



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:42 PM UTC

PDB ID : 8P3H / pdb_00008p3h
Title : Fusion hSlp2-a_Rab27A bound to covalent hit fragment IMP-1712
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 : 2.76 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

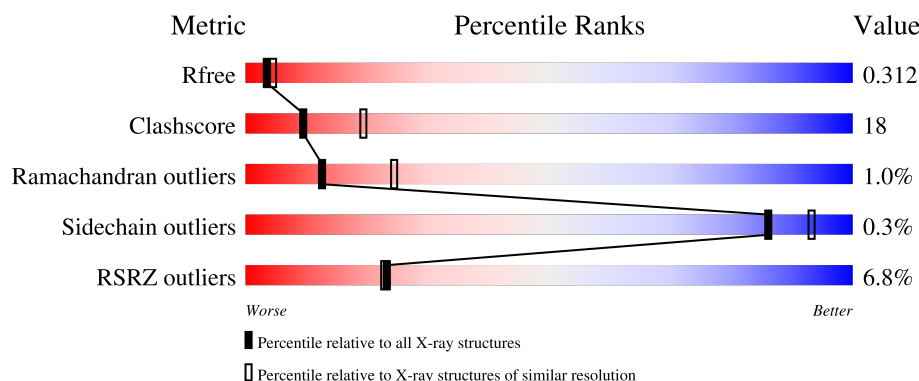
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	4% 61% 27% 10%
1	B	230	8% 63% 24% 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	WTO	A	205	-	X	-	-
4	WTO	B	203	-	X	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3459 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.

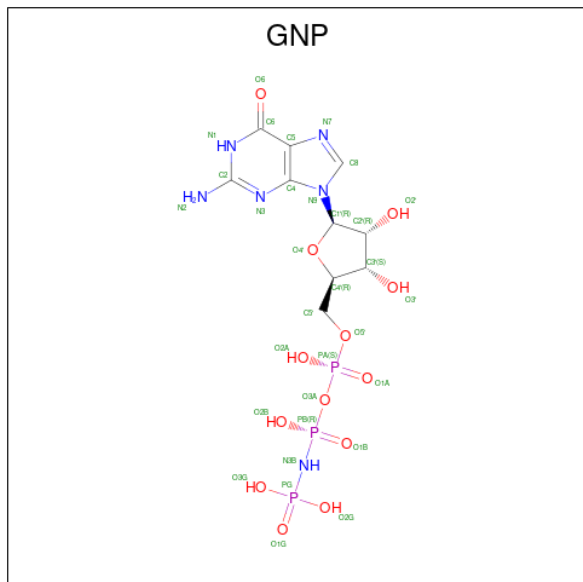
- Molecule 1 is a protein called Synaptotagmin-like protein 2,Ras-related protein Rab-27A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	1	0
			1661	1051	284	318	8			
1	B	203	Total	C	N	O	S	0	0	0
			1615	1028	276	303	8			

There are 24 discrepancies between the modelled and reference sequences:

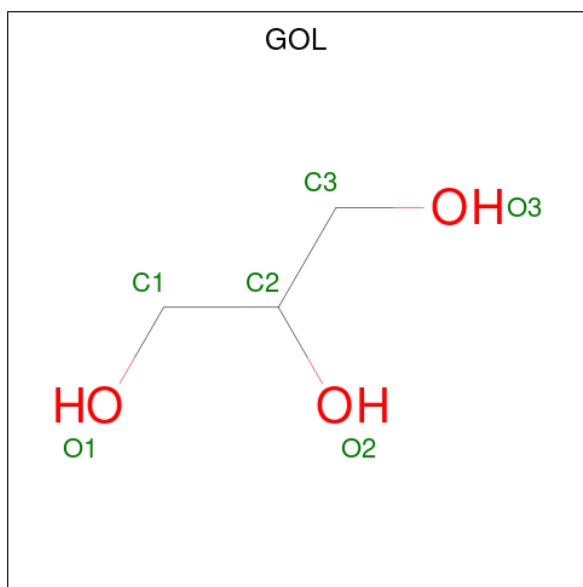
Chain	Residue	Modelled	Actual	Comment	Reference
A	-38	GLY	-	expression tag	UNP Q9HCH5
A	-37	HIS	-	expression tag	UNP Q9HCH5
A	-36	MET	-	expression tag	UNP Q9HCH5
A	-9B	GLY	-	linker	UNP Q9HCH5
A	-9C	SER	-	linker	UNP Q9HCH5
A	-9D	GLY	-	linker	UNP Q9HCH5
A	-9E	SER	-	linker	UNP Q9HCH5
A	-9F	GLY	-	linker	UNP Q9HCH5
A	-9G	SER	-	linker	UNP Q9HCH5
A	-9H	GLY	-	linker	UNP Q9HCH5
A	60	LEU	GLN	engineered mutation	UNP P51159
A	170	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	57	LEU	GLN	engineered mutation	UNP P51159
B	167	SER	CYS	engineered mutation	UNP P51159

