



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:05 PM UTC

PDB ID : 8P3I / pdb_00008p3i
Title : Fusion hSlp2-a_Rab27A bound to covalent hit fragment IMP-1721
Authors : De Vita, E.; Brustur, D.; Tersa, M.; Petracca, R.; Morgan, R.M.L.; Lanyon-Hogg, T.; Norman, J.C.; Cota, E.; Tate, E.W.
Deposited on : 2023-05-17
Resolution : 2.00 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

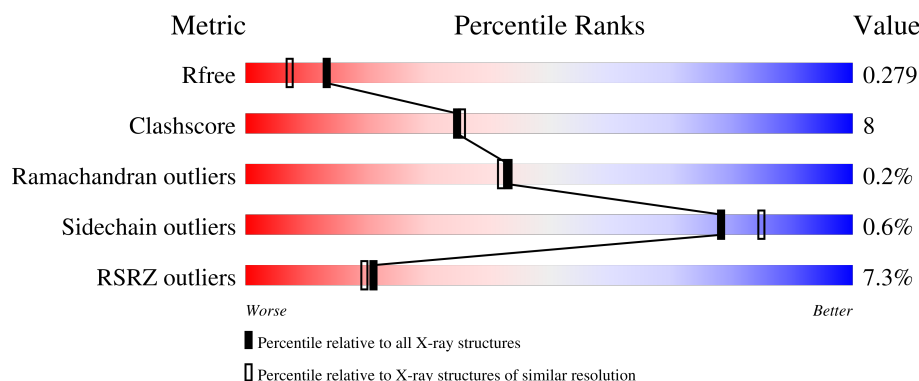
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	230	
1	B	230	

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
3	GOL	B	204	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3586 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.

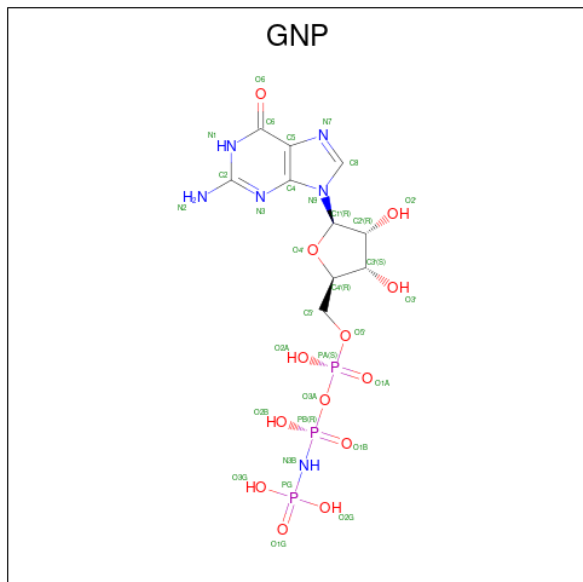
- Molecule 1 is a protein called Synaptotagmin-like protein 2,Ras-related protein Rab-27A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1680	1066	289	316	9			
1	B	212	Total	C	N	O	S	0	0	0
			1669	1059	290	312	8			

There are 24 discrepancies between the modelled and reference sequences:

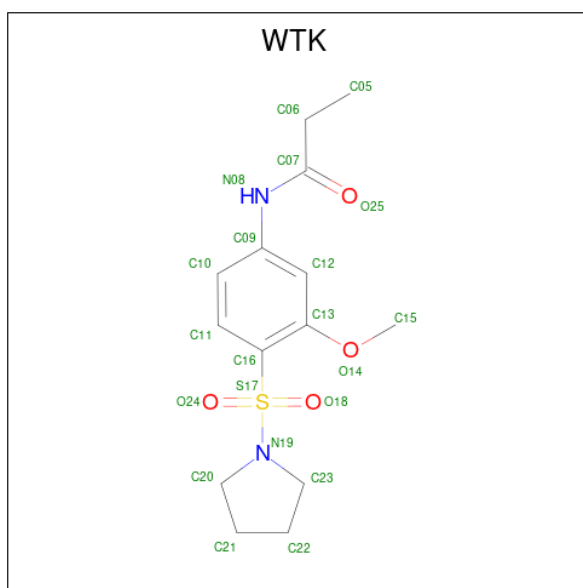
Chain	Residue	Modelled	Actual	Comment	Reference
A	-38	GLY	-	expression tag	UNP Q9HCH5
A	-37	HIS	-	expression tag	UNP Q9HCH5
A	-36	MET	-	expression tag	UNP Q9HCH5
A	-9B	GLY	-	linker	UNP Q9HCH5
A	-9C	SER	-	linker	UNP Q9HCH5
A	-9D	GLY	-	linker	UNP Q9HCH5
A	-9E	SER	-	linker	UNP Q9HCH5
A	-9F	GLY	-	linker	UNP Q9HCH5
A	-9G	SER	-	linker	UNP Q9HCH5
A	-9H	GLY	-	linker	UNP Q9HCH5
A	65	LEU	GLN	engineered mutation	UNP P51159
A	175	SER	CYS	engineered mutation	UNP P51159
B	-38	GLY	-	expression tag	UNP Q9HCH5
B	-37	HIS	-	expression tag	UNP Q9HCH5
B	-36	MET	-	expression tag	UNP Q9HCH5
B	-9B	GLY	-	linker	UNP Q9HCH5
B	-9C	SER	-	linker	UNP Q9HCH5
B	-9D	GLY	-	linker	UNP Q9HCH5
B	-9E	SER	-	linker	UNP Q9HCH5
B	-9F	GLY	-	linker	UNP Q9HCH5
B	-9G	SER	-	linker	UNP Q9HCH5
B	-9H	GLY	-	linker	UNP Q9HCH5
B	64	LEU	GLN	engineered mutation	UNP P51159
B	174	SER	CYS	engineered mutation	UNP P51159

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



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

- Molecule 4 is {N}-(3-methoxy-4-pyrrolidin-1-ylsulfonyl-phenyl)propanamide (CCD ID: WTK) (formula: C₁₄H₂₀N₂O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	1	0
			21	14	2	4	1		
4	B	1	Total	C	N	O	S	0	0
			21	14	2	4	1		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

