2	C	201	GNP	PB-N3B-PG-O1G
2	C	201	GNP	PG-N3B-PB-O1B
2	C	201	GNP	PG-N3B-PB-O3A
4	C	203	6IC	O01-C09-C25-C26
6	A	208	GOL	O1-C1-C2-C3
6	A	209	GOL	O1-C1-C2-O2
6	A	209	GOL	O1-C1-C2-C3
6	A	209	GOL	C1-C2-C3-O3
6	B	210	GOL	C1-C2-C3-O3
6	A	208	GOL	O1-C1-C2-O2
6	A	209	GOL	O2-C2-C3-O3
6	B	210	GOL	O2-C2-C3-O3
6	B	210	GOL	O1-C1-C2-O2
2	A	201	GNP	PG-N3B-PB-O3A
4	C	203	6IC	C01-C04-N04-C10
4	B	203	6IC	C01-C04-N04-C10
6	B	210	GOL	O1-C1-C2-C3
4	A	203	6IC	C01-C04-N04-C10

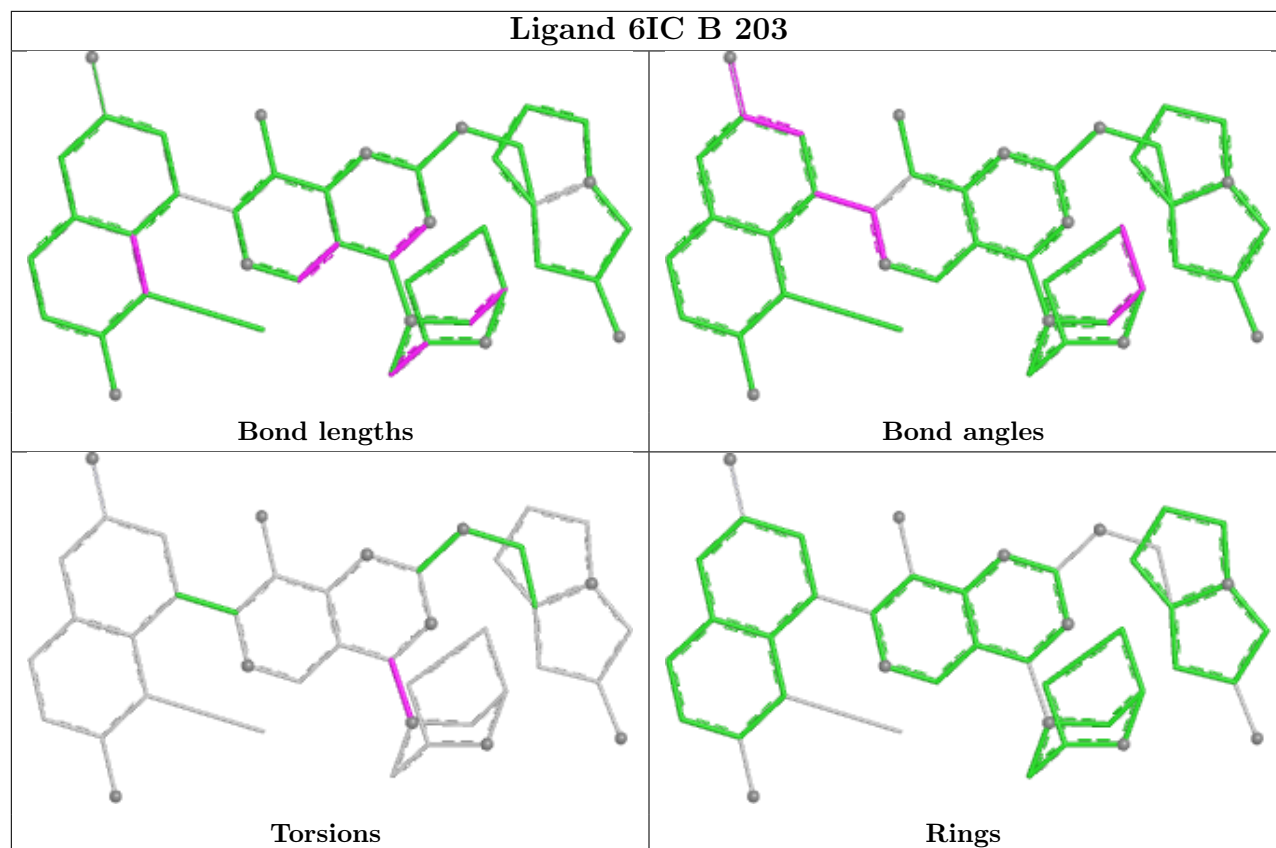
There are no ring outliers.

