



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 01:57 PM UTC

PDB ID : 8P3J / pdb_00008p3j
Title : Fusion hSlp2-a_Rab27A non-covalent complex with hit fragment IMP-1704
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 : 2.16 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

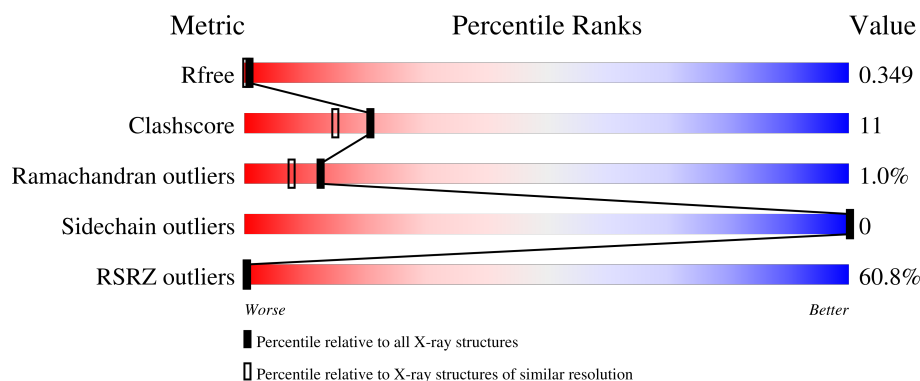
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	53% 75% 17% 8%
1	B	230	60% 69% 24% 7%

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
2	WT6	A	201	-	X	-	X
2	WT6	A	202	-	-	-	X
2	WT6	B	201	-	X	-	-
2	WT6	B	203	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3686 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	212	Total	C	N	O	S	0	2	0
			1710	1083	295	324	8			
1	B	214	Total	C	N	O	S	0	2	0
			1719	1085	298	328	8			

There are 26 discrepancies between the modelled and reference sequences:

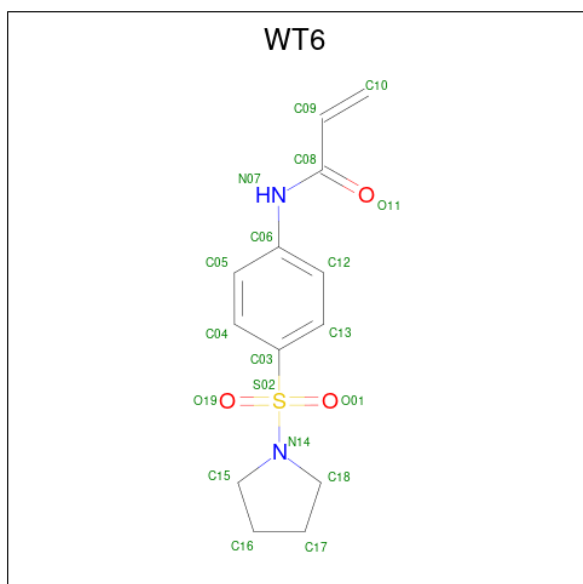
Chain	Residue	Modelled	Actual	Comment	Reference
A	-38	GLY	-	expression tag	UNP Q9HCH5
A	-37	HIS	-	expression tag	UNP Q9HCH5
A	-36	MET	-	expression tag	UNP Q9HCH5
A	-6	GLY	-	linker	UNP Q9HCH5
A	-5	SER	-	linker	UNP Q9HCH5
A	-4	GLY	-	linker	UNP Q9HCH5
A	-3	SER	-	linker	UNP Q9HCH5
A	-2	GLY	-	linker	UNP Q9HCH5
A	-1	SER	-	linker	UNP Q9HCH5
A	0	GLY	-	linker	UNP Q9HCH5
A	78	LEU	GLN	engineered mutation	UNP P51159
A	123	ALA	CYS	engineered mutation	UNP P51159
A	188	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	-6	GLY	-	linker	UNP Q9HCH5
B	-5	SER	-	linker	UNP Q9HCH5
B	-4	GLY	-	linker	UNP Q9HCH5
B	-3	SER	-	linker	UNP Q9HCH5
B	-2	GLY	-	linker	UNP Q9HCH5
B	-1	SER	-	linker	UNP Q9HCH5
B	0	GLY	-	linker	UNP Q9HCH5
B	78	LEU	GLN	engineered mutation	UNP P51159
B	123	ALA	CYS	engineered mutation	UNP P51159

Continued on next page...

Continued from previous page...

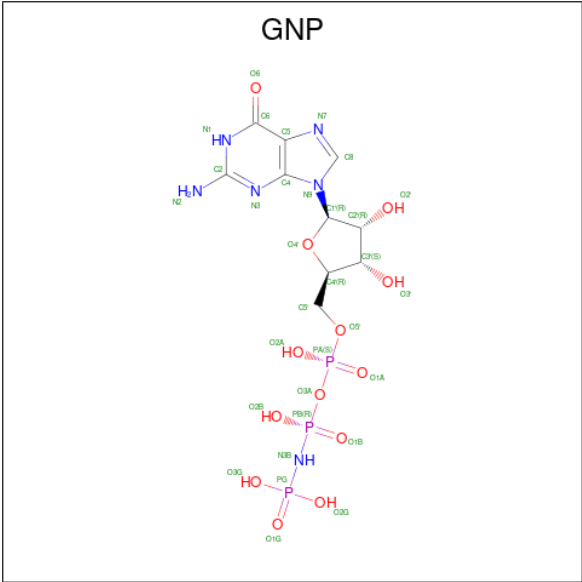
Chain	Residue	Modelled	Actual	Comment	Reference
B	188	SER	CYS	engineered mutation	UNP P51159

- Molecule 2 is {N}-(4-pyrrolidin-1-ylsulfonylphenyl)prop-2-enamide (CCD ID: WT6) (formula: C₁₃H₁₆N₂O₃S) (labeled as "Ligand of Interest" by depositor).



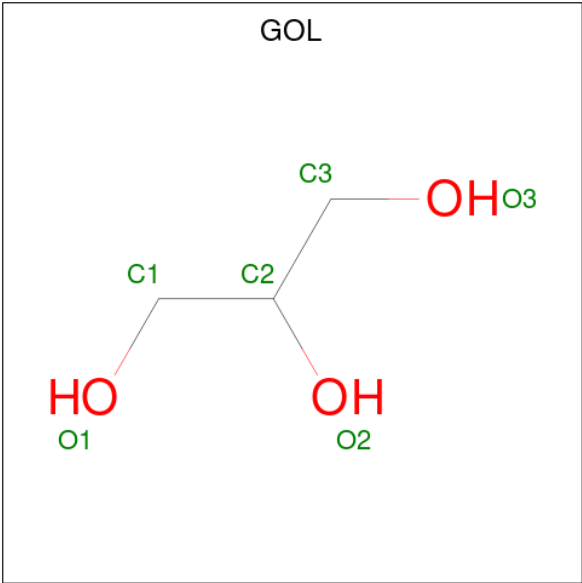
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			19	13	2	3	1		
2	A	1	Total	C	N	O	S	0	0
			19	13	2	3	1		
2	B	1	Total	C	N	O	S	0	0
			19	13	2	3	1		
2	B	1	Total	C	N	O	S	0	0
			19	13	2	3	1		

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).



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

- 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	B	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

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

- 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		

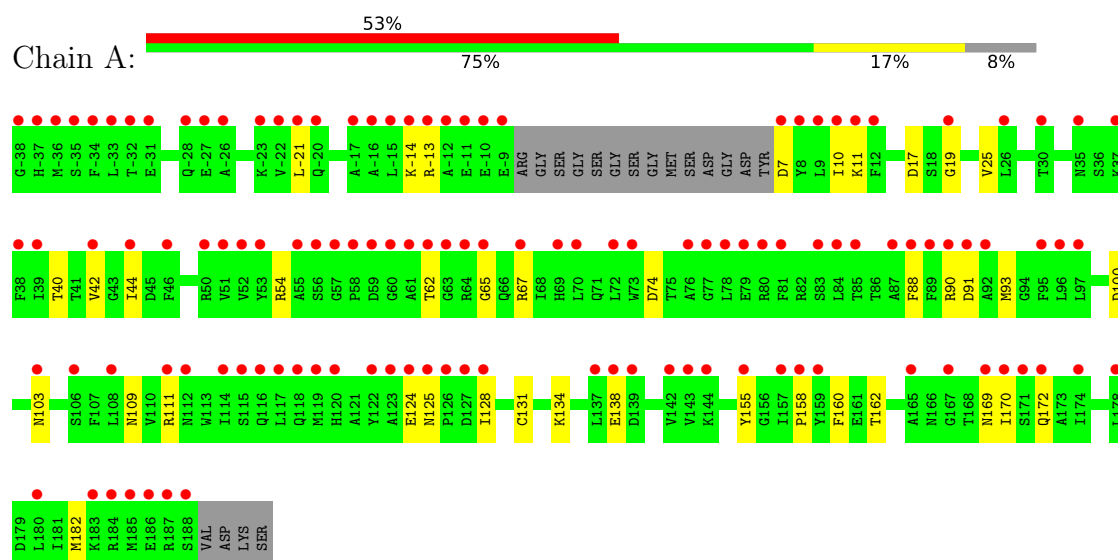
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	68	Total	O	0	0
			68	68		
6	B	29	Total	O	0	0
			29	29		