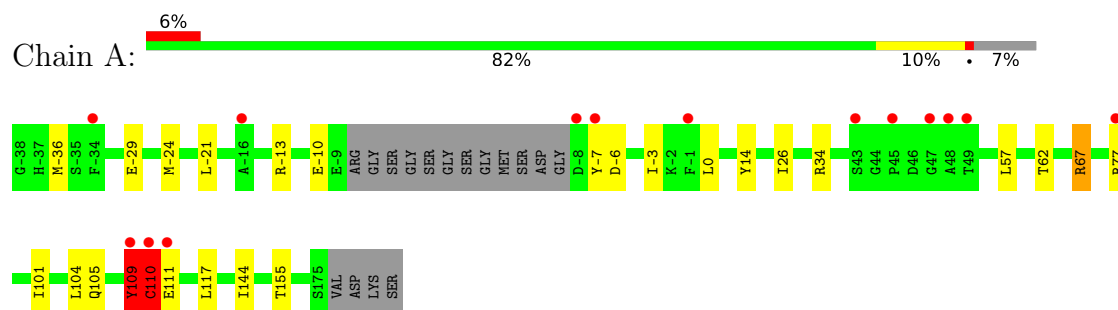
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	28	Total	O	0	0
			28	28		
6	B	29	Total	O	0	0
			29	29		

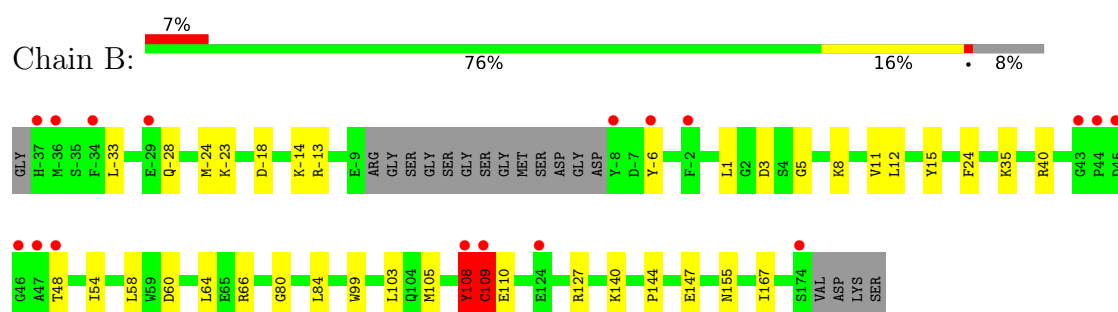
3 Residue-property plots [i](#)

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: Synaptotagmin-like protein 2,Ras-related protein Rab-27A



- Molecule 1: Synaptotagmin-like protein 2,Ras-related protein Rab-27A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.37Å 76.60Å 118.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	64.36 – 2.00 64.36 – 2.00	Depositor EDS
% Data completeness (in resolution range)	88.0 (64.36-2.00) 88.1 (64.36-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.93 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.17_3644: ???)	Depositor
R, R_{free}	0.229 , 0.280 0.234 , 0.279	Depositor DCC
R_{free} test set	1967 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3586	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 6.72% 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, WTK, GOL, MG

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	0.47	2/1708 (0.1%)	1.09	6/2301 (0.3%)
1	B	0.45	2/1697 (0.1%)	0.70	4/2287 (0.2%)
All	All	0.46	4/3405 (0.1%)	0.92	10/4588 (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	4
1	B	0	2
All	All	0	6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	109	CYS	C-N	7.70	1.43	1.33
1	A	109	TYR	C-N	6.97	1.43	1.33
1	A	110	CYS	C-N	6.93	1.43	1.33
1	B	108	TYR	C-N	6.77	1.43	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	109	TYR	O-C-N	-25.00	83.14	121.89
1	A	109	TYR	CA-C-N	23.64	166.69	121.54
1	A	109	TYR	C-N-CA	23.64	166.69	121.54
1	B	108	TYR	O-C-N	14.33	138.48	122.15
1	A	110	CYS	O-C-N	-14.27	103.61	122.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	109	CYS	O-C-N	-8.65	111.98	123.23
1	B	109	CYS	CA-C-N	-6.76	111.65	120.44
1	B	109	CYS	C-N-CA	-6.76	111.65	120.44
1	A	-6	ASP	CA-C-O	-5.82	114.25	120.42
1	A	-6	ASP	CB-CA-C	5.06	119.45	110.85

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	TYR	Mainchain,Peptide
1	A	110	CYS	Mainchain,Peptide
1	B	108	TYR	Peptide
1	B	109	CYS	Mainchain

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	1680	0	1642	21	0
1	B	1669	0	1635	30	1
2	A	32	0	13	2	0
2	B	32	0	13	2	0
3	A	36	0	48	8	0
3	B	36	0	48	7	0
4	A	21	0	0	0	0
4	B	21	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	28	0	0	0	0
6	B	29	0	0	2	0
All	All	3586	0	3399	52	1

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 8.

All (52) 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:155:THR:HG21	3:A:203:GOL:H31	1.72	0.72
1:B:15:TYR:O	1:B:35:LYS:NZ	2.25	0.69
1:B:140:LYS:NZ	6:B:302:HOH:O	2.29	0.65
1:B:66:ARG:HH21	3:B:204:GOL:H12	1.61	0.64
1:B:80:GLY:HA3	1:B:167:ILE:HD11	1.82	0.62
1:B:5:GLY:H	2:B:201:GNP:HNB3	1.46	0.62
1:A:-13:ARG:HH22	1:B:105:MET:C	2.13	0.57
1:B:66:ARG:NH2	3:B:204:GOL:H12	2.22	0.54
1:A:-36:MET:HE3	1:B:-33:LEU:O	2.08	0.54
1:A:-10:GLU:HG2	1:A:-10:GLU:O	2.08	0.53
1:B:12:LEU:HD22	1:B:58:LEU:HD23	1.91	0.52
1:A:-7:TYR:CD2	1:A:-7:TYR:C	2.87	0.52
1:A:-10:GLU:OE2	1:B:108:TYR:O	2.28	0.51
1:B:127:ARG:HH22	1:B:147:GLU:CD	2.19	0.51
1:B:147:GLU:O	1:B:155:ASN:ND2	2.34	0.50
1:A:111:GLU:HG3	1:B:-13:ARG:HG2	1.94	0.50
1:B:-28:GLN:O	1:B:-24:MET:HG2	2.11	0.49
3:B:204:GOL:O3	3:B:204:GOL:O1	2.26	0.49
1:A:77:ARG:HA	1:A:109:TYR:CD1	2.47	0.49
2:A:201:GNP:N3	3:A:205:GOL:H11	2.28	0.49
1:B:24:PHE:CD1	2:B:201:GNP:H5'1	2.47	0.48
1:A:34:ARG:HA	3:A:207:GOL:H2	1.96	0.48
3:A:203:GOL:O3	3:A:203:GOL:O1	2.28	0.48
1:B:12:LEU:HD12	1:B:60:ASP:HB2	1.96	0.47
1:B:144:PRO:HB3	3:B:207:GOL:H2	1.95	0.47
1:B:99:TRP:CE2	3:B:205:GOL:H32	2.49	0.46
1:A:-3:ILE:HB	1:A:57:LEU:HD23	1.98	0.46
1:B:40:ARG:HG2	1:B:40:ARG:HH11	1.81	0.46
2:A:201:GNP:H1'	3:A:205:GOL:H11	1.98	0.45
1:A:-7:TYR:CD2	1:A:-7:TYR:O	2.70	0.45
1:B:66:ARG:HE	3:B:204:GOL:H12	1.82	0.45
1:B:-6:TYR:HB2	1:B:54:ILE:HD13	2.00	0.44
1:B:64:LEU:HD23	1:B:64:LEU:HA	1.89	0.44
1:B:127:ARG:NH2	1:B:147:GLU:OE1	2.47	0.43
1:A:101:ILE:O	1:A:105:GLN:HG2	2.18	0.43
1:B:1:LEU:HD12	1:B:99:TRP:CE3	2.54	0.43
1:A:14:TYR:CZ	3:A:206:GOL:H12	2.54	0.43
1:A:26:ILE:H	3:A:202:GOL:HO1	1.62	0.43
1:B:11:VAL:HG21	1:B:84:LEU:HD21	2.01	0.42
1:A:26:ILE:HD12	3:A:202:GOL:O2	2.18	0.42
1:A:117:LEU:HB2	1:A:144:ILE:HD12	2.02	0.42
1:B:109:CYS:O	1:B:110:GLU:C	2.60	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:0:LEU:HD21	1:A:62:THR:HG21	2.02	0.41
1:B:-18:ASP:OD1	1:B:-14:LYS:NZ	2.48	0.41
1:B:40:ARG:HG2	1:B:40:ARG:NH1	2.35	0.41
1:A:-24:MET:HE3	1:A:-24:MET:HB3	1.92	0.41
1:B:103:LEU:HD23	1:B:103:LEU:HA	1.76	0.41
1:B:3:ASP:O	1:B:8:LYS:NZ	2.54	0.41
1:A:-21:LEU:HD23	1:A:-21:LEU:HA	1.83	0.40
1:A:-29:GLU:OE1	1:A:67:ARG:NH2	2.52	0.40
1:A:104:LEU:HD23	1:A:104:LEU:HA	1.85	0.40
3:B:202:GOL:H31	6:B:311:HOH:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:-23:LYS:NZ	1:B:48:THR:O[3_545]	2.17	0.03