6 monomers are involved in 14 short contacts:

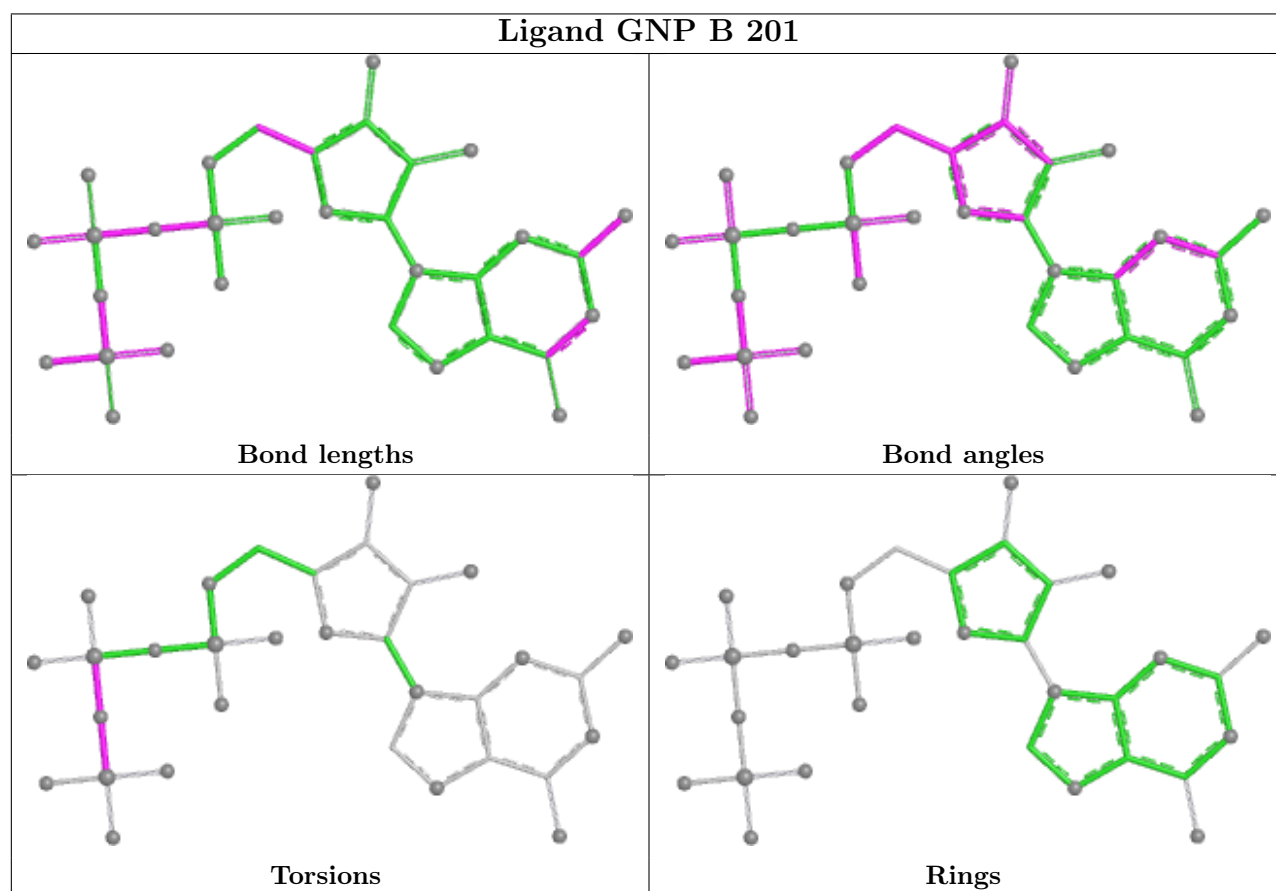
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	208	GOL	2	0
4	B	203	6IC	2	0
4	A	203	6IC	2	0
4	C	203	6IC	6	0
2	C	201	GNP	1	0
5	C	204	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