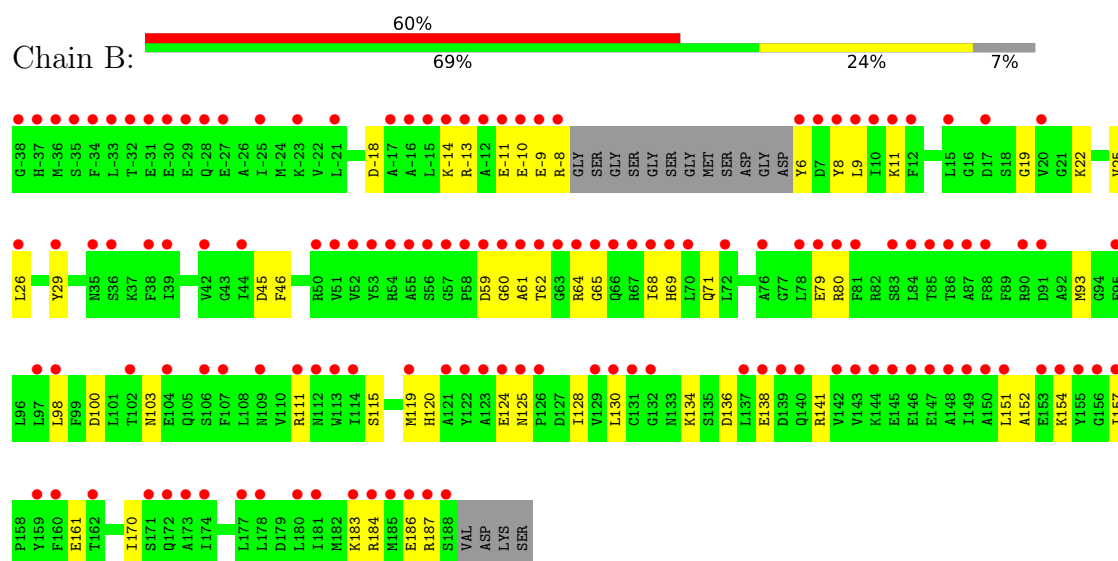
3 Residue-property plots [i](#)

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	62.44Å 75.83Å 118.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.88 – 2.16 63.88 – 2.16	Depositor EDS
% Data completeness (in resolution range)	96.4 (63.88-2.16) 96.5 (63.88-2.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 2.16Å)	Xtriage
Refinement program	PHENIX (1.17_3644: ???)	Depositor
R, R_{free}	0.284 , 0.351 0.285 , 0.349	Depositor DCC
R_{free} test set	1579 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	4.5	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 33.4	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	0.74	EDS
Total number of atoms	3686	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.22% 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: GOL, GNP, WT6, 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	0.36	0/1741	0.55	0/2340
1	B	0.36	0/1745	0.58	0/2345
All	All	0.36	0/3486	0.57	0/4685

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	7	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	1710	0	1688	41	3
1	B	1719	0	1695	53	3
2	A	38	0	0	2	0
2	B	38	0	0	6	0
3	A	32	0	13	4	0
3	B	32	0	13	1	0
4	A	6	0	8	0	0
4	B	12	0	15	3	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	68	0	0	3	0
6	B	29	0	0	1	0
All	All	3686	0	3432	78	3

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 11.

All (78) 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:125:ASN:ND2	2:B:203:WT6:C04	1.68	1.55
1:A:124:GLU:CG	1:B:-13:ARG:HD2	1.61	1.28
1:B:125:ASN:ND2	2:B:203:WT6:C05	1.98	1.27
1:A:124:GLU:HG3	1:B:-13:ARG:CD	1.73	1.17
1:A:124:GLU:HG3	1:B:-13:ARG:HD2	1.14	1.11
1:A:124:GLU:HG2	1:B:-13:ARG:HH11	1.26	0.99
1:A:124:GLU:CG	1:B:-13:ARG:CD	2.37	0.98
1:A:19:GLY:H	3:A:203:GNP:HNB3	1.20	0.86
1:B:-18:ASP:OD1	1:B:-14:LYS:NZ	2.10	0.85
1:B:19:GLY:H	3:B:202:GNP:HNB3	1.30	0.80
1:A:124:GLU:HG2	1:B:-13:ARG:HD2	1.64	0.77
1:B:125:ASN:CG	2:B:203:WT6:C04	2.57	0.77
1:A:111:ARG:HD3	1:A:155:TYR:OH	1.88	0.72
1:B:141:ARG:NH2	1:B:161:GLU:OE1	2.23	0.71
1:A:11:LYS:HE3	1:A:93:MET:HE3	1.74	0.69
1:A:90[B]:ARG:NH1	1:B:-18:ASP:OD2	2.25	0.69
1:A:-13:ARG:HD2	1:B:124:GLU:HG3	1.76	0.66
1:A:124:GLU:HG2	1:B:-13:ARG:CD	2.23	0.64
1:B:25:VAL:HG21	1:B:98:LEU:HD21	1.81	0.61
1:A:-13:ARG:CD	1:B:124:GLU:HG3	2.30	0.61
1:A:124:GLU:HG2	1:B:-13:ARG:NH1	2.08	0.61
1:A:-13:ARG:HD2	1:B:124:GLU:CG	2.31	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:GLU:HG3	1:B:-13:ARG:HD3	1.77	0.61
1:B:59:ASP:O	1:B:61:ALA:N	2.35	0.59
1:A:-14:LYS:O	6:A:301:HOH:O	2.17	0.56
1:A:124:GLU:CD	1:B:-13:ARG:HD2	2.26	0.56
1:A:40:THR:OG1	3:A:203:GNP:O2G	2.23	0.54
1:B:111:ARG:HG3	6:B:308:HOH:O	2.08	0.53
1:A:124:GLU:CG	1:B:-13:ARG:HD3	2.35	0.52
1:A:90[B]:ARG:HH22	1:B:-14:LYS:HE2	1.74	0.51
1:A:-14:LYS:NZ	1:A:91:ASP:OD2	2.39	0.51
1:B:125:ASN:HD22	2:B:203:WT6:C04	2.04	0.50
1:B:8:TYR:HB2	1:B:68:ILE:HD13	1.94	0.50
1:A:125:ASN:ND2	6:A:304:HOH:O	2.37	0.49
1:B:128:ILE:H	2:B:203:WT6:C09	2.25	0.49
1:B:-10:GLU:O	1:B:-8:ARG:N	2.43	0.49
1:B:100:ASP:HB3	1:B:103:ASN:HB3	1.94	0.49
1:B:79:GLU:HB2	4:B:205:GOL:H32	1.95	0.48
1:A:-21:LEU:HD21	1:A:88:PHE:HZ	1.79	0.47
1:A:158:PRO:HD3	2:A:202:WT6:C10	2.44	0.47
1:B:183:LYS:O	1:B:186:GLU:HG2	2.14	0.47
1:B:136:ASP:O	4:B:204:GOL:H31	2.14	0.47
1:A:25:VAL:HG13	1:A:170:ILE:HD12	1.97	0.47
1:A:128:ILE:H	2:A:202:WT6:C09	2.29	0.46
1:A:90[B]:ARG:HH12	1:B:-14:LYS:HZ3	1.64	0.46
1:B:151:LEU:HA	1:B:154[B]:LYS:HE2	1.98	0.46
1:B:80:ARG:N	4:B:205:GOL:O2	2.39	0.45
1:A:54:ARG:HG2	1:A:65:GLY:HA2	1.98	0.45
1:B:11:LYS:HG2	1:B:71:GLN:HB3	1.99	0.45
1:B:125:ASN:HD22	1:B:125:ASN:C	2.25	0.44
1:B:6:TYR:N	1:B:69:HIS:HB2	2.33	0.44
1:A:17:ASP:OD2	1:A:109:ASN:ND2	2.47	0.44
1:A:62:THR:HG23	6:A:337:HOH:O	2.17	0.44
1:B:184:ARG:HA	1:B:187:ARG:NH1	2.32	0.44
1:B:100:ASP:CG	1:B:134:LYS:HD2	2.43	0.44
1:B:-11:GLU:CD	1:B:9:LEU:HB2	2.43	0.43
1:A:134:LYS:HG2	3:A:203:GNP:C6	2.48	0.43
1:A:10:ILE:HG13	1:A:182:MET:HE3	1.99	0.43
1:B:64:ARG:HA	1:B:64:ARG:HD2	1.65	0.43
1:A:-21:LEU:HD21	1:A:88:PHE:CZ	2.54	0.43
1:A:44:ILE:HD12	1:A:74:ASP:O	2.19	0.42
1:A:169:ASN:HA	1:A:172:GLN:NE2	2.34	0.42
1:B:45:ASP:OD1	1:B:46:PHE:N	2.51	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ARG:HH22	1:B:161:GLU:CD	2.22	0.42
1:B:64:ARG:NH1	1:B:65:GLY:H	2.17	0.42
1:A:17:ASP:CG	1:A:109:ASN:HD22	2.27	0.42
1:B:119:MET:HG2	1:B:120:HIS:CD2	2.55	0.42
1:B:130:LEU:HD23	1:B:152:ALA:HB2	2.02	0.42
1:B:152:ALA:HB1	1:B:157:ILE:O	2.20	0.41
1:A:100:ASP:HB3	1:A:103:ASN:HB3	2.03	0.41
1:B:29:TYR:HB2	1:B:170:ILE:CG2	2.51	0.41
1:B:93:MET:HA	2:B:201:WT6:C08	2.51	0.41
1:B:-11:GLU:OE2	1:B:9:LEU:HB2	2.21	0.41
1:B:22:LYS:O	1:B:26:LEU:HG	2.21	0.41
1:A:131:CYS:HA	1:A:160:PHE:O	2.22	0.40
1:A:111:ARG:HD3	1:A:155:TYR:HH	1.84	0.40
3:A:203:GNP:H5'2	3:A:203:GNP:H8	2.04	0.40
1:A:162:THR:HB	1:A:170:ILE:HD13	2.04	0.40