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	210/230 (91%)	203 (97%)	6 (3%)	1 (0%)	24	21
1	B	208/230 (90%)	198 (95%)	10 (5%)	0	100	100
All	All	418/460 (91%)	401 (96%)	16 (4%)	1 (0%)	43	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	CYS

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	173/193 (90%)	172 (99%)	1 (1%)	78	85
1	B	172/193 (89%)	171 (99%)	1 (1%)	78	85
All	All	345/386 (89%)	343 (99%)	2 (1%)	78	85

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	ARG
1	B	109	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-37	HIS
1	A	53	GLN
1	A	92	GLN
1	A	127	GLN
1	B	106	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

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
3	GOL	A	207	-	5,5,5	0.94	0	5,5,5	1.10	0
3	GOL	A	204	-	5,5,5	0.95	0	5,5,5	1.06	0
3	GOL	B	203	-	5,5,5	1.12	0	5,5,5	0.90	0
4	WTK	A	208	1	22,22,22	3.48	13 (59%)	31,31,31	2.62	7 (22%)
3	GOL	B	206	-	5,5,5	0.94	0	5,5,5	1.05	0
2	GNP	A	201	5	34,34,34	1.40	5 (14%)	47,54,54	1.01	3 (6%)
3	GOL	A	202	-	5,5,5	0.87	0	5,5,5	1.00	0
4	WTK	B	208	1	22,22,22	3.67	12 (54%)	31,31,31	3.00	9 (29%)
3	GOL	B	205	-	5,5,5	0.68	0	5,5,5	1.14	0
3	GOL	A	205	-	5,5,5	1.13	1 (20%)	5,5,5	1.00	0
3	GOL	B	202	-	5,5,5	0.73	0	5,5,5	1.06	1 (20%)
3	GOL	B	204	-	5,5,5	1.09	0	5,5,5	1.31	1 (20%)
3	GOL	A	203	-	5,5,5	0.70	0	5,5,5	1.57	1 (20%)
3	GOL	B	207	-	5,5,5	0.85	0	5,5,5	0.99	0
2	GNP	B	201	5	34,34,34	1.36	5 (14%)	47,54,54	0.99	2 (4%)
3	GOL	A	206	-	5,5,5	1.15	0	5,5,5	0.80	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
3	GOL	A	207	-	-	3/4/4/4	-
3	GOL	A	204	-	-	3/4/4/4	-
3	GOL	B	203	-	-	0/4/4/4	-
4	WTK	A	208	1	-	4/20/27/27	0/2/2/2
3	GOL	B	206	-	-	2/4/4/4	-
2	GNP	A	201	5	-	7/18/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	202	-	-	2/4/4/4	-
4	WTK	B	208	1	-	7/20/27/27	0/2/2/2
3	GOL	B	205	-	-	1/4/4/4	-
3	GOL	A	205	-	-	4/4/4/4	-
3	GOL	B	202	-	-	2/4/4/4	-
3	GOL	B	204	-	-	2/4/4/4	-
3	GOL	A	203	-	-	0/4/4/4	-
3	GOL	B	207	-	-	2/4/4/4	-
2	GNP	B	201	5	-	2/18/38/38	0/3/3/3
3	GOL	A	206	-	-	4/4/4/4	-