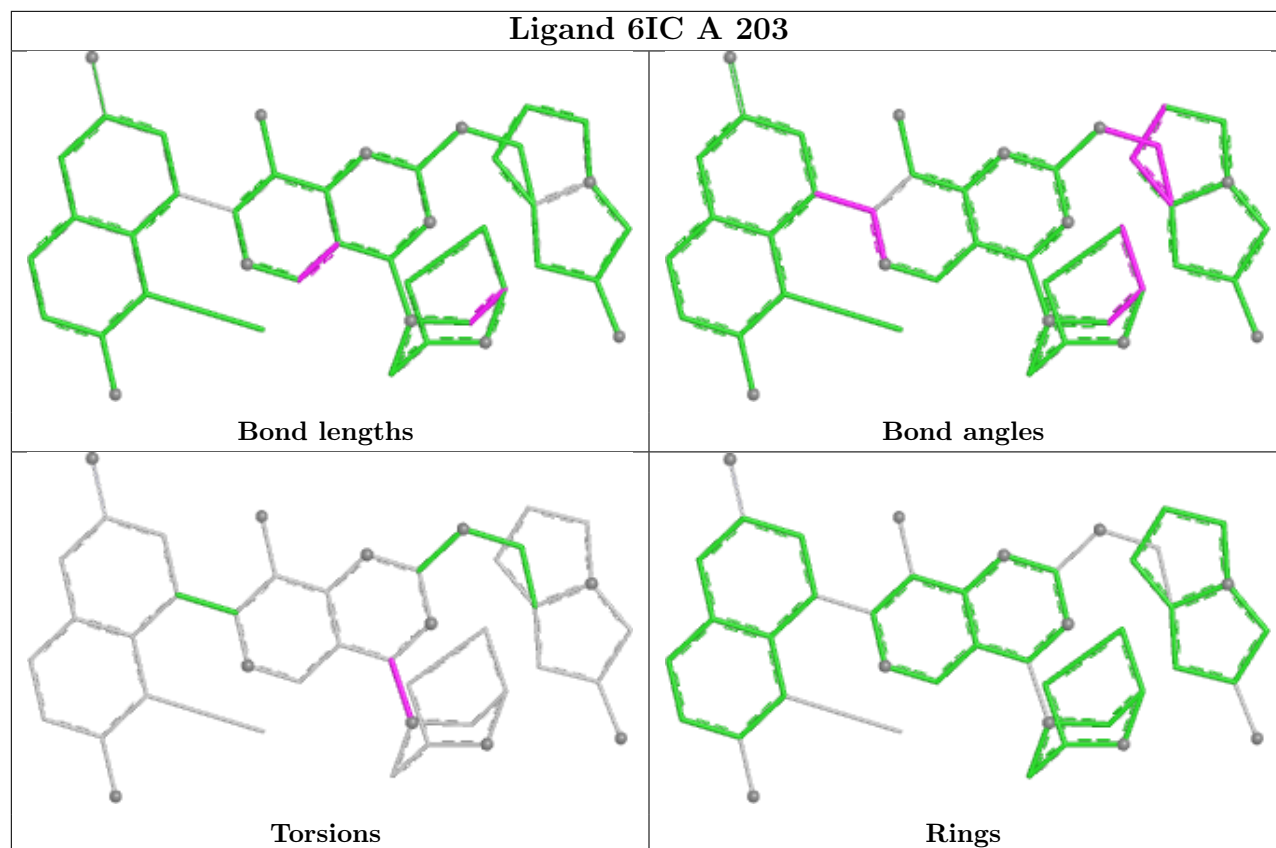
Ligand 6IC B 203



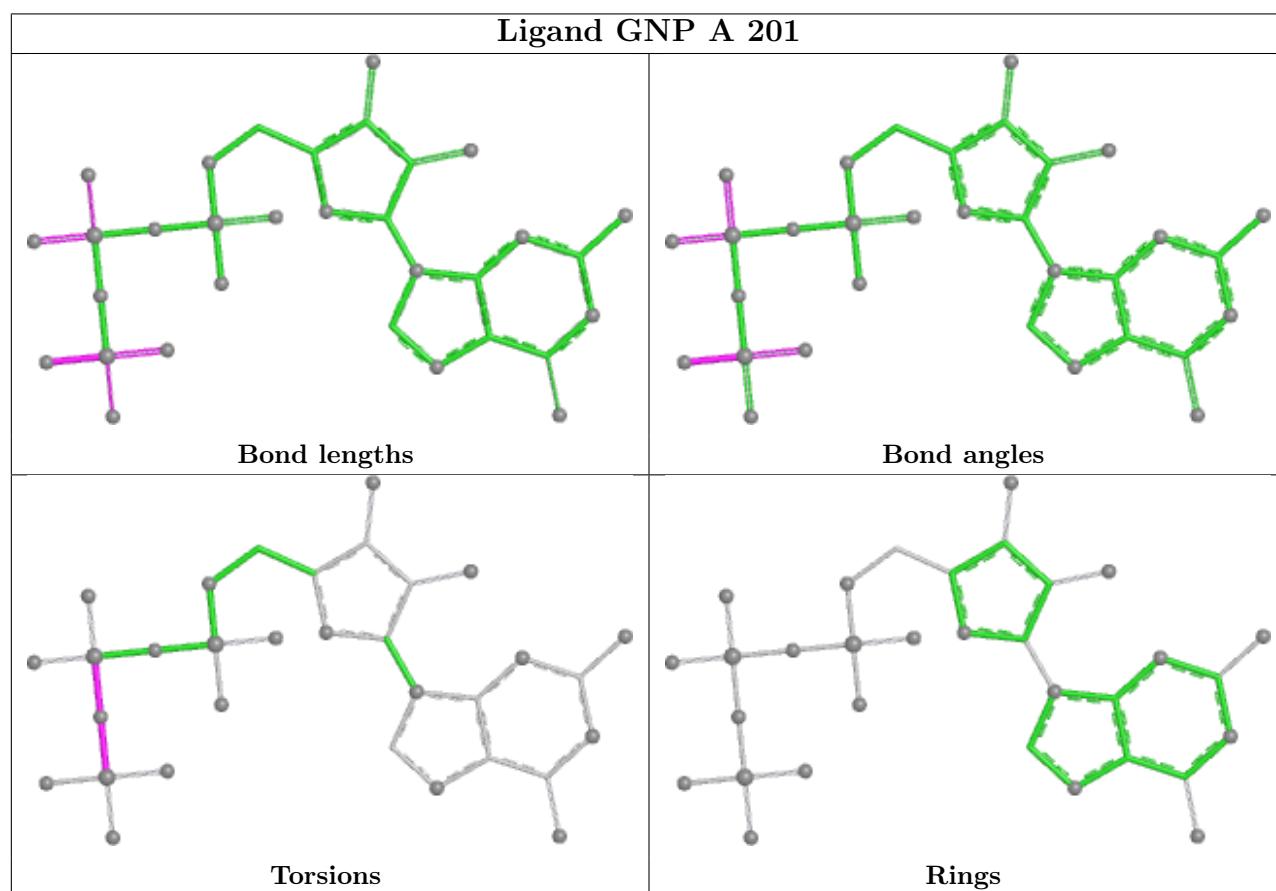
Ligand GNP B 201



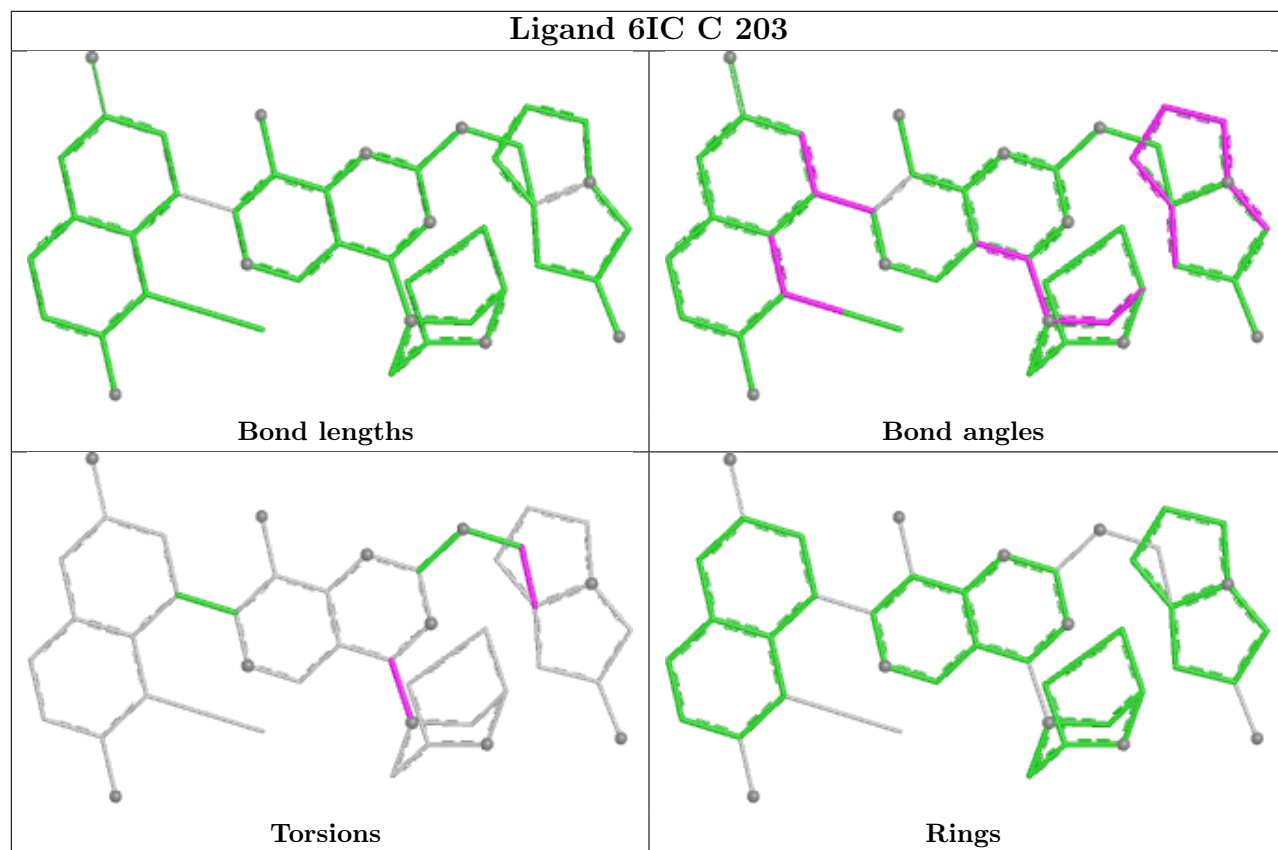
Ligand 6IC A 203



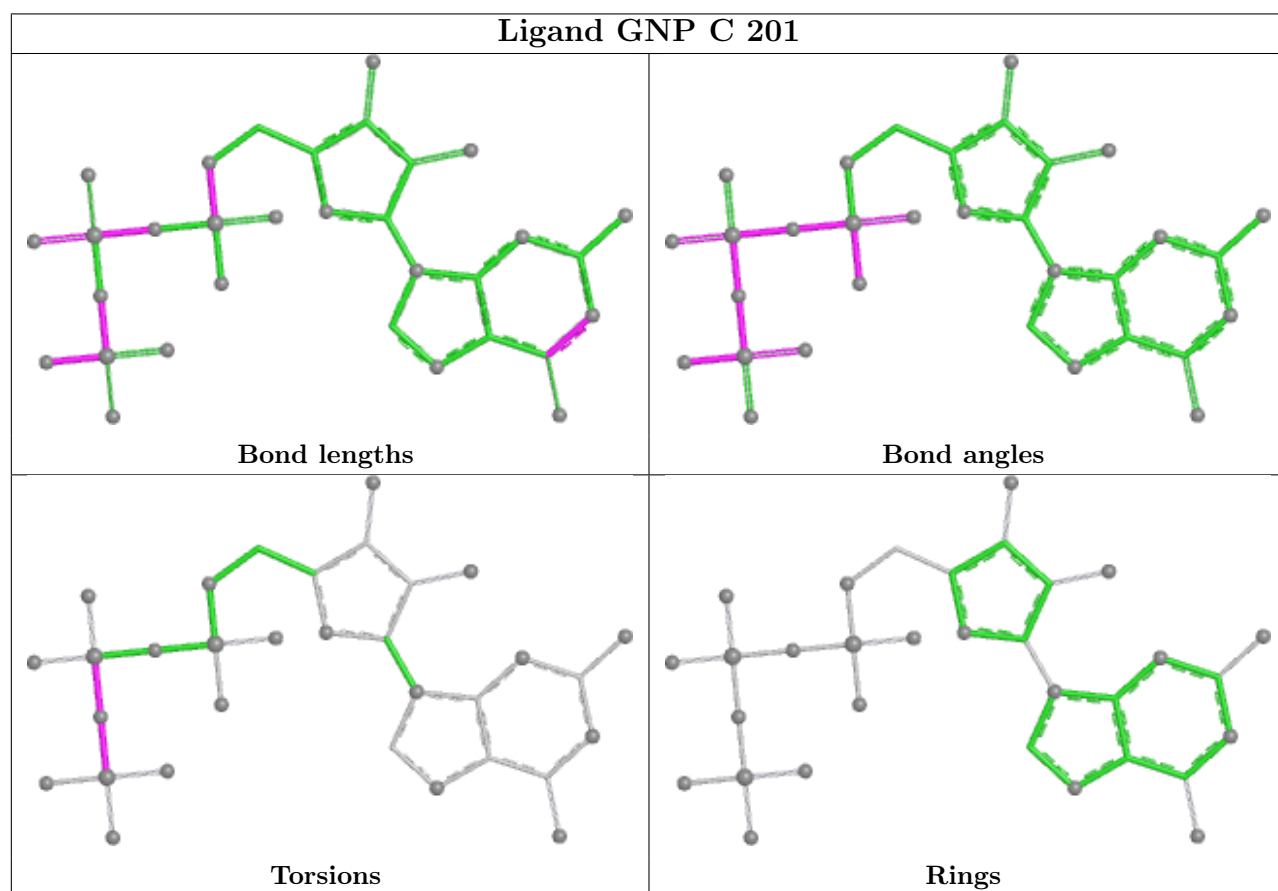
Ligand GNP A 201



Ligand 6IC C 203



Ligand GNP C 201



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	169/179 (94%)	-0.14	4 (2%) 59 63	28, 38, 67, 106	0
1	B	168/179 (93%)	0.14	8 (4%) 35 38	21, 47, 84, 94	1 (0%)
1	C	168/179 (93%)	1.39	47 (27%) 1 1	38, 79, 123, 134	0