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



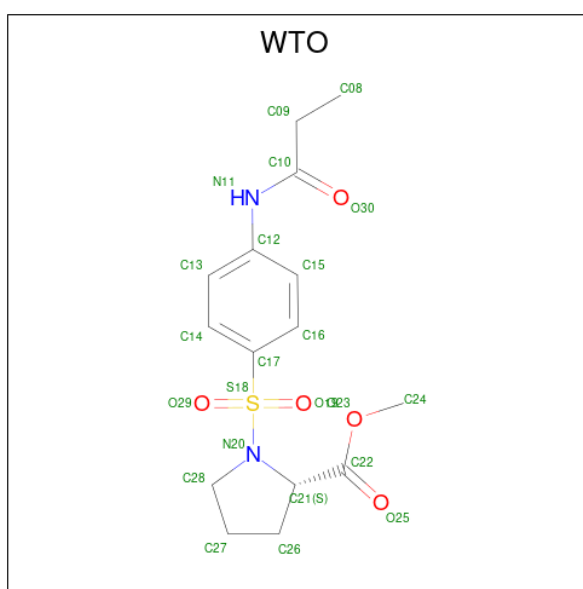
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
2	B	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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	B	1	Total C O 6 3 3	0	0

- Molecule 4 is methyl (2 {S})-1-[4-(propanoylamino)phenyl]sulfonylpyrrolidine-2-carboxylate (CCD ID: WTO) (formula: C₁₅H₂₀N₂O₅S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O S 23 15 2 5 1	0	0
4	B	1	Total C N O S 23 15 2 5 1	0	0

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

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

- Molecule 6 is water.

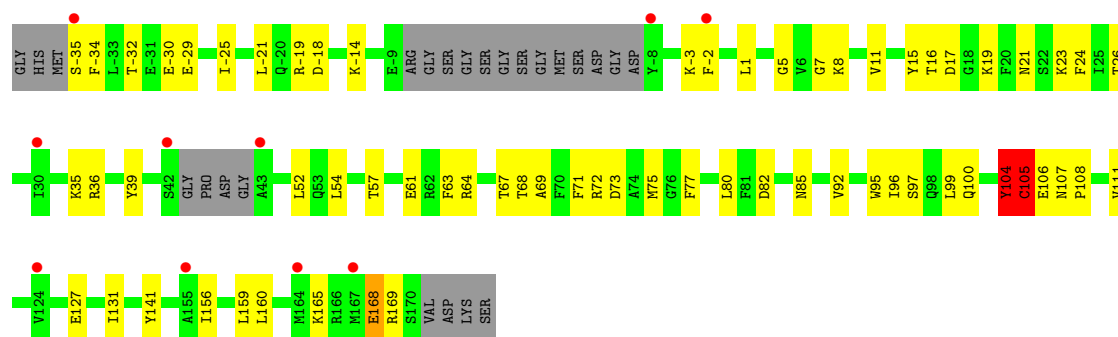
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	23	Total 23	O 23	0	0
6	B	24	Total 24	O 24	0	0

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.

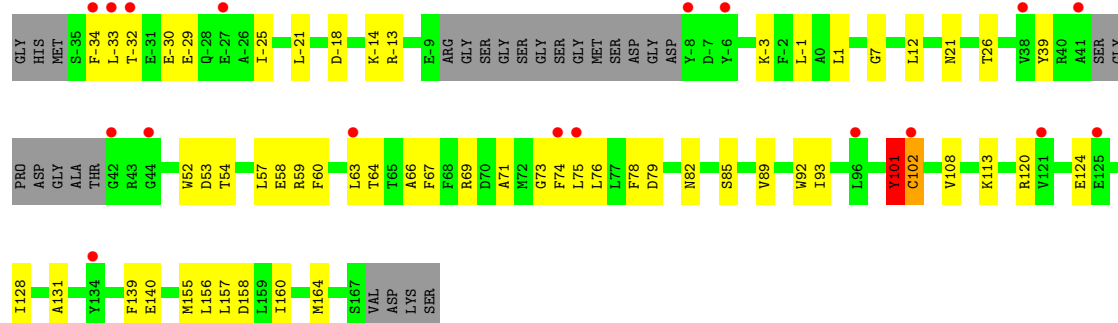
- Molecule 1: Synaptotagmin-like protein 2,Ras-related protein Rab-27A