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	208	WTK	S17-N19	8.99	1.76	1.63
4	A	208	WTK	S17-N19	8.51	1.75	1.63
4	A	208	WTK	O24-S17	6.59	1.50	1.43
4	B	208	WTK	O24-S17	6.30	1.50	1.43
4	B	208	WTK	C07-N08	5.62	1.47	1.35
4	B	208	WTK	C21-C20	-5.09	1.34	1.51
2	A	201	GNP	PB-O3A	5.03	1.65	1.59
4	A	208	WTK	C21-C20	-5.01	1.34	1.51
4	A	208	WTK	C07-N08	4.93	1.46	1.35
2	B	201	GNP	PB-O3A	4.90	1.65	1.59
4	A	208	WTK	C22-C23	-4.73	1.35	1.51
4	B	208	WTK	C22-C23	-4.61	1.36	1.51
4	B	208	WTK	C20-N19	4.53	1.57	1.48
4	A	208	WTK	C20-N19	4.51	1.57	1.48
4	B	208	WTK	C09-N08	4.13	1.50	1.41
4	B	208	WTK	C23-N19	4.13	1.56	1.48
4	A	208	WTK	C23-N19	3.96	1.56	1.48
4	B	208	WTK	C16-S17	3.67	1.83	1.78
4	A	208	WTK	C09-N08	3.63	1.49	1.41
2	B	201	GNP	PB-O1B	3.59	1.51	1.46
2	A	201	GNP	PB-O1B	3.04	1.50	1.46
2	A	201	GNP	PG-O1G	2.94	1.50	1.46
2	B	201	GNP	PG-O1G	2.92	1.50	1.46
2	A	201	GNP	PG-N3B	2.79	1.70	1.63
2	B	201	GNP	PG-N3B	2.70	1.70	1.63
4	B	208	WTK	O18-S17	2.38	1.46	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	GNP	PB-O2B	-2.37	1.50	1.56
4	B	208	WTK	O14-C13	2.26	1.40	1.37
4	A	208	WTK	C16-S17	2.24	1.81	1.78
3	A	205	GOL	C3-C2	2.21	1.60	1.51
4	A	208	WTK	O14-C13	2.18	1.40	1.37
4	A	208	WTK	C22-C21	2.12	1.62	1.48
4	B	208	WTK	C22-C21	2.11	1.62	1.48
4	A	208	WTK	O18-S17	2.07	1.45	1.43
2	B	201	GNP	PB-O2B	-2.07	1.51	1.56
4	A	208	WTK	O14-C15	-2.01	1.37	1.42

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	208	WTK	O24-S17-O18	-12.06	100.77	119.59
4	A	208	WTK	O24-S17-O18	-8.94	105.64	119.59
4	A	208	WTK	O18-S17-N19	5.56	111.92	106.69
2	B	201	GNP	O1G-PG-N3B	-5.47	103.72	111.77
4	B	208	WTK	O18-S17-N19	4.81	111.22	106.69
4	B	208	WTK	C23-N19-C20	-4.71	104.71	111.22
4	B	208	WTK	O24-S17-N19	4.70	111.11	106.69
4	A	208	WTK	C23-N19-S17	4.43	126.94	119.81
4	A	208	WTK	O24-S17-N19	4.21	110.65	106.69
2	A	201	GNP	O5'-PA-O1A	-3.89	93.51	108.94
4	A	208	WTK	C20-N19-S17	3.84	126.00	119.81
4	A	208	WTK	O14-C13-C16	3.58	119.23	116.49
4	B	208	WTK	C20-N19-S17	3.47	125.39	119.81
4	A	208	WTK	C23-N19-C20	-3.37	106.56	111.22
4	B	208	WTK	C23-N19-S17	3.36	125.22	119.81
2	A	201	GNP	O2A-PA-O5'	3.32	122.61	107.57
4	B	208	WTK	C16-S17-N19	3.15	112.54	106.69
4	B	208	WTK	O14-C13-C16	3.05	118.82	116.49
3	A	203	GOL	C3-C2-C1	-2.48	102.72	111.80
2	A	201	GNP	O1G-PG-N3B	-2.33	108.34	111.77
3	B	204	GOL	C3-C2-C1	-2.23	103.62	111.80
4	B	208	WTK	C11-C16-S17	2.18	120.46	117.48
2	B	201	GNP	O2A-PA-O5'	2.04	116.79	107.57
3	B	202	GOL	C3-C2-C1	-2.01	104.41	111.80

There are no chirality outliers.

All (45) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	GNP	PG-N3B-PB-O1B
2	A	201	GNP	C5'-O5'-PA-O3A
2	A	201	GNP	C5'-O5'-PA-O2A
2	A	201	GNP	O4'-C4'-C5'-O5'
2	B	201	GNP	PA-O3A-PB-O2B
3	A	202	GOL	C1-C2-C3-O3
3	A	205	GOL	O1-C1-C2-C3
3	A	205	GOL	C1-C2-C3-O3
3	A	205	GOL	O2-C2-C3-O3
3	B	206	GOL	O1-C1-C2-C3
3	B	207	GOL	O1-C1-C2-C3
4	B	208	WTK	C13-C16-S17-O24
4	A	208	WTK	C16-C13-O14-C15
4	A	208	WTK	C12-C13-O14-C15
3	B	202	GOL	O2-C2-C3-O3
3	B	207	GOL	O1-C1-C2-O2
2	A	201	GNP	C3'-C4'-C5'-O5'
3	A	204	GOL	O1-C1-C2-C3
3	A	204	GOL	C1-C2-C3-O3
3	A	206	GOL	O1-C1-C2-C3
3	B	202	GOL	C1-C2-C3-O3
4	A	208	WTK	C20-N19-S17-O18
3	A	202	GOL	O2-C2-C3-O3
3	A	204	GOL	O1-C1-C2-O2
4	B	208	WTK	C23-N19-S17-O24
3	B	206	GOL	O1-C1-C2-O2
4	B	208	WTK	C16-C13-O14-C15
3	A	207	GOL	O1-C1-C2-C3
3	B	204	GOL	O1-C1-C2-C3
2	A	201	GNP	C5'-O5'-PA-O1A
3	A	205	GOL	O1-C1-C2-O2
4	B	208	WTK	C05-C06-C07-N08
4	B	208	WTK	C12-C13-O14-C15
3	A	206	GOL	C1-C2-C3-O3
3	B	204	GOL	C1-C2-C3-O3
3	A	206	GOL	O1-C1-C2-O2
2	A	201	GNP	PA-O3A-PB-O2B
3	A	206	GOL	O2-C2-C3-O3
3	B	205	GOL	O2-C2-C3-O3
4	B	208	WTK	C05-C06-C07-O25
4	B	208	WTK	C13-C16-S17-O18
4	A	208	WTK	C20-N19-S17-C16
2	B	201	GNP	PA-O3A-PB-O1B

Continued on next page...

Continued from previous page...