All (3) 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:A:138:GLU:OE2	1:B:138:GLU:OE1[2_554]	1.46	0.74
1:A:138:GLU:CD	1:B:138:GLU:OE1[2_554]	1.87	0.33
1:A:67:ARG:NH2	1:B:115:SER:OG[4_455]	2.15	0.05

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%)	205 (98%)	4 (2%)	1 (0%)	24	20
1	B	212/230 (92%)	198 (93%)	11 (5%)	3 (1%)	9	4
All	All	422/460 (92%)	403 (96%)	15 (4%)	4 (1%)	12	9

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	-9	GLU
1	B	60	GLY
1	A	42	VAL
1	B	62	THR

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	180/192 (94%)	180 (100%)	0	100	100
1	B	180/192 (94%)	180 (100%)	0	100	100
All	All	360/384 (94%)	360 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	133	ASN
1	B	-20	GLN
1	B	105	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	B	204	-	5,5,5	0.94	0	5,5,5	0.81	0
3	GNP	A	203	5	34,34,34	1.31	5 (14%)	47,54,54	0.86	3 (6%)
4	GOL	B	205	-	5,5,5	1.35	1 (20%)	5,5,5	1.39	1 (20%)
2	WT6	B	201	-	20,20,20	4.05	13 (65%)	28,28,28	3.60	12 (42%)
2	WT6	B	203	-	20,20,20	4.12	13 (65%)	28,28,28	6.17	18 (64%)
2	WT6	A	201	-	20,20,20	4.17	14 (70%)	28,28,28	4.78	10 (35%)
3	GNP	B	202	5	34,34,34	1.40	5 (14%)	47,54,54	0.84	1 (2%)
4	GOL	A	204	-	5,5,5	0.65	0	5,5,5	1.62	1 (20%)
2	WT6	A	202	-	20,20,20	3.89	11 (55%)	28,28,28	3.53	9 (32%)

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	B	204	-	-	1/4/4/4	-
3	GNP	A	203	5	-	8/18/38/38	0/3/3/3
4	GOL	B	205	-	-	3/4/4/4	-
2	WT6	B	201	-	-	5/18/25/25	0/2/2/2
2	WT6	B	203	-	-	13/18/25/25	0/2/2/2
2	WT6	A	201	-	-	8/18/25/25	0/2/2/2
3	GNP	B	202	5	-	4/18/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	204	-	-	2/4/4/4	-
2	WT6	A	202	-	-	5/18/25/25	0/2/2/2

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	202	WT6	S02-N14	10.34	1.78	1.63
2	B	201	WT6	S02-N14	10.11	1.77	1.63
2	A	201	WT6	S02-N14	10.02	1.77	1.63
2	B	203	WT6	S02-N14	9.71	1.77	1.63
2	B	203	WT6	C08-N07	8.44	1.51	1.35
2	A	201	WT6	C08-N07	7.69	1.49	1.35
2	B	201	WT6	C08-N07	7.10	1.48	1.35
2	A	202	WT6	C08-N07	6.63	1.47	1.35
2	B	203	WT6	C04-C03	6.02	1.48	1.38
2	A	201	WT6	O11-C08	-5.06	1.14	1.24
3	B	202	GNP	PB-O3A	4.99	1.65	1.59
2	A	201	WT6	C17-C18	-4.90	1.35	1.51
2	A	202	WT6	C18-N14	4.82	1.58	1.48
2	B	201	WT6	C17-C18	-4.77	1.35	1.51
2	A	202	WT6	C17-C18	-4.74	1.35	1.51
2	A	202	WT6	O11-C08	-4.72	1.15	1.24
3	A	203	GNP	PB-O3A	4.70	1.64	1.59
2	A	202	WT6	C16-C15	-4.69	1.35	1.51
2	B	201	WT6	C15-N14	4.63	1.57	1.48
2	B	201	WT6	C18-N14	4.63	1.57	1.48
2	B	201	WT6	C16-C15	-4.61	1.36	1.51
2	A	201	WT6	C16-C15	-4.59	1.36	1.51
2	A	201	WT6	C15-N14	4.59	1.57	1.48
2	A	201	WT6	C03-S02	4.58	1.82	1.76
2	B	201	WT6	O11-C08	-4.57	1.15	1.24
2	B	201	WT6	C03-S02	4.51	1.82	1.76
2	A	201	WT6	C18-N14	4.48	1.57	1.48
2	B	203	WT6	C17-C18	-4.46	1.36	1.51
2	B	203	WT6	C16-C15	-4.45	1.36	1.51
2	A	202	WT6	C15-N14	4.42	1.57	1.48
2	B	203	WT6	C15-N14	4.01	1.56	1.48
2	B	203	WT6	O11-C08	-3.91	1.16	1.24
2	B	203	WT6	C03-S02	3.90	1.81	1.76
2	B	203	WT6	C18-N14	3.65	1.55	1.48
2	A	201	WT6	O19-S02	3.61	1.47	1.43
2	A	201	WT6	C12-C06	3.53	1.45	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	WT6	C12-C06	3.45	1.45	1.39
3	A	203	GNP	PG-N3B	3.28	1.71	1.63
2	A	202	WT6	C03-S02	3.22	1.80	1.76
2	B	201	WT6	C06-N07	3.19	1.48	1.41
2	B	203	WT6	C13-C03	3.17	1.43	1.38
2	A	202	WT6	C12-C06	3.12	1.44	1.39
2	A	201	WT6	C06-N07	2.98	1.47	1.41
3	B	202	GNP	PG-N3B	2.92	1.71	1.63
3	B	202	GNP	PB-O1B	2.90	1.50	1.46
3	A	203	GNP	PG-O1G	2.88	1.50	1.46
2	B	201	WT6	C09-C08	2.86	1.52	1.48
2	B	201	WT6	C04-C03	2.74	1.43	1.38
3	B	202	GNP	PG-O1G	2.71	1.50	1.46
2	A	201	WT6	C04-C03	2.67	1.43	1.38
3	B	202	GNP	PB-O2B	-2.58	1.50	1.56
4	B	205	GOL	O2-C2	-2.52	1.36	1.43
3	A	203	GNP	PB-O1B	2.44	1.49	1.46
2	A	202	WT6	C04-C03	2.42	1.42	1.38
2	B	203	WT6	C06-N07	2.42	1.46	1.41
2	A	202	WT6	O19-S02	2.22	1.45	1.43
3	A	203	GNP	PB-O2B	-2.19	1.51	1.56
2	A	201	WT6	C17-C16	2.07	1.62	1.48
2	B	203	WT6	C09-C08	2.07	1.51	1.48
2	B	201	WT6	C17-C16	2.05	1.62	1.48
2	B	203	WT6	C17-C16	2.05	1.62	1.48
2	A	201	WT6	C09-C08	2.01	1.51	1.48