All	All	505/537 (94%)	0.46	59 (11%) 9 10	21, 49, 110, 134	1 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	41	ASP	7.3
1	C	119	PHE	5.2
1	C	42	TYR	4.8
1	C	111	LEU	4.7
1	C	113	VAL	4.5
1	C	108	GLN	4.3
1	C	120	PRO	4.2
1	C	44	PRO	4.1
1	C	46	ILE	3.9
1	C	70	GLY	3.9
1	A	46	ILE	3.8
1	C	74	TYR	3.7
1	C	45	THR	3.7
1	B	46	ILE	3.6
1	C	81	TYR	3.5
1	C	110	ILE	3.5
1	C	116	ARG	3.4
1	A	138	ARG	3.4
1	B	138	ARG	3.4
1	C	105	HIS	3.2
1	C	66	LEU	3.2
1	B	53	HIS	3.1
1	A	81	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	77	MET	3.0
1	C	68	THR	3.0
1	C	50	TYR	2.9
1	C	11	LEU	2.9
1	C	76	ALA	2.9
1	C	112	ARG	2.9
1	C	75	SER	2.8
1	C	90	ILE	2.7
1	B	81	TYR	2.7
1	C	150	ILE	2.7
1	A	45	THR	2.6
1	C	31	ILE	2.6
1	C	71	GLN	2.6
1	C	118	SER	2.5
1	C	145	ALA	2.5
1	B	41	ASP	2.5
1	C	34	PHE	2.4
1	C	13	THR	2.4
1	C	117	GLU	2.4
1	C	148	HIS	2.4
1	C	109	GLN	2.3
1	C	19	VAL	2.3
1	C	174	VAL	2.3
1	C	175	ILE	2.3
1	C	121	MET	2.3
1	C	53	HIS	2.3
1	C	69	ALA	2.2
1	C	73	GLU	2.2
1	C	106	TYR	2.2
1	C	82	MET	2.1
1	C	171	LEU	2.1
1	B	11	LEU	2.1
1	B	37	ILE	2.1
1	B	77	MET	2.0
1	C	78	ARG	2.0
1	C	40	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