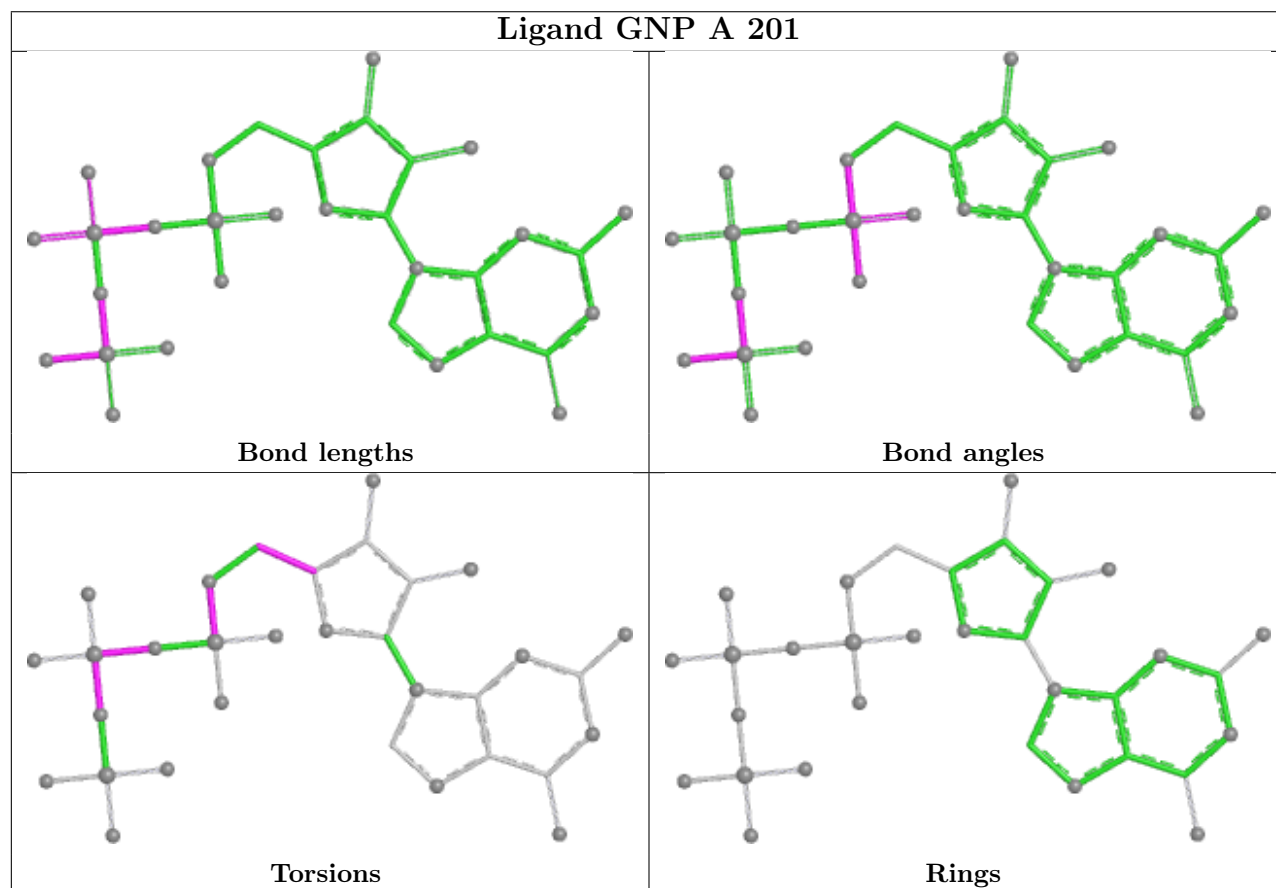
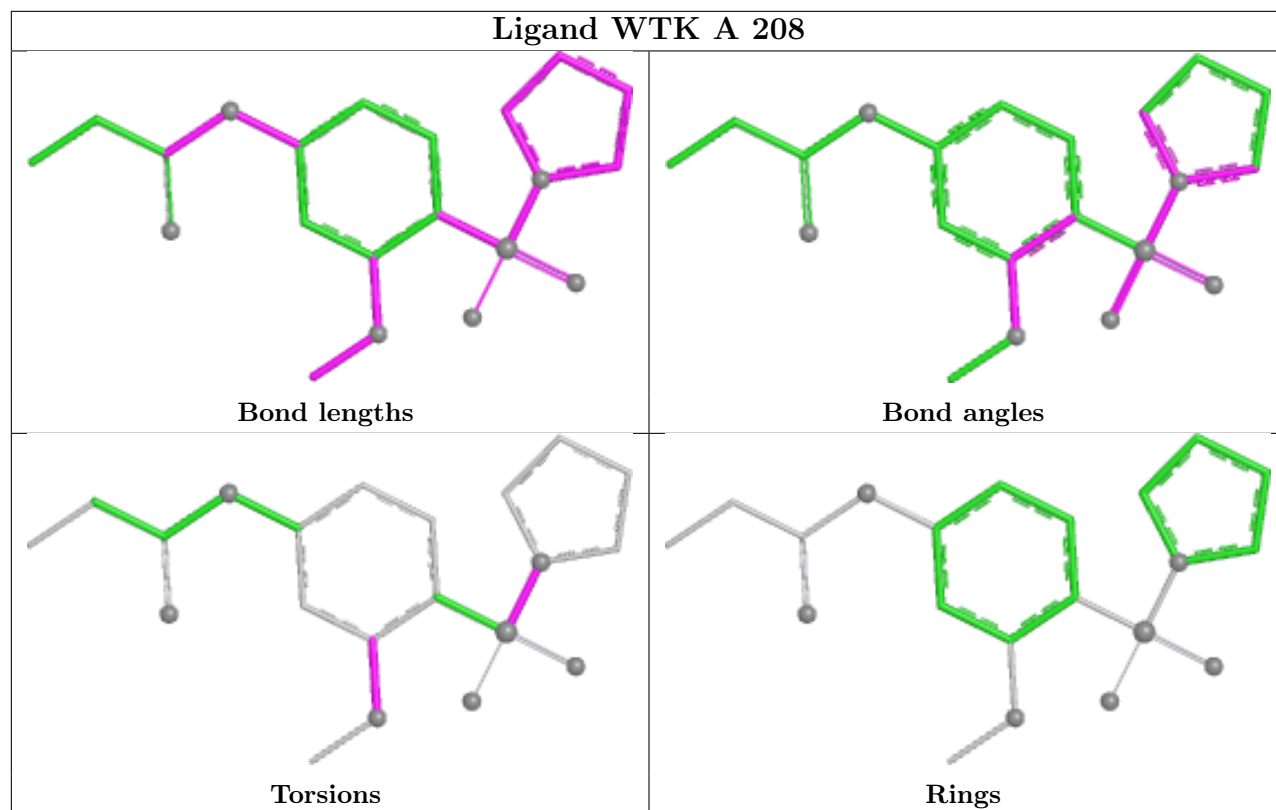
Mol	Chain	Res	Type	Atoms
3	A	207	GOL	O1-C1-C2-O2
3	A	207	GOL	O2-C2-C3-O3