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	WT6	C09-C08-N07	15.94	124.67	113.84
2	B	203	WT6	C13-C03-S02	-15.31	104.53	119.73
2	B	203	WT6	C03-S02-N14	15.10	125.51	107.28
2	A	201	WT6	O19-S02-O01	-12.33	100.34	119.59
2	B	201	WT6	O19-S02-O01	-12.03	100.81	119.59
2	B	203	WT6	C04-C03-S02	11.84	131.50	119.73
2	A	202	WT6	O19-S02-O01	-11.65	101.41	119.59
2	B	203	WT6	O19-S02-O01	-10.27	103.56	119.59
2	B	203	WT6	C18-N14-C15	-9.80	97.66	111.22
2	B	201	WT6	C09-C08-N07	9.42	120.23	113.84
2	A	202	WT6	C10-C09-C08	-7.72	113.73	122.22
2	B	203	WT6	C05-C04-C03	-7.09	112.55	119.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	WT6	C18-N14-C15	-6.68	101.98	111.22
2	A	201	WT6	C10-C09-C08	-6.21	115.39	122.22
2	A	202	WT6	C03-S02-N14	6.12	114.66	107.28
2	A	201	WT6	O11-C08-C09	-5.99	113.72	122.70
2	A	201	WT6	C03-S02-N14	5.98	114.49	107.28
2	A	202	WT6	C18-N14-C15	-5.79	103.21	111.22
2	B	203	WT6	C09-C08-N07	5.65	117.67	113.84
2	B	203	WT6	C12-C06-C05	5.52	126.37	119.04
2	B	203	WT6	O19-S02-C03	-5.51	101.25	108.10
2	A	202	WT6	O19-S02-N14	5.40	111.77	106.69
2	A	201	WT6	C06-N07-C08	-5.25	118.20	128.07
2	B	201	WT6	C18-N14-C15	-5.10	104.17	111.22
2	B	203	WT6	O19-S02-N14	4.88	111.28	106.69
2	B	203	WT6	C13-C12-C06	-4.77	114.80	120.30
2	B	201	WT6	O01-S02-N14	4.52	110.94	106.69
2	A	202	WT6	O01-S02-N14	4.52	110.94	106.69
2	B	201	WT6	O19-S02-N14	4.36	110.79	106.69
2	B	201	WT6	C03-S02-N14	4.07	112.19	107.28
2	B	203	WT6	C15-N14-S02	4.03	126.30	119.81
2	A	201	WT6	O19-S02-C03	3.96	113.03	108.10
2	B	203	WT6	C12-C06-N07	-3.62	108.26	120.41
3	B	202	GNP	O1B-PB-N3B	-3.58	106.49	111.77
2	A	201	WT6	O01-S02-N14	3.16	109.66	106.69
2	A	201	WT6	O19-S02-N14	3.12	109.62	106.69
2	B	201	WT6	O11-C08-C09	-3.12	118.02	122.70
2	B	203	WT6	O11-C08-C09	-2.81	118.48	122.70
4	A	204	GOL	C3-C2-C1	-2.72	101.80	111.80
2	B	203	WT6	C13-C03-C04	2.69	123.97	120.47
2	B	201	WT6	C15-N14-S02	2.63	124.05	119.81
2	A	202	WT6	C15-N14-S02	2.54	123.91	119.81
3	A	203	GNP	O3G-PG-O1G	-2.49	107.21	113.45
2	B	203	WT6	C10-C09-C08	-2.42	119.56	122.22
2	B	203	WT6	O01-S02-C03	-2.41	105.11	108.10
2	B	203	WT6	C17-C18-N14	2.34	107.71	103.52
2	A	202	WT6	C17-C18-N14	2.26	107.57	103.52
2	B	201	WT6	C13-C03-S02	2.19	121.90	119.73
2	B	201	WT6	O01-S02-C03	2.16	110.79	108.10
2	B	201	WT6	O19-S02-C03	2.16	110.78	108.10
2	B	201	WT6	C16-C15-N14	2.15	107.36	103.52
2	A	202	WT6	O11-C08-N07	2.09	125.86	123.11
4	B	205	GOL	O1-C1-C2	-2.05	101.15	110.38
3	A	203	GNP	O2A-PA-O3A	2.03	112.76	107.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	203	GNP	O2B-PB-O3A	2.01	111.35	104.64

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	202	WT6	N07-C08-C09-C10
2	A	202	WT6	O11-C08-C09-C10
2	B	201	WT6	N07-C08-C09-C10
2	B	201	WT6	O11-C08-C09-C10
2	B	201	WT6	C15-N14-S02-C03
2	B	203	WT6	N07-C08-C09-C10
2	B	203	WT6	O11-C08-C09-C10
2	B	203	WT6	C09-C08-N07-C06
2	B	203	WT6	O11-C08-N07-C06
3	A	203	GNP	PG-N3B-PB-O1B
3	A	203	GNP	PA-O3A-PB-O2B
3	A	203	GNP	C5'-O5'-PA-O3A
3	A	203	GNP	C5'-O5'-PA-O2A
3	B	202	GNP	PB-N3B-PG-O1G
3	B	202	GNP	PA-O3A-PB-O1B
3	B	202	GNP	PA-O3A-PB-O2B
2	A	202	WT6	C18-N14-S02-O01
2	B	201	WT6	C15-N14-S02-O01
2	A	201	WT6	C15-N14-S02-O01
2	A	202	WT6	C18-N14-S02-C03
2	B	201	WT6	C18-N14-S02-C03
2	B	203	WT6	C18-N14-S02-C03
2	B	203	WT6	C18-N14-S02-O01
2	B	203	WT6	C04-C03-S02-N14
2	A	201	WT6	C15-N14-S02-C03
2	B	203	WT6	C13-C03-S02-N14
3	A	203	GNP	O4'-C4'-C5'-O5'
2	A	201	WT6	C18-N14-S02-O19
2	A	201	WT6	C15-N14-S02-O19
3	A	203	GNP	C3'-C4'-C5'-O5'
4	A	204	GOL	O1-C1-C2-C3
4	B	204	GOL	O1-C1-C2-C3
4	B	205	GOL	C1-C2-C3-O3
2	A	201	WT6	C04-C03-S02-O19
2	A	201	WT6	C13-C03-S02-O19
2	B	203	WT6	C13-C03-S02-O01

Continued on next page...

Continued from previous page...

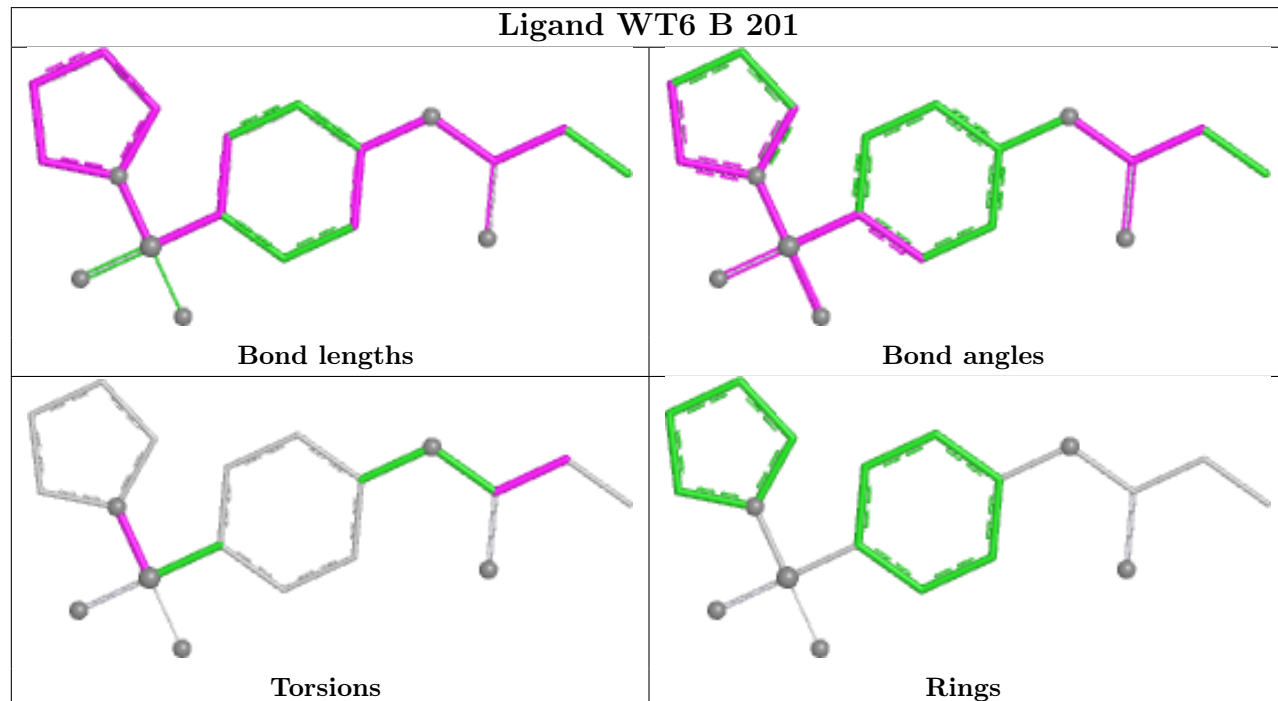
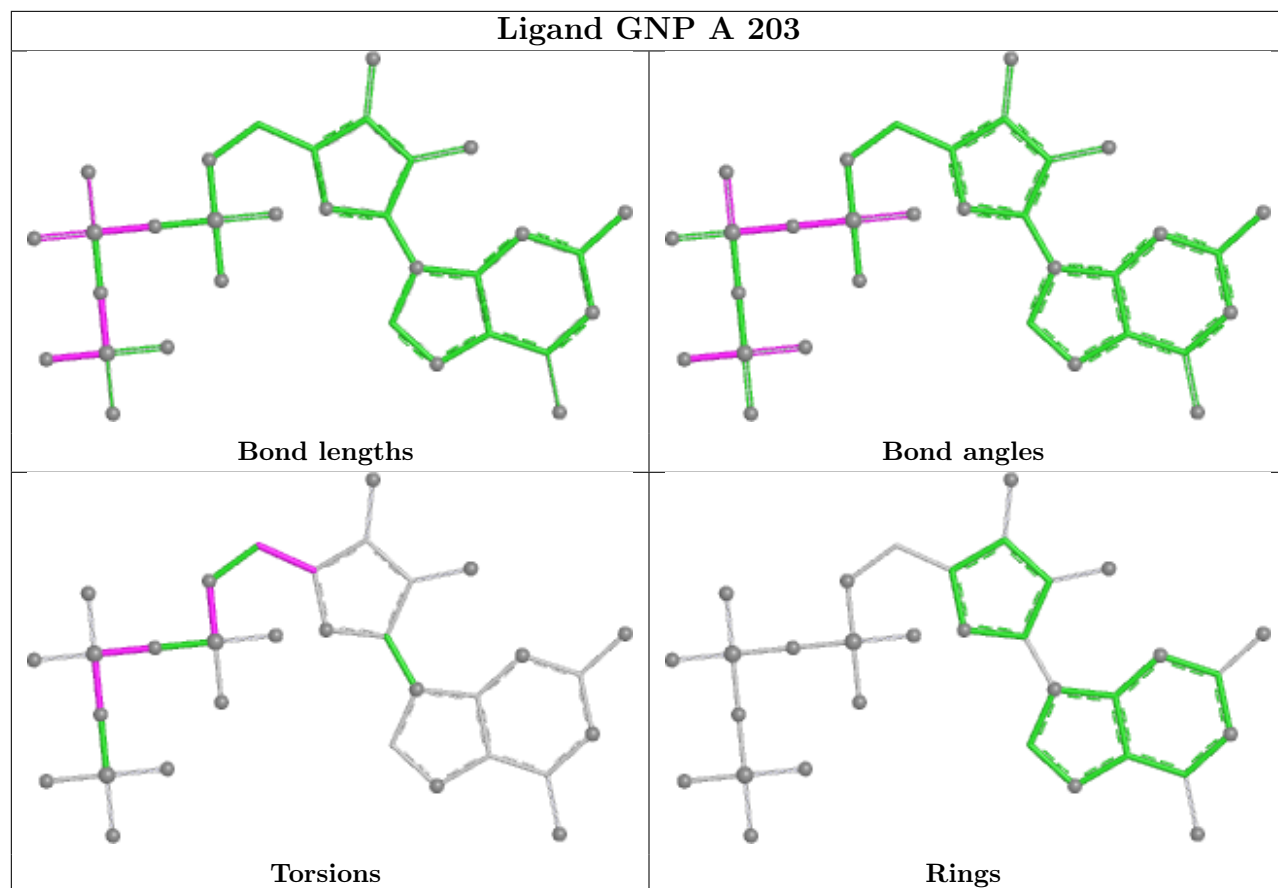
Mol	Chain	Res	Type	Atoms
2	B	203	WT6	C04-C03-S02-O01
2	B	203	WT6	C15-N14-S02-O19
4	B	205	GOL	O2-C2-C3-O3
3	A	203	GNP	C5'-O5'-PA-O1A
3	B	202	GNP	C5'-O5'-PA-O1A
2	A	202	WT6	C18-N14-S02-O19
2	B	203	WT6	C12-C06-N07-C08
4	B	205	GOL	O1-C1-C2-C3
2	B	203	WT6	C18-N14-S02-O19
3	A	203	GNP	PA-O3A-PB-O1B
2	A	201	WT6	C13-C03-S02-N14
4	A	204	GOL	O1-C1-C2-O2
2	A	201	WT6	C04-C03-S02-N14