Chain A: 



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

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.17Å 77.70Å 116.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.08 – 2.76 58.08 – 2.76	Depositor EDS
% Data completeness (in resolution range)	99.4 (58.08-2.76) 100.0 (58.08-2.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.17_3644: ???)	Depositor
R, R_{free}	0.227 , 0.313 0.228 , 0.312	Depositor DCC
R_{free} test set	727 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	53.5	Xtriage
Anisotropy	0.985	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.3	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	0.93	EDS
Total number of atoms	3459	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.13% 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: WTO, GOL, GNP, 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	0.45	2/1685 (0.1%)	1.06	5/2264 (0.2%)
1	B	0.47	2/1640 (0.1%)	1.03	4/2207 (0.2%)
All	All	0.46	4/3325 (0.1%)	1.04	9/4471 (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	2
1	B	0	3
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	CYS	C-N	7.16	1.44	1.33
1	A	104	TYR	C-N	7.02	1.43	1.33
1	B	101	TYR	C-N	7.02	1.43	1.33
1	B	102	CYS	C-N	6.54	1.43	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	101	TYR	O-C-N	-34.33	76.06	122.06
1	A	104	TYR	O-C-N	-30.89	89.90	122.03
1	A	105	CYS	CA-C-N	-18.04	88.09	123.09
1	A	105	CYS	C-N-CA	-18.04	88.09	123.09
1	B	102	CYS	O-C-N	-13.92	104.08	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	101	TYR	CA-C-N	7.96	136.75	121.54
1	B	101	TYR	C-N-CA	7.96	136.75	121.54
1	A	104	TYR	CA-C-N	5.89	132.80	121.54
1	A	104	TYR	C-N-CA	5.89	132.80	121.54

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	104	TYR	Mainchain
1	A	105	CYS	Peptide
1	B	101	TYR	Mainchain
1	B	102	CYS	Peptide,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	1661	0	1641	67	0
1	B	1615	0	1588	65	0
2	A	32	0	13	4	0
2	B	32	0	13	1	0
3	A	18	0	24	3	0
3	B	6	0	8	1	0
4	A	23	0	0	1	0
4	B	23	0	0	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	23	0	0	2	0
6	B	24	0	0	0	0
All	All	3459	0	3287	120	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 18.