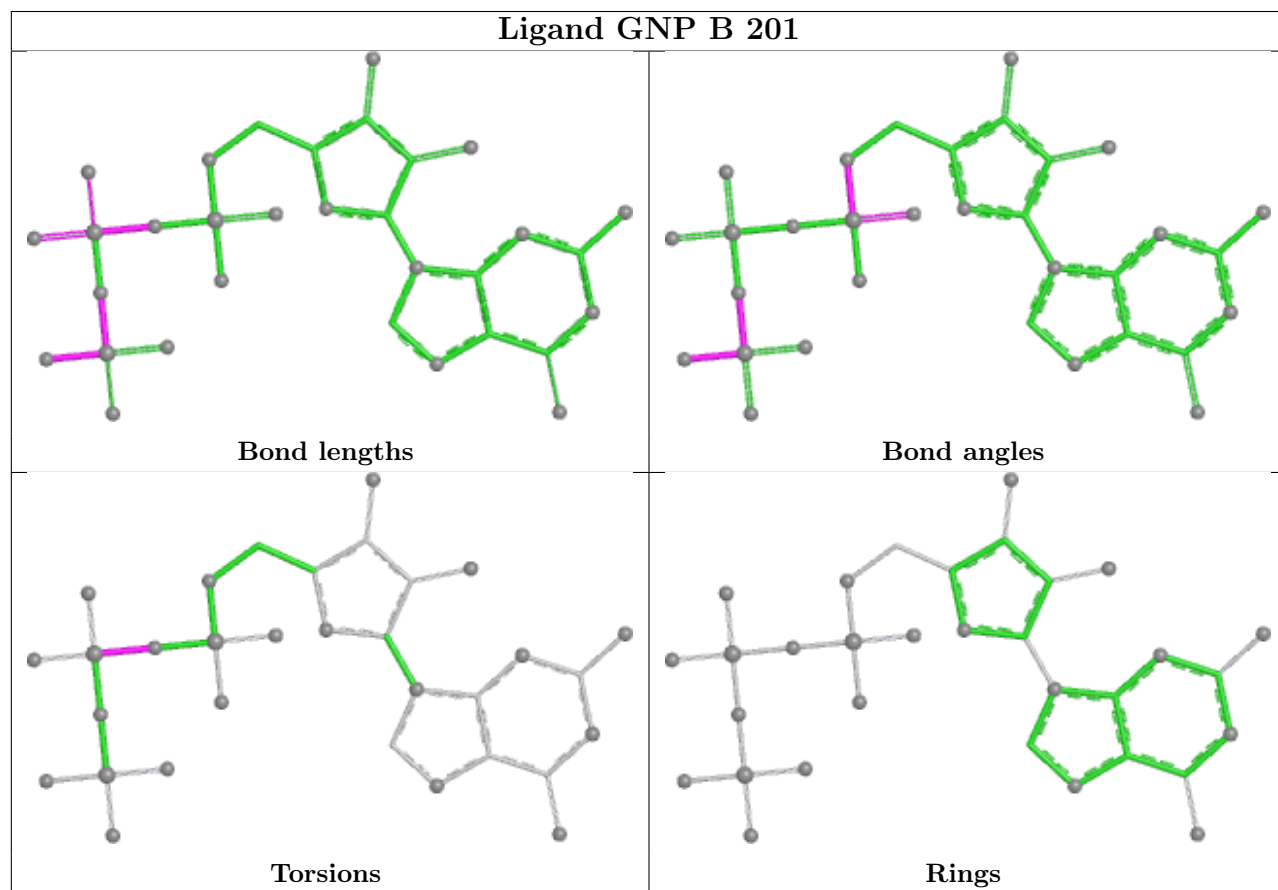
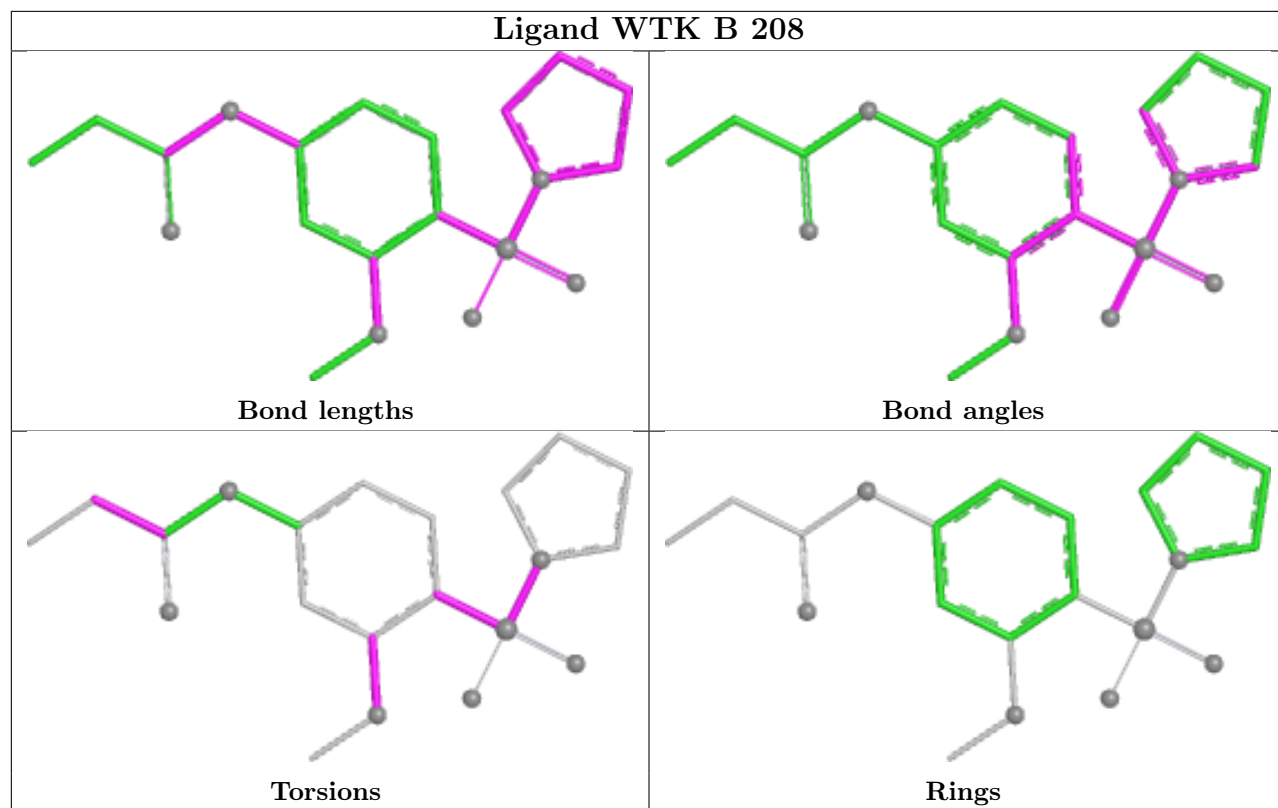
There are no ring outliers.

11 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	207	GOL	1	0
2	A	201	GNP	2	0
3	A	202	GOL	2	0
3	B	205	GOL	1	0
3	A	205	GOL	2	0
3	B	202	GOL	1	0
3	B	204	GOL	4	0
3	A	203	GOL	2	0
3	B	207	GOL	1	0
2	B	201	GNP	2	0
3	A	206	GOL	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.