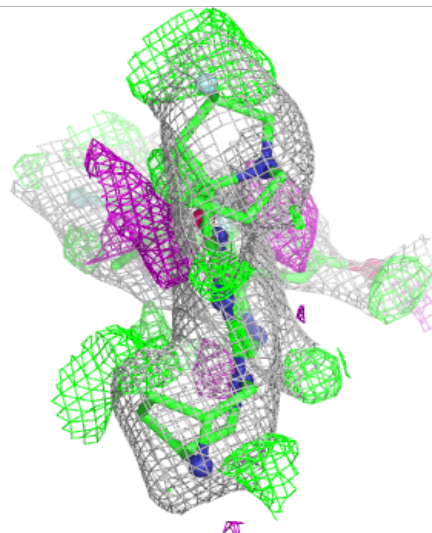
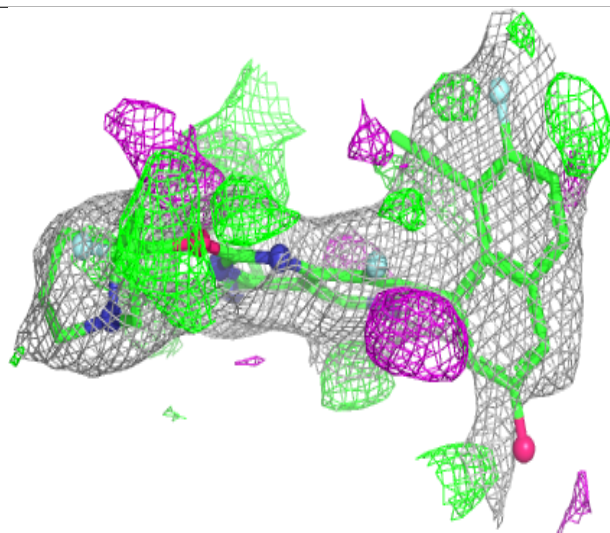
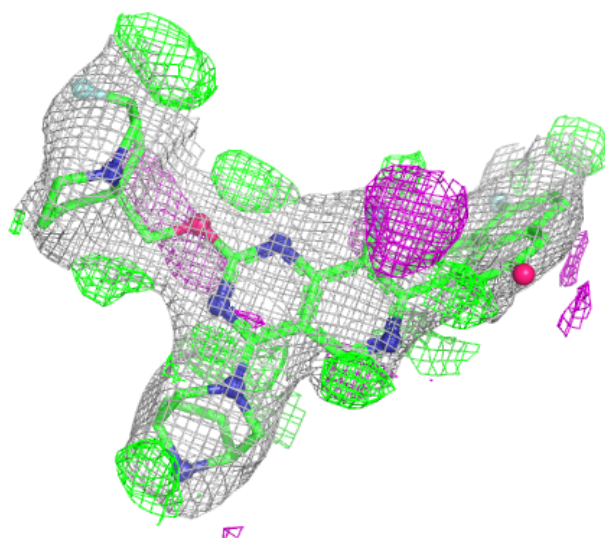
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	GOL	B	211	6/6	0.56	0.18	79,91,97,100	0
6	GOL	B	210	6/6	0.79	0.17	74,78,86,88	0
5	SO4	B	206	5/5	0.79	0.08	98,100,110,118	0
5	SO4	A	206	5/5	0.80	0.11	84,87,100,109	0
6	GOL	A	209	6/6	0.80	0.16	67,74,76,83	0
4	6IC	C	203	44/44	0.81	0.20	76,88,94,110	0
6	GOL	A	208	6/6	0.82	0.15	52,54,62,63	0
5	SO4	A	207	5/5	0.84	0.10	74,86,108,134	0
5	SO4	A	205	5/5	0.87	0.11	52,86,92,102	0
5	SO4	B	207	5/5	0.87	0.08	83,84,118,128	0
5	SO4	B	208	5/5	0.88	0.10	69,80,103,103	0
5	SO4	B	205	5/5	0.89	0.11	75,83,97,107	0
5	SO4	B	209	5/5	0.89	0.09	56,58,74,84	0
7	CL	C	205	1/1	0.90	0.14	88,88,88,88	0
5	SO4	C	204	5/5	0.93	0.07	64,67,92,96	0
2	GNP	C	201	32/32	0.94	0.08	37,49,66,69	0
5	SO4	B	204	5/5	0.95	0.07	59,66,72,75	0
7	CL	B	212	1/1	0.95	0.13	85,85,85,85	0
4	6IC	B	203	44/44	0.95	0.08	36,46,51,55	0
4	6IC	A	203	44/44	0.97	0.06	25,32,35,38	0
5	SO4	A	204	5/5	0.97	0.06	52,53,56,60	0
2	GNP	B	201	32/32	0.98	0.05	32,38,44,45	0
2	GNP	A	201	32/32	0.98	0.05	28,31,35,37	0
3	MG	A	202	1/1	0.99	0.02	33,33,33,33	0
3	MG	C	202	1/1	0.99	0.04	62,62,62,62	0
3	MG	B	202	1/1	1.00	0.02	41,41,41,41	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.