All (120) 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:58:GLU:OE2	1:B:59:ARG:NH1	2.06	0.89
1:A:-32:THR:HG22	1:A:-30:GLU:H	1.41	0.84
1:A:72:ARG:NH2	1:B:-18:ASP:OD2	2.15	0.79
1:A:168:GLU:HG3	1:A:169:ARG:HD3	1.66	0.77
2:A:201:GNP:N3	3:A:204:GOL:H32	2.04	0.73
1:A:72:ARG:HD2	1:A:72:ARG:H	1.56	0.71
1:A:72:ARG:HG2	1:A:72:ARG:HH21	1.58	0.69
1:A:23:LYS:O	3:A:202:GOL:H11	1.97	0.64
1:A:97:SER:HA	1:A:100:GLN:HG3	1.80	0.64
1:A:127:GLU:O	1:A:131:ILE:HD12	1.98	0.63
1:A:-19[B]:ARG:NH2	6:A:302:HOH:O	2.33	0.62
1:A:106:GLU:HB2	1:B:-13:ARG:HD2	1.82	0.61
1:B:73:GLY:HA3	1:B:160:ILE:HD11	1.83	0.60
1:B:120:ARG:NH1	1:B:140:GLU:OE1	2.31	0.60
1:A:11:VAL:HG21	1:A:80:LEU:HD21	1.83	0.60
1:B:57:LEU:HD23	1:B:59:ARG:NH1	2.17	0.59
1:B:75:LEU:HD12	1:B:108:VAL:HB	1.84	0.59
1:B:76:LEU:HD11	1:B:92:TRP:HB3	1.85	0.58
1:A:92:VAL:O	1:A:96:ILE:HG13	2.02	0.58
1:B:-3:LYS:NZ	4:B:203:WTO:O29	2.37	0.58
1:A:106:GLU:CD	1:A:107:ASN:H	2.12	0.58
1:A:111:VAL:HG23	1:A:159:LEU:HD13	1.87	0.57
1:A:57:THR:HB	1:A:67:THR:HB	1.86	0.56
1:B:-32:THR:HG22	1:B:-30:GLU:H	1.70	0.56
1:B:-32:THR:HB	1:B:-29:GLU:HB2	1.87	0.56
1:B:1:LEU:HG	1:B:76:LEU:HD12	1.87	0.55
1:A:-34:PHE:CE1	1:B:59:ARG:HB3	2.41	0.55
1:B:89:VAL:O	1:B:93:ILE:HG13	2.06	0.55
1:A:21:ASN:HB3	3:A:202:GOL:H12	1.87	0.55
1:A:1:LEU:HD12	1:A:95:TRP:CE3	2.41	0.55
1:A:100:GLN:O	6:A:301:HOH:O	2.18	0.55
1:A:-14:LYS:HG3	1:B:101:TYR:CE1	2.42	0.55
1:A:26:THR:OG1	2:A:201:GNP:O1G	2.25	0.55
1:B:59:ARG:HH11	1:B:59:ARG:HG3	1.72	0.55
1:B:57:LEU:HB3	1:B:59:ARG:NH1	2.23	0.54
1:A:-14:LYS:HG3	1:B:101:TYR:CZ	2.43	0.53
1:A:16:THR:HG22	1:A:35:LYS:HB2	1.90	0.53
1:A:104:TYR:CE2	1:B:-14:LYS:HG3	2.44	0.53
1:A:63:PHE:O	1:A:67:THR:HG23	2.09	0.52
1:A:72:ARG:NH1	1:B:-21:LEU:O	2.42	0.52
1:B:21:ASN:HB3	3:B:202:GOL:H2	1.92	0.52
1:B:108:VAL:HG23	1:B:156:LEU:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:LYS:NZ	1:A:24:PHE:H	2.08	0.51
1:B:82:ASN:HB3	1:B:85:SER:OG	2.11	0.50
1:B:69:ARG:HD3	1:B:101:TYR:OH	2.12	0.50
1:A:5:GLY:H	2:A:201:GNP:HNB3	1.60	0.49
1:A:-35:SER:HA	1:B:-34:PHE:HB3	1.94	0.49
1:B:-25:ILE:HG21	1:B:63:LEU:HD21	1.94	0.49
1:B:79:ASP:CG	1:B:113:LYS:HD2	2.38	0.49
1:B:79:ASP:H	1:B:85:SER:HB3	1.78	0.48
1:B:155:MET:HB3	1:B:155:MET:HE3	1.67	0.48
1:A:-34:PHE:N	1:B:-34:PHE:HB3	2.29	0.48
1:A:96:ILE:O	1:A:100:GLN:HG2	2.13	0.48
1:B:54:THR:HB	1:B:64:THR:CG2	2.43	0.48
1:A:-2:PHE:CZ	1:A:54:LEU:HD22	2.48	0.48
1:A:-32:THR:HB	1:A:-29:GLU:HB2	1.95	0.48
1:A:-32:THR:HG22	1:A:-30:GLU:N	2.19	0.48
1:B:66:ALA:O	1:B:69:ARG:NE	2.34	0.48
1:A:77:PHE:HE2	1:A:108:PRO:HB2	1.79	0.47
1:A:-18:ASP:OD2	1:B:101:TYR:OH	2.29	0.47
1:B:39:TYR:CD1	1:B:157:LEU:HD22	2.49	0.47
1:A:82:ASP:HB3	1:A:85:ASN:HB3	1.96	0.47