There are no ring outliers.

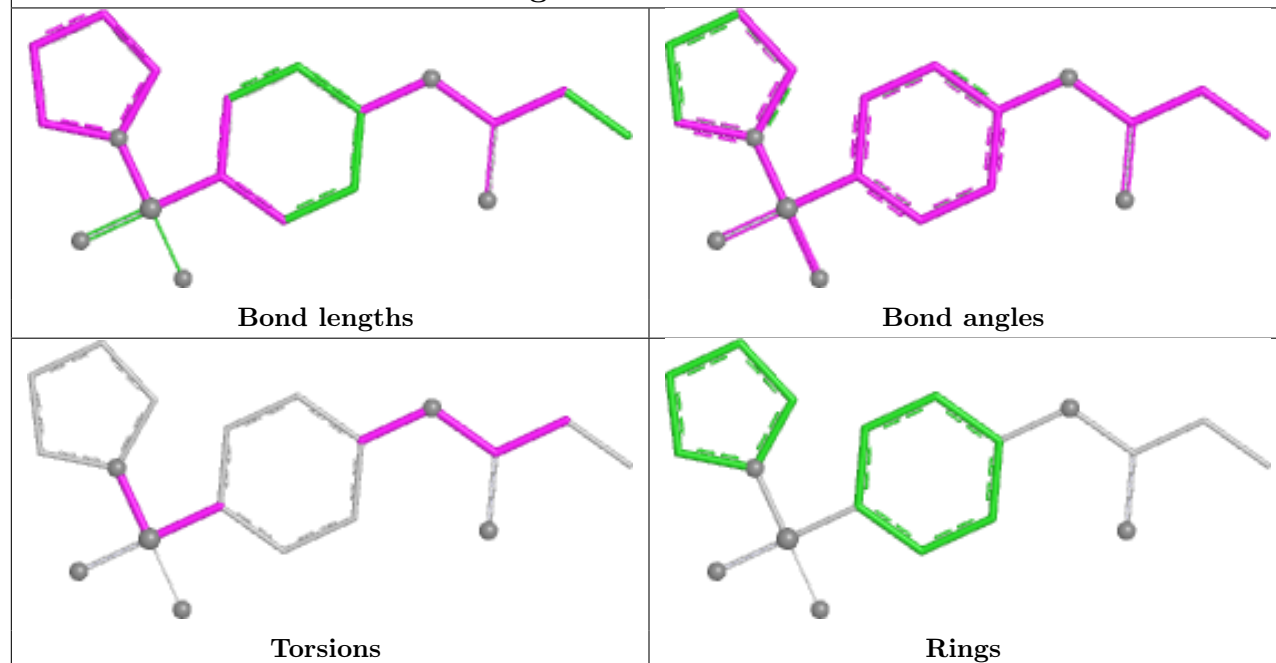
7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	204	GOL	1	0
3	A	203	GNP	4	0
4	B	205	GOL	2	0
2	B	201	WT6	1	0
2	B	203	WT6	5	0
3	B	202	GNP	1	0
2	A	202	WT6	2	0

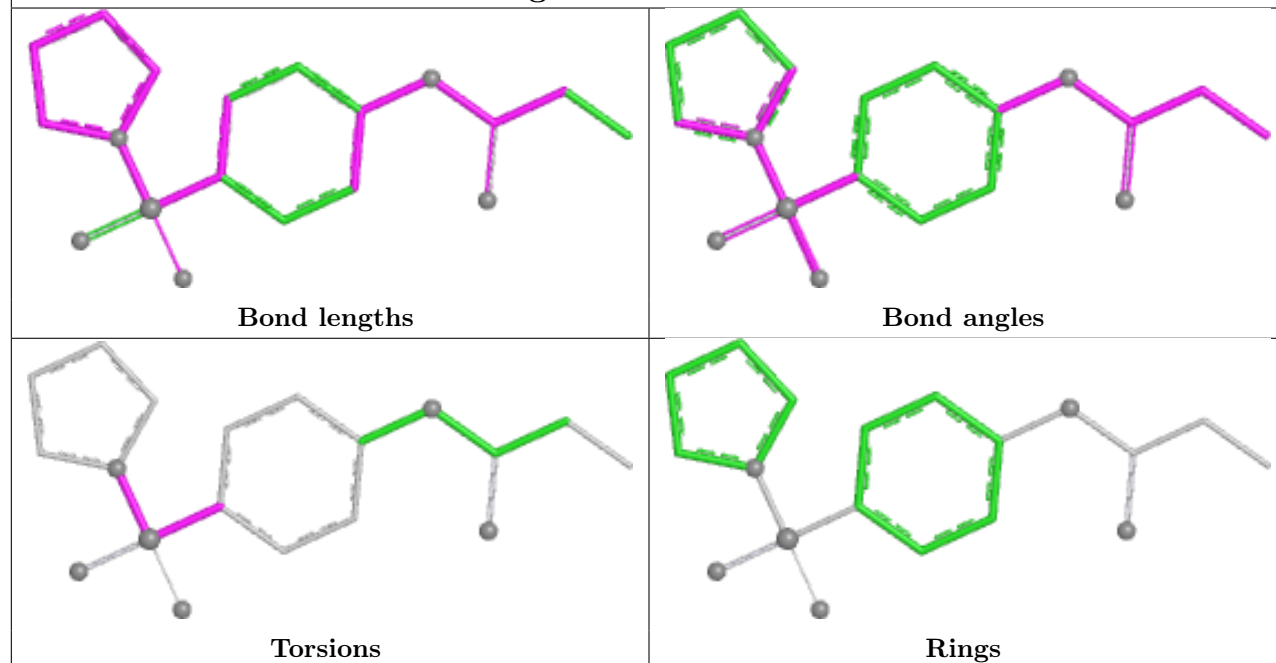
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