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	214/230 (93%)	0.55	14 (6%) 25 23	39, 52, 77, 115	0
1	B	212/230 (92%)	0.83	17 (8%) 18 17	43, 56, 95, 112	0
All	All	426/460 (92%)	0.69	31 (7%) 21 19	39, 54, 90, 115	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	111	GLU	5.0
1	B	47	ALA	4.8
1	B	46	GLY	4.2
1	B	-34	PHE	3.9
1	B	45	ASP	3.8
1	A	47	GLY	3.6
1	B	-8	TYR	3.5
1	B	44	PRO	3.4
1	B	-37	HIS	3.1
1	A	-7	TYR	3.1
1	A	49	THR	3.1
1	B	-36	MET	3.0
1	A	-8	ASP	3.0
1	A	45	PRO	2.9
1	B	43	GLY	2.7
1	B	-2	PHE	2.7
1	B	174	SER	2.7
1	A	-1	PHE	2.6
1	B	108	TYR	2.5
1	A	109	TYR	2.4
1	B	-6	TYR	2.4
1	B	124	GLU	2.3
1	B	48	THR	2.2
1	A	77	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	48	ALA	2.2
1	A	110	CYS	2.1
1	A	43	SER	2.1
1	A	-34	PHE	2.1
1	A	-16	ALA	2.1
1	B	109	CYS	2.0
1	B	-29	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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.

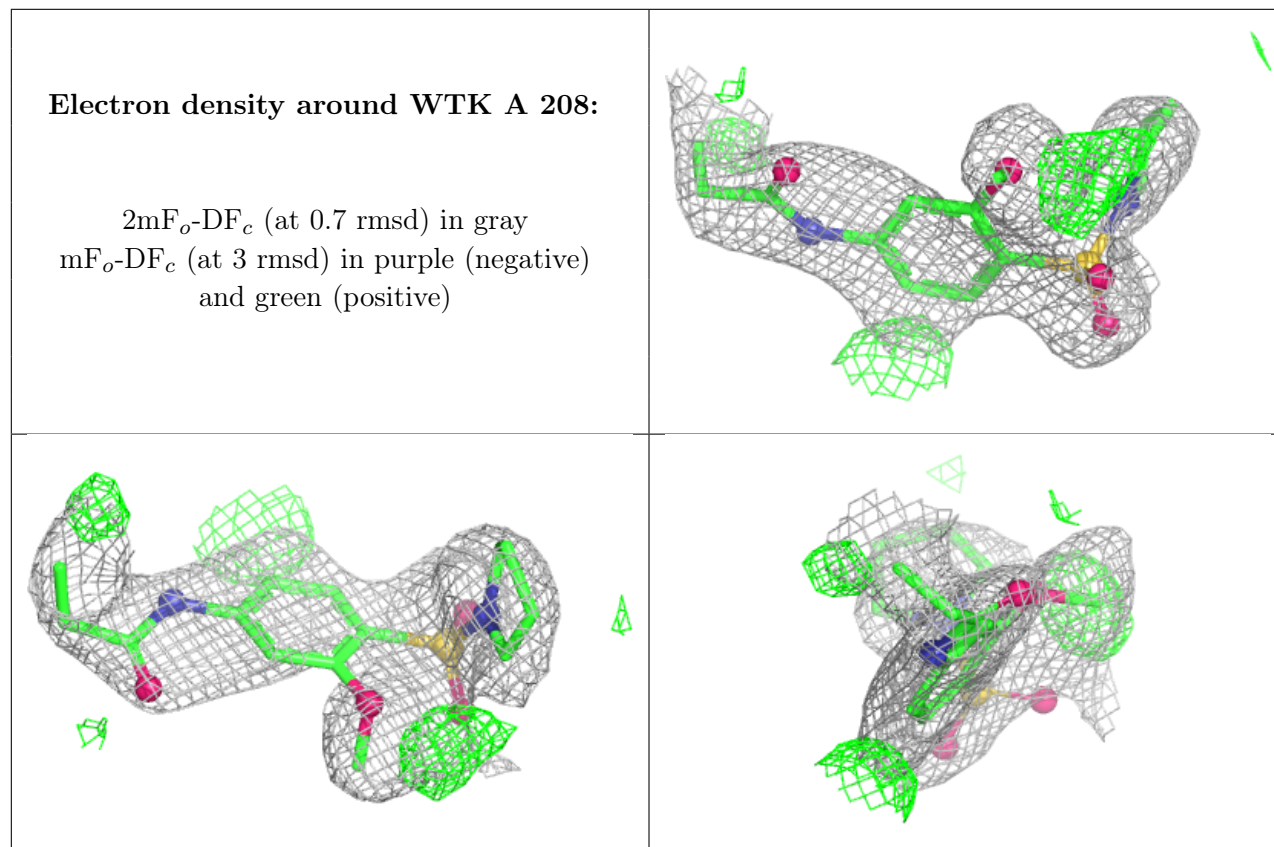
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	WTK	A	208	21/21	0.72	0.19	56,62,71,74	9
3	GOL	B	203	6/6	0.74	0.16	66,73,76,76	0
3	GOL	B	207	6/6	0.76	0.13	63,65,67,69	0
3	GOL	B	206	6/6	0.77	0.15	61,66,69,75	0
3	GOL	A	207	6/6	0.82	0.12	55,60,60,64	0
4	WTK	B	208	21/21	0.82	0.15	62,68,73,78	7
3	GOL	A	205	6/6	0.85	0.12	47,50,58,66	0
3	GOL	B	204	6/6	0.85	0.12	58,63,66,71	0
3	GOL	A	206	6/6	0.86	0.10	59,62,65,71	0
3	GOL	B	205	6/6	0.86	0.11	53,61,62,64	0
3	GOL	A	202	6/6	0.90	0.11	46,52,57,59	0
3	GOL	A	203	6/6	0.91	0.11	52,62,64,67	0
3	GOL	B	202	6/6	0.92	0.09	47,50,54,56	0
3	GOL	A	204	6/6	0.92	0.10	52,62,64,66	0
2	GNP	A	201	32/32	0.97	0.06	37,43,47,50	0
2	GNP	B	201	32/32	0.97	0.06	39,45,50,53	0

Continued on next page...

Continued from previous page...