1:A:1:LEU:HD11	1:A:99:LEU:HD11	1.96	0.47
1:B:71:ALA:HB3	1:B:74:PHE:CE1	2.50	0.47
1:A:104:TYR:CZ	1:B:-14:LYS:HE2	2.49	0.47
1:B:124:GLU:O	1:B:128:ILE:HG13	2.15	0.46
1:B:59:ARG:NH1	1:B:59:ARG:HG3	2.30	0.46
1:A:36:ARG:HG2	1:A:36:ARG:HH11	1.81	0.46
1:B:26:THR:OG1	1:B:57:LEU:HD11	2.15	0.46
1:A:15:TYR:CD1	1:A:156:ILE:HD12	2.50	0.46
1:B:128:ILE:HA	1:B:131:ALA:HB3	1.97	0.46
1:B:71:ALA:O	4:B:203:WTO:N11	2.49	0.46
1:A:17:ASP:O	1:A:19:LYS:HG3	2.15	0.46
1:A:97:SER:HA	1:A:100:GLN:CG	2.46	0.45
1:B:57:LEU:HD12	1:B:57:LEU:H	1.81	0.45
1:B:-1:LEU:HA	1:B:52:TRP:HB2	1.99	0.45
1:B:57:LEU:HD23	1:B:59:ARG:CZ	2.46	0.45
1:A:7:GLY:HA2	2:A:201:GNP:O2A	2.16	0.45
1:B:76:LEU:CD2	1:B:89:VAL:HG13	2.47	0.45
1:A:131:ILE:HG13	1:A:141:TYR:CD2	2.53	0.44
1:B:1:LEU:HD21	1:B:74:PHE:HB3	1.99	0.44
1:B:78:PHE:HB2	1:B:85:SER:CB	2.47	0.44
1:B:39:TYR:OH	1:B:158:ASP:OD1	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ALA:O	1:A:72:ARG:HD3	2.18	0.43
1:A:-3:LYS:NZ	1:A:73:ASP:OD1	2.47	0.43
1:A:61:GLU:HA	1:A:64:ARG:NH1	2.33	0.43
1:A:72:ARG:NH2	1:A:72:ARG:HG2	2.29	0.43
1:B:54:THR:HB	1:B:64:THR:HB	2.01	0.42
1:B:57:LEU:HB2	1:B:60:PHE:HD2	1.84	0.42
1:A:-21:LEU:HA	1:A:-18:ASP:HB3	2.01	0.42
1:A:71:PHE:N	1:A:71:PHE:CD1	2.87	0.42
1:B:7:GLY:HA2	2:B:201:GNP:PA	2.59	0.42
1:B:157:LEU:HD23	1:B:157:LEU:O	2.18	0.42
1:A:77:PHE:CE2	1:A:108:PRO:HB2	2.55	0.42
1:B:-32:THR:HG22	1:B:-30:GLU:N	2.33	0.42
1:B:76:LEU:HD11	1:B:92:TRP:CB	2.49	0.42
1:A:-35:SER:OG	1:A:-34:PHE:O	2.36	0.42
1:A:75:MET:HE2	4:A:205:WTO:C16	2.50	0.42
1:A:64:ARG:O	1:A:68:THR:OG1	2.25	0.42
1:A:165:LYS:HA	1:A:168:GLU:HB2	2.02	0.42
1:B:69:ARG:HB2	1:B:101:TYR:CE1	2.55	0.42
1:B:120:ARG:HH22	1:B:140:GLU:CD	2.27	0.42
1:A:169:ARG:HA	1:A:169:ARG:HD2	1.77	0.41
1:A:72:ARG:HH21	1:A:72:ARG:CG	2.29	0.41
1:A:16:THR:HA	1:A:35:LYS:HD3	2.02	0.41
1:A:52:LEU:HB3	1:A:54:LEU:HD21	2.01	0.41
1:B:-1:LEU:HB2	1:B:71:ALA:HB2	2.02	0.41
1:B:139:PHE:HZ	1:B:155:MET:HG3	1.86	0.41
1:A:-2:PHE:CE1	1:A:54:LEU:HD22	2.55	0.41
1:B:69:ARG:HB2	1:B:101:TYR:CD1	2.56	0.41
1:A:39:TYR:HB2	1:A:160:LEU:HD21	2.03	0.41
1:B:76:LEU:HD21	1:B:89:VAL:HG13	2.03	0.41
1:A:72:ARG:NH2	1:A:72:ARG:CG	2.83	0.41
1:A:-29:GLU:O	1:A:-25:ILE:HG13	2.21	0.40
1:A:8:LYS:HB2	1:A:8:LYS:HE3	1.74	0.40
1:A:-21:LEU:HB3	1:B:69:ARG:NH2	2.36	0.40
1:B:12:LEU:HD12	1:B:53:ASP:HB2	2.03	0.40
1:A:-21:LEU:HB3	1:B:69:ARG:HH22	1.87	0.40
1:B:-21:LEU:HD21	1:B:67:PHE:HZ	1.86	0.40
1:B:79:ASP:OD1	1:B:113:LYS:HD2	2.20	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	201/230 (87%)	184 (92%)	15 (8%)	2 (1%)	12	24
1	B	197/230 (86%)	179 (91%)	16 (8%)	2 (1%)	12	24
All	All	398/460 (86%)	363 (91%)	31 (8%)	4 (1%)	12	24