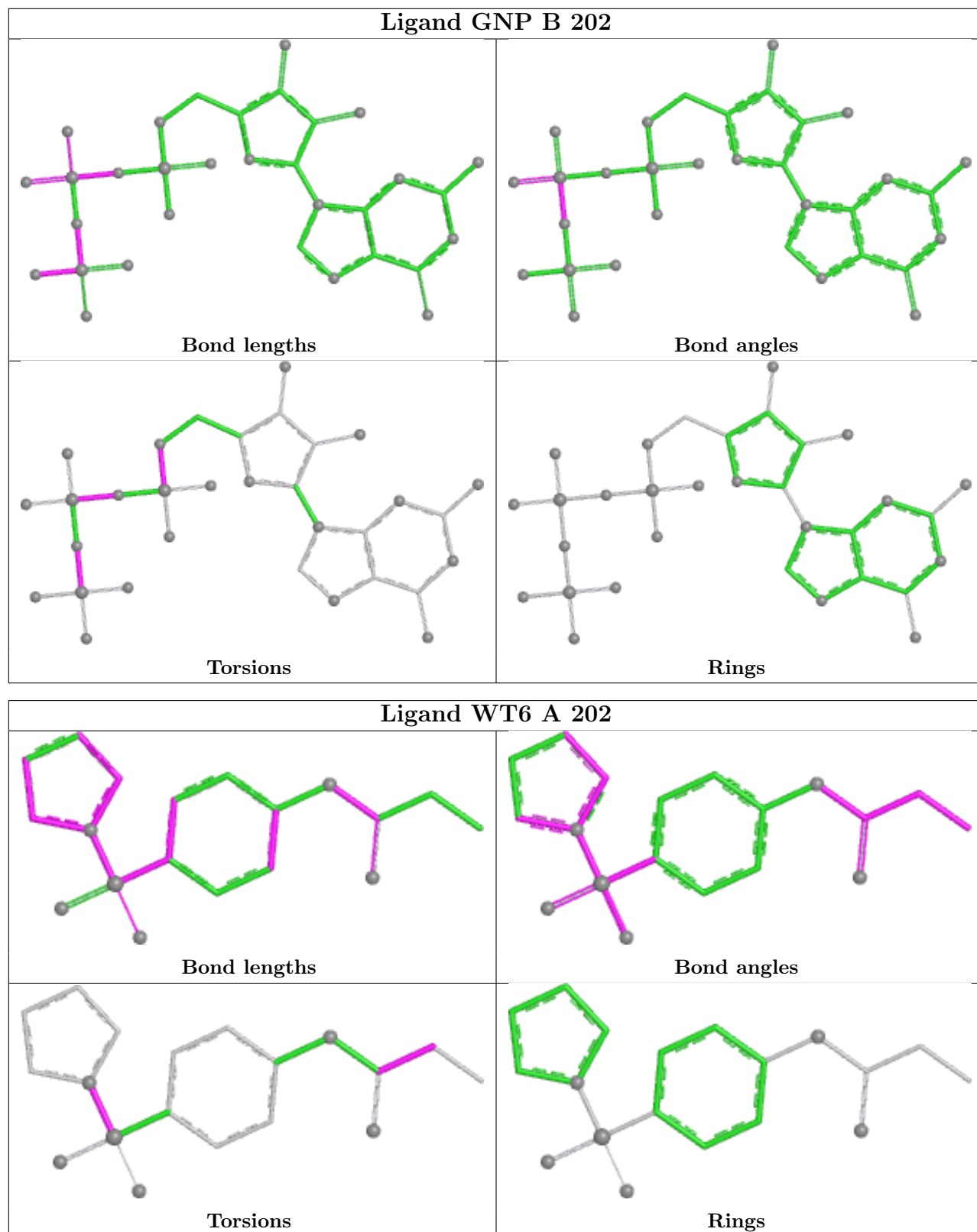


Ligand WT6 B 203



Ligand WT6 A 201





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	212/230 (92%)	2.42	122 (57%) 0 0	13, 23, 44, 91	2 (0%)
1	B	214/230 (93%)	2.84	137 (64%) 0 0	10, 25, 63, 93	2 (0%)
All	All	426/460 (92%)	2.63	259 (60%) 0 0	10, 24, 60, 93	4 (0%)

All (259) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	58	PRO	10.2
1	B	60	GLY	9.5
1	B	61	ALA	9.3
1	B	57	GLY	8.8
1	A	58	PRO	8.8
1	B	-38	GLY	7.7
1	A	57	GLY	7.3
1	A	59	ASP	7.3
1	A	61	ALA	7.3
1	B	-36	MET	7.2
1	B	8	TYR	7.0
1	B	59	ASP	6.7
1	B	55	ALA	6.6
1	B	62	THR	6.5
1	B	63	GLY	6.4
1	B	-34	PHE	6.4
1	B	-37	HIS	6.3
1	B	-33	LEU	6.2
1	B	6	TYR	6.1
1	B	124	GLU	5.9
1	B	188	SER	5.6
1	A	124	GLU	5.6
1	A	8	TYR	5.6
1	A	-9	GLU	5.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	122	TYR	5.5
1	A	60	GLY	5.3
1	B	-9	GLU	5.2
1	A	-34	PHE	5.1
1	B	-31	GLU	5.1
1	B	187	ARG	5.0
1	A	125	ASN	4.9
1	A	188	SER	4.9
1	B	186	GLU	4.8
1	A	7	ASP	4.8
1	B	56	SER	4.8
1	A	-37	HIS	4.7
1	B	139	ASP	4.7
1	A	186	GLU	4.6
1	B	35[A]	ASN	4.6
1	B	-8	ARG	4.6
1	B	39	ILE	4.6
1	B	7	ASP	4.5
1	B	88	PHE	4.4
1	A	-38	GLY	4.4
1	B	-27	GLU	4.4
1	A	62	THR	4.3
1	A	56	SER	4.3
1	B	-35	SER	4.3
1	A	122	TYR	4.2
1	A	12[A]	PHE	4.2
1	B	12	PHE	4.2
1	A	123	ALA	4.1
1	B	64	ARG	4.1
1	A	91	ASP	4.0
1	B	65	GLY	4.0
1	A	187	ARG	4.0
1	B	26	LEU	3.9
1	A	-16	ALA	3.9
1	B	9	LEU	3.9
1	B	-12	ALA	3.9
1	B	143	VAL	3.8
1	B	183	LYS	3.8
1	B	79	GLU	3.8
1	B	-11	GLU	3.7
1	B	52	VAL	3.7
1	A	-27	GLU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	111	ARG	3.7
1	A	42	VAL	3.7
1	A	-23	LYS	3.6
1	B	-32	THR	3.6
1	B	97	LEU	3.6
1	B	-10	GLU	3.6
1	B	184	ARG	3.5
1	A	-10	GLU	3.5
1	A	90[A]	ARG	3.5
1	B	111	ARG	3.5
1	A	-31	GLU	3.5
1	B	54	ARG	3.5
1	B	68	ILE	3.5
1	A	83	SER	3.5
1	B	-29	GLU	3.5
1	A	19	GLY	3.4
1	A	157	ILE	3.4
1	B	80	ARG	3.4
1	B	-25	ILE	3.4
1	B	51	VAL	3.3
1	B	157	ILE	3.3
1	A	-36	MET	3.3
1	B	-23	LYS	3.3
1	A	35	ASN	3.3
1	B	90	ARG	3.2
1	A	-12	ALA	3.2
1	B	123	ALA	3.2
1	B	185	MET	3.2
1	B	144	LYS	3.2
1	A	10	ILE	3.2
1	A	-35	SER	3.2
1	B	138	GLU	3.2
1	A	-26	ALA	3.2
1	B	177	LEU	3.2
1	A	88	PHE	3.2
1	A	89	PHE	3.2
1	B	81	PHE	3.2
1	B	-28	GLN	3.2
1	B	151	LEU	3.1
1	B	174	ILE	3.1
1	B	-13	ARG	3.1
1	B	125	ASN	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	70	LEU	3.1
1	B	178	LEU	3.1
1	A	-17	ALA	3.1
1	B	67	ARG	3.1
1	A	-33	LEU	3.1
1	A	178	LEU	3.1
1	B	98	LEU	3.1
1	B	146	GLU	3.0
1	A	184	ARG	3.0
1	A	85	THR	3.0
1	B	-30	GLU	3.0
1	A	87	ALA	3.0
1	B	42	VAL	3.0
1	B	154[A]	LYS	3.0
1	B	66	GLN	3.0
1	A	79	GLU	2.9
1	A	72	LEU	2.9
1	B	-15	LEU	2.9
1	B	149	ILE	2.9
1	B	121	ALA	2.9
1	A	81	PHE	2.9
1	B	76	ALA	2.9
1	A	70	LEU	2.9
1	B	91	ASP	2.9
1	B	53	TYR	2.9
1	A	185	MET	2.8
1	B	-21	LEU	2.8
1	B	180	LEU	2.8
1	B	85	THR	2.8
1	B	50	ARG	2.8
1	A	-11	GLU	2.8
1	B	10	ILE	2.8
1	A	138	GLU	2.8
1	A	165	ALA	2.8
1	A	-32	THR	2.8
1	A	142	VAL	2.8
1	B	126	PRO	2.8
1	A	50	ARG	2.8
1	B	107	PHE	2.8
1	A	96	LEU	2.8
1	A	119	MET	2.7
1	A	-20	GLN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	145	GLU	2.7
1	B	147	GLU	2.7
1	A	55	ALA	2.7
1	A	84	LEU	2.7
1	A	53	TYR	2.7
1	A	170	ILE	2.7
1	B	-14	LYS	2.7
1	A	77	GLY	2.7
1	B	173	ALA	2.7
1	B	84	LEU	2.7
1	A	67	ARG	2.7
1	A	126	PRO	2.6
1	A	65	GLY	2.6
1	B	140	GLN	2.6
1	A	155	TYR	2.6
1	B	142	VAL	2.6
1	A	78	LEU	2.6
1	B	95	PHE	2.6
1	A	183	LYS	2.6
1	B	87	ALA	2.6
1	B	106	SER	2.6
1	B	160	PHE	2.5
1	A	44	ILE	2.5
1	B	171	SER	2.5
1	B	130	LEU	2.5
1	A	37	LYS	2.5
1	B	-16	ALA	2.5
1	B	119	MET	2.5
1	A	63	GLY	2.5
1	B	114	ILE	2.5
1	A	112	ASN	2.5
1	B	86	THR	2.5
1	A	128	ILE	2.5
1	A	92	ALA	2.4
1	A	51	VAL	2.4
1	A	171	SER	2.4
1	B	83	SER	2.4
1	A	144	LYS	2.4
1	B	156	GLY	2.4
1	B	112	ASN	2.4
1	B	38	PHE	2.4
1	A	-22	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	181	ILE	2.4
1	A	180	LEU	2.4
1	B	72	LEU	2.4
1	B	137	LEU	2.4
1	A	103	ASN	2.4
1	B	44	ILE	2.4
1	A	64	ARG	2.4
1	B	150	ALA	2.3
1	B	129	VAL	2.3
1	B	69	HIS	2.3
1	B	104	GLU	2.3
1	A	108	LEU	2.3
1	A	117	LEU	2.3
1	A	174	ILE	2.3
1	A	30	THR	2.3
1	B	102	THR	2.3
1	A	169	ASN	2.3
1	B	131	CYS	2.3
1	A	97	LEU	2.3
1	A	137	LEU	2.3
1	B	78	LEU	2.3
1	B	159	TYR	2.3
1	A	11	LYS	2.3
1	A	76	ALA	2.3
1	B	-17	ALA	2.3
1	A	167	GLY	2.3
1	A	-15	LEU	2.3
1	A	120	HIS	2.2
1	A	-28	GLN	2.2
1	A	52	VAL	2.2
1	B	15	LEU	2.2
1	B	155	TYR	2.2
1	B	113	TRP	2.2
1	A	-13	ARG	2.2
1	B	20	VAL	2.2
1	A	9	LEU	2.2
1	B	172	GLN	2.2
1	B	36	SER	2.2
1	B	132	GLY	2.2
1	A	172	GLN	2.2
1	A	115	SER	2.2
1	A	38	PHE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	127	ASP	2.1
1	A	39	ILE	2.1
1	A	114	ILE	2.1
1	B	148	ALA	2.1
1	A	-14	LYS	2.1
1	A	26	LEU	2.1
1	B	109	ASN	2.1
1	B	29	TYR	2.1
1	A	46	PHE	2.1
1	A	95	PHE	2.1
1	A	106	SER	2.1
1	B	153	GLU	2.1
1	A	118	GLN	2.1
1	A	80	ARG	2.1
1	A	158	PRO	2.1
1	B	11	LYS	2.1
1	A	143	VAL	2.1
1	A	73	TRP	2.1
1	A	116	GLN	2.0
1	B	17	ASP	2.0
1	B	162	THR	2.0
1	A	159	TYR	2.0
1	A	-21	LEU	2.0
1	A	139	ASP	2.0
1	A	69	HIS	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 ⓘ