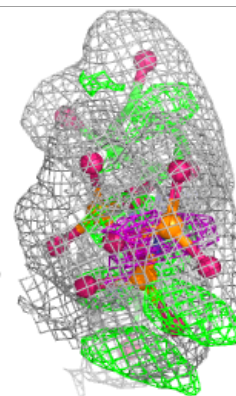
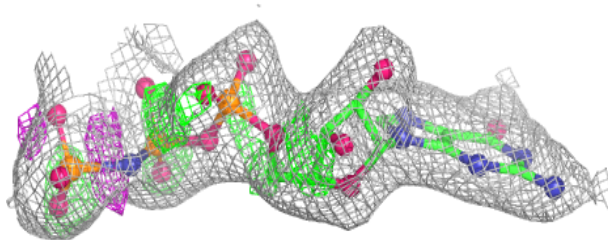
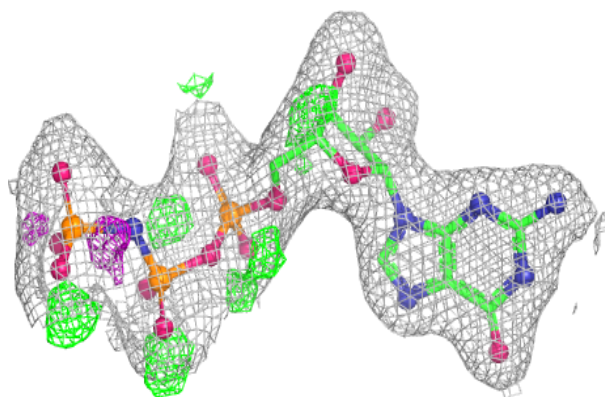
Electron density around 6IC C 203:

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



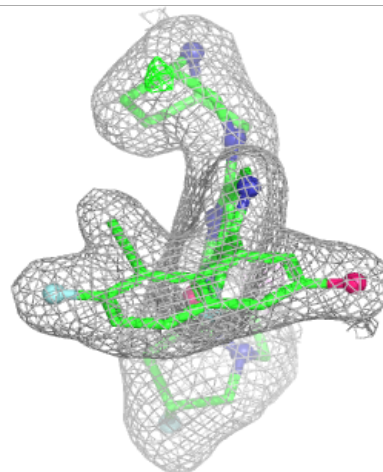
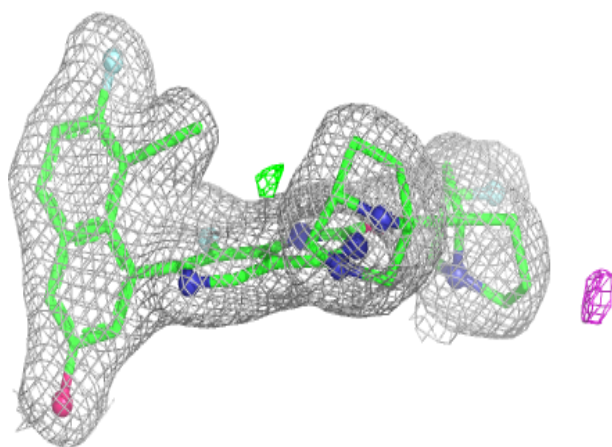
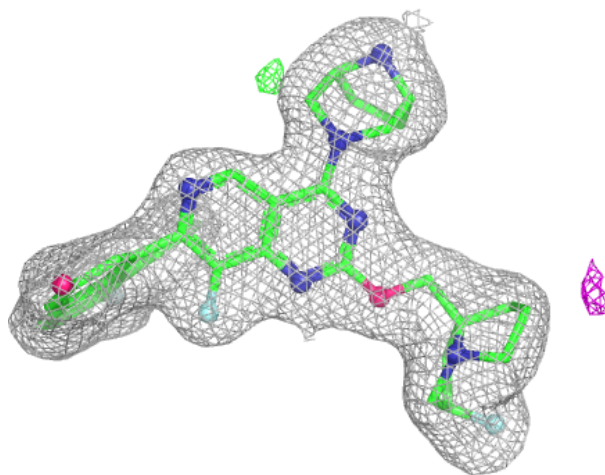
Electron density around GNP C 201:

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



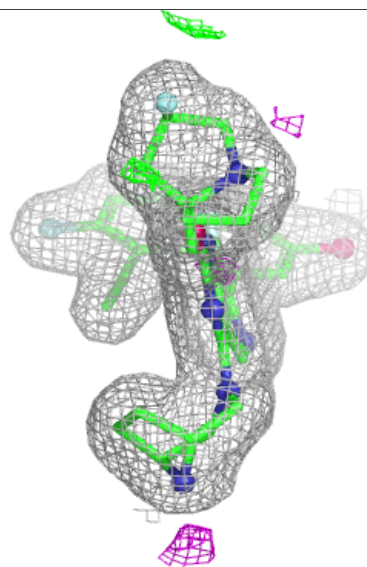
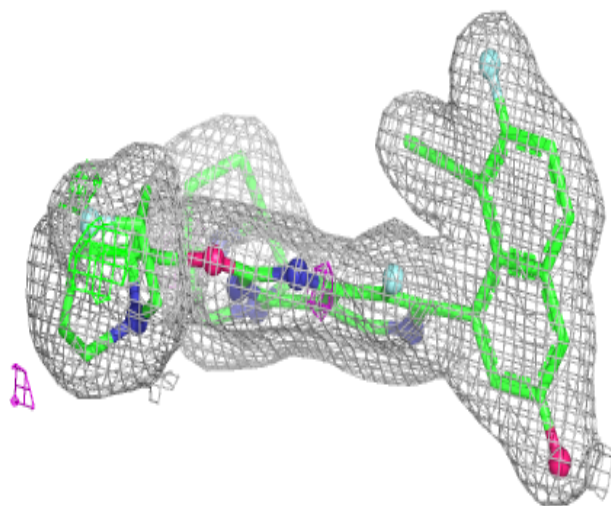
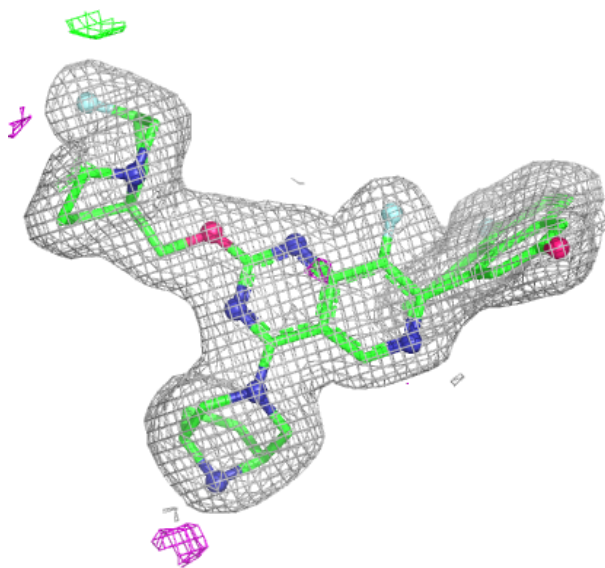
Electron density around 6IC B 203:

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



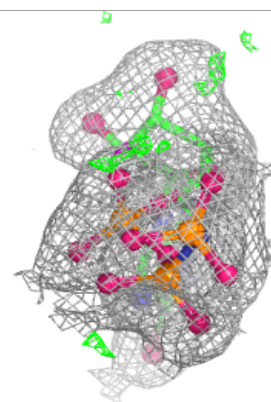
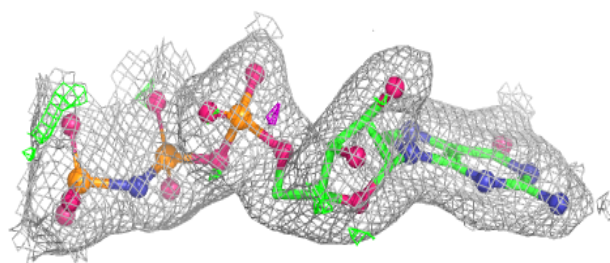
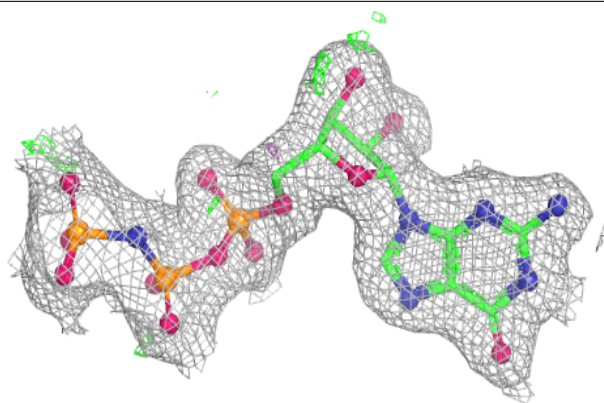
Electron density around 6IC A 203:

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

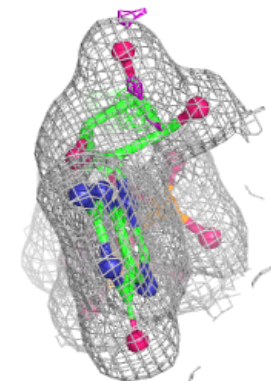
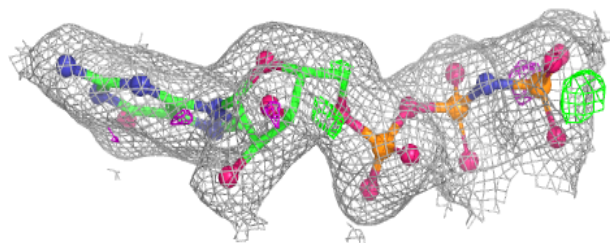
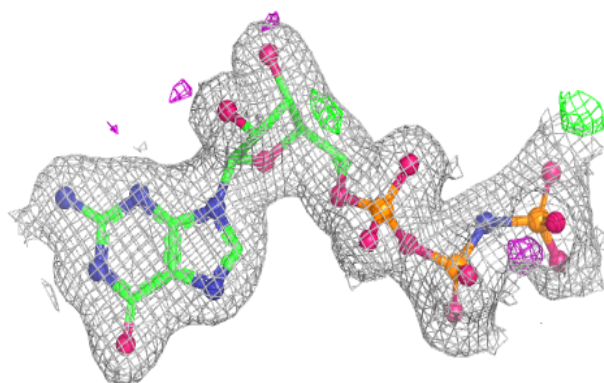


Electron density around GNP B 201:

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

**Electron density around GNP A 201:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.