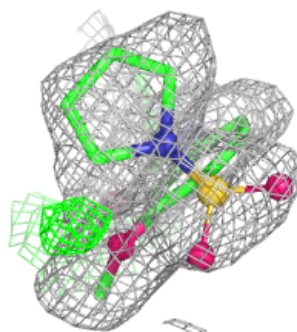
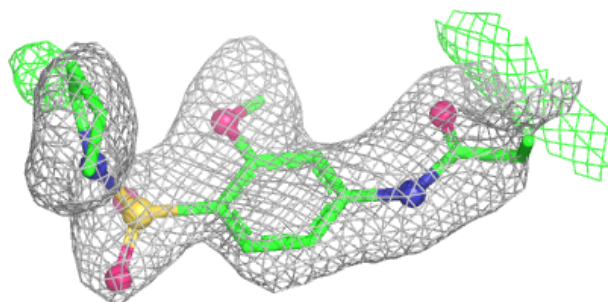
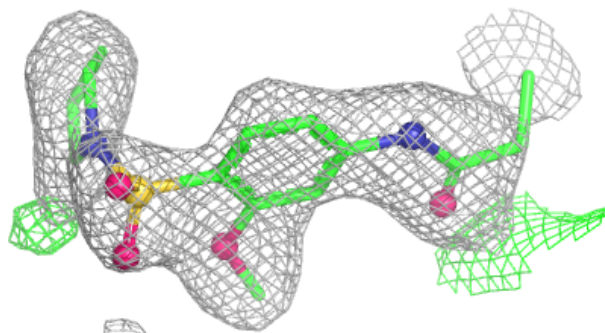
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	A	209	1/1	0.99	0.03	44,44,44,44	0
5	MG	B	209	1/1	1.00	0.03	45,45,45,45	0

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.

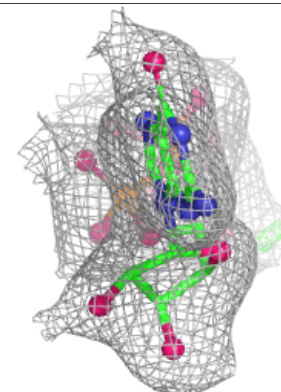
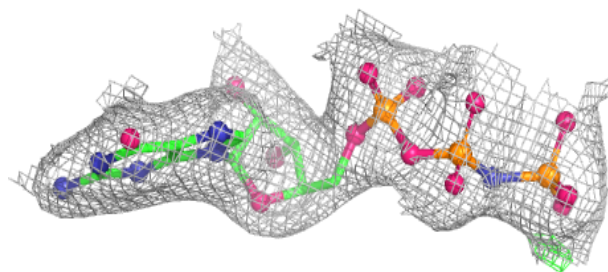
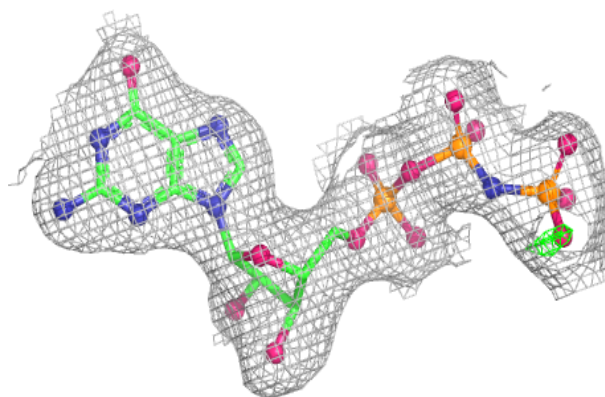


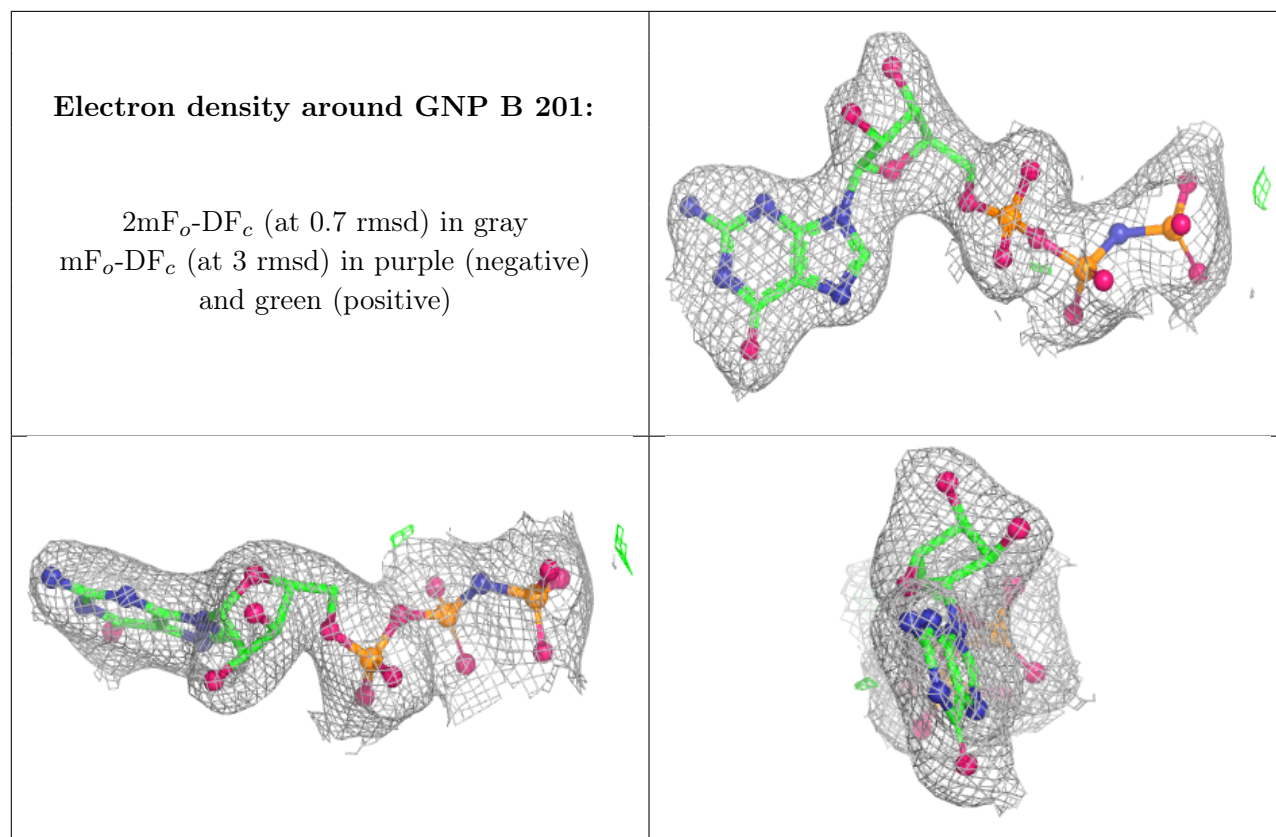
Electron density around WTK B 208:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.