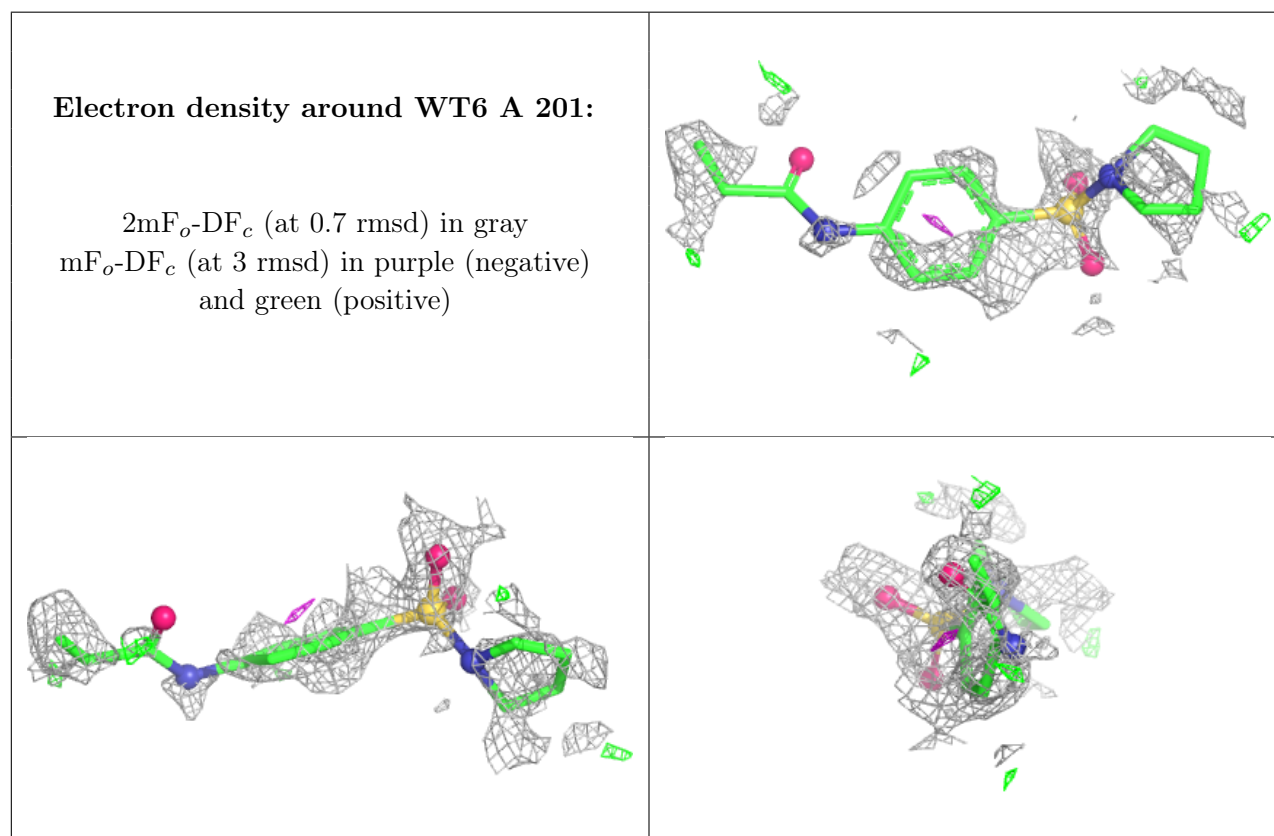
There are no oligosaccharides in this entry.

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.

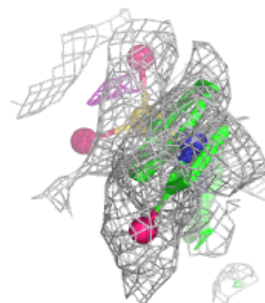
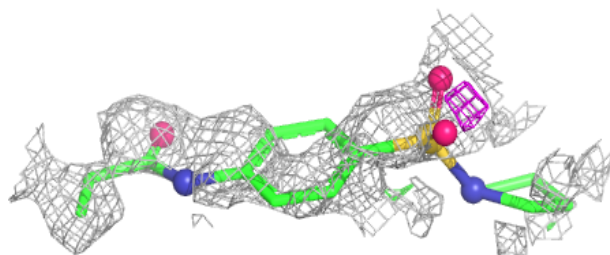
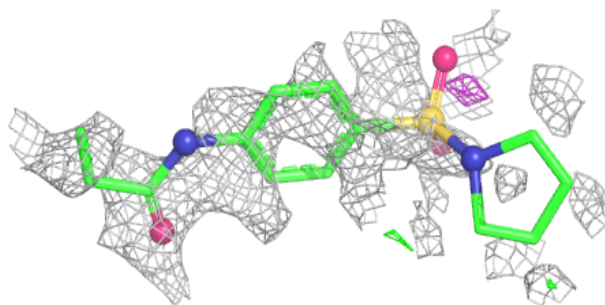
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	WT6	A	201	19/19	0.36	0.41	30,41,57,71	19
2	WT6	A	202	19/19	0.39	0.42	19,52,84,96	19
2	WT6	B	203	19/19	0.39	0.31	37,53,71,82	19
2	WT6	B	201	19/19	0.49	0.33	29,35,50,59	9
4	GOL	B	204	6/6	0.52	0.25	20,27,39,48	0
4	GOL	B	205	6/6	0.68	0.20	26,29,36,42	0
4	GOL	A	204	6/6	0.70	0.23	27,28,29,29	0
5	MG	A	205	1/1	0.70	0.09	21,21,21,21	0
3	GNP	B	202	32/32	0.90	0.11	10,17,22,30	0
3	GNP	A	203	32/32	0.92	0.10	8,17,23,28	0
5	MG	B	206	1/1	0.95	0.09	8,8,8,8	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.

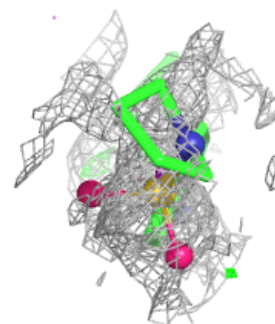
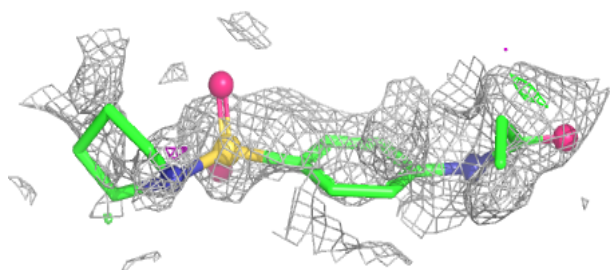
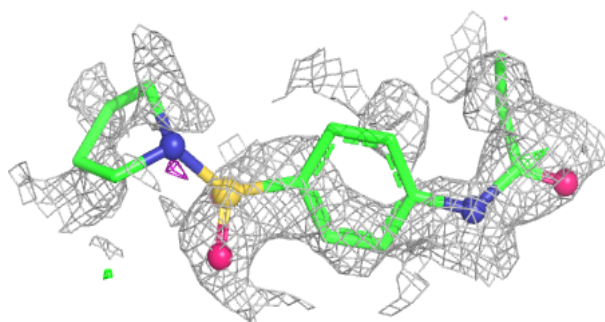


Electron density around WT6 A 202:

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

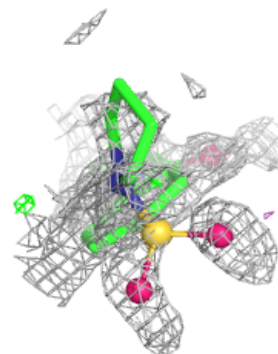
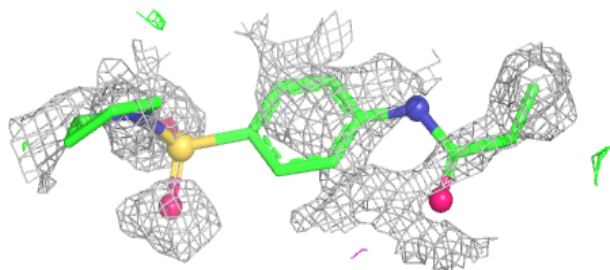
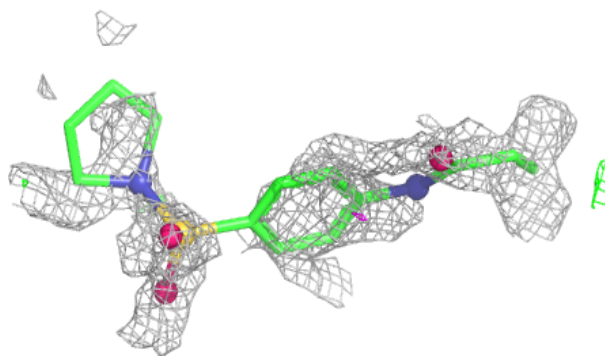
**Electron density around WT6 B 203:**

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

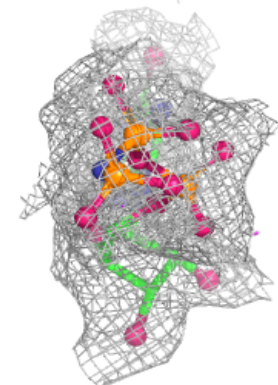
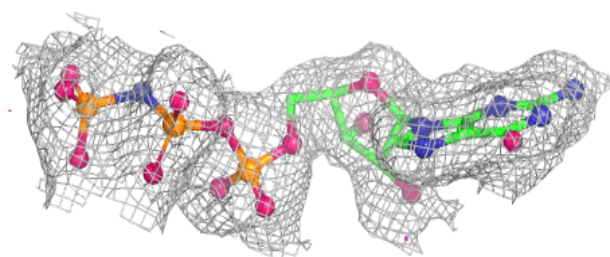
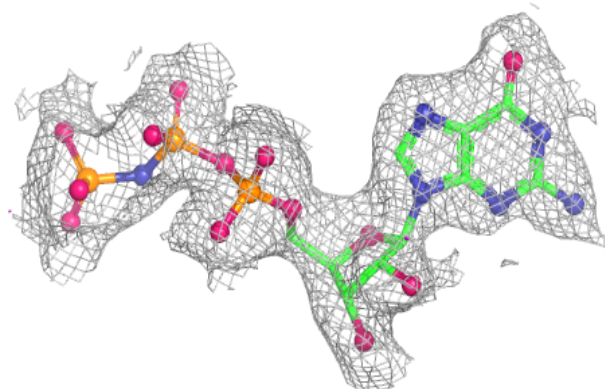


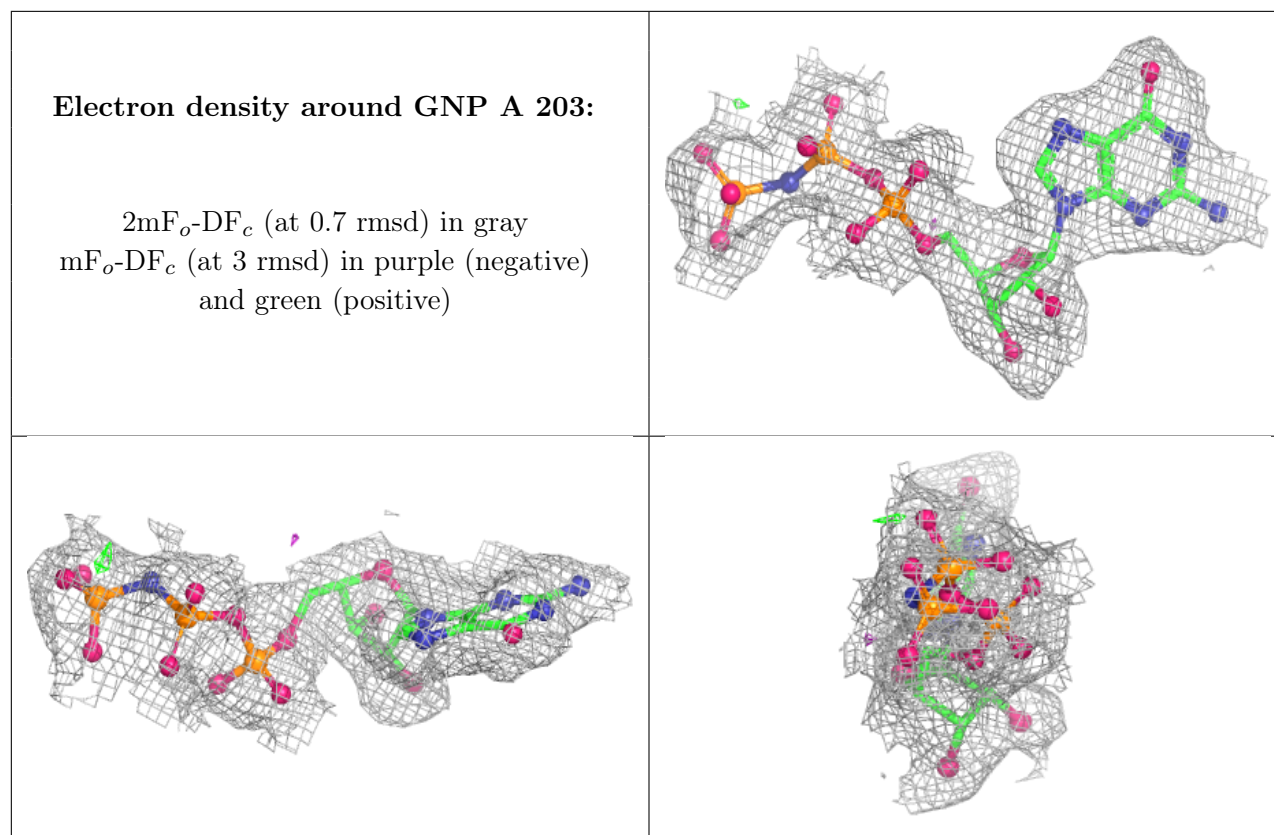
Electron density around WT6 B 201:

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

**Electron density around GNP B 202:**

$2mF_o-DF_c$ (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.