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	-33	LEU
1	A	105	CYS
1	B	164	MET
1	A	168	GLU

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	176/193 (91%)	175 (99%)	1 (1%)	78	88
1	B	168/193 (87%)	168 (100%)	0	100	100
All	All	344/386 (89%)	343 (100%)	1 (0%)	86	93

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	CYS

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	-28	GLN
1	B	95	GLN
1	B	112	ASN
1	B	119	GLN

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 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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
2	GNP	A	201	5	34,34,34	1.39	6 (17%)	47,54,54	1.05	3 (6%)
3	GOL	A	204	-	5,5,5	1.37	1 (20%)	5,5,5	1.04	0
2	GNP	B	201	5	34,34,34	1.35	4 (11%)	47,54,54	0.73	2 (4%)
4	WTO	A	205	1	24,24,24	4.65	12 (50%)	34,34,34	3.53	14 (41%)
3	GOL	A	202	-	5,5,5	0.76	0	5,5,5	1.47	1 (20%)
3	GOL	B	202	-	5,5,5	0.91	0	5,5,5	1.22	1 (20%)
4	WTO	B	203	1	24,24,24	4.74	10 (41%)	34,34,34	3.74	18 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	A	203	-	5,5,5	0.98	0	5,5,5	1.05	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GNP	A	201	5	-	5/18/38/38	0/3/3/3
3	GOL	A	204	-	-	4/4/4/4	-
2	GNP	B	201	5	-	3/18/38/38	0/3/3/3
4	WTO	A	205	1	-	12/24/34/34	0/2/2/2
3	GOL	A	202	-	-	0/4/4/4	-
3	GOL	B	202	-	-	1/4/4/4	-
4	WTO	B	203	1	-	15/24/34/34	0/2/2/2
3	GOL	A	203	-	-	2/4/4/4	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	205	WTO	C28-N20	-12.32	1.31	1.48
4	B	203	WTO	C28-N20	-12.13	1.31	1.48
4	B	203	WTO	C21-N20	11.30	1.65	1.48
4	A	205	WTO	C21-N20	10.90	1.64	1.48
4	A	205	WTO	C26-C21	-9.83	1.30	1.53
4	B	203	WTO	C26-C21	-9.82	1.30	1.53
4	B	203	WTO	C17-S18	6.11	1.84	1.76
4	B	203	WTO	S18-N20	6.03	1.72	1.63
4	B	203	WTO	C10-N11	5.63	1.47	1.35
4	A	205	WTO	C17-S18	5.62	1.84	1.76
4	A	205	WTO	S18-N20	5.48	1.71	1.63
2	A	201	GNP	PB-O3A	5.39	1.65	1.59
4	A	205	WTO	C10-N11	5.23	1.46	1.35
2	B	201	GNP	PB-O3A	4.54	1.64	1.59
4	A	205	WTO	O19-S18	4.25	1.48	1.43
2	B	201	GNP	PB-O1B	3.81	1.52	1.46
2	B	201	GNP	PG-O1G	3.64	1.51	1.46
4	B	203	WTO	O19-S18	3.53	1.47	1.43
4	B	203	WTO	O23-C22	3.52	1.41	1.33
4	A	205	WTO	O29-S18	3.38	1.47	1.43
4	B	203	WTO	C12-N11	3.27	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	GNP	PG-O1G	3.16	1.51	1.46
4	B	203	WTO	O29-S18	3.12	1.46	1.43
4	A	205	WTO	O23-C22	3.04	1.40	1.33
2	A	201	GNP	PB-O1B	2.83	1.50	1.46
3	A	204	GOL	C1-C2	2.58	1.61	1.51
4	A	205	WTO	C21-C22	2.37	1.56	1.52
2	A	201	GNP	PG-N3B	2.31	1.69	1.63
2	A	201	GNP	PB-O2B	-2.29	1.50	1.56
2	A	201	GNP	PA-O2A	-2.18	1.45	1.55
2	B	201	GNP	PB-O2B	-2.10	1.51	1.56
4	A	205	WTO	C12-N11	2.02	1.45	1.41
4	A	205	WTO	O23-C24	-2.01	1.40	1.45

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	205	WTO	O29-S18-O19	-14.36	97.19	119.59
4	B	203	WTO	O29-S18-O19	-13.84	97.99	119.59
4	A	205	WTO	O19-S18-C17	7.21	117.07	108.10
4	B	203	WTO	C12-N11-C10	6.61	139.22	127.52
4	B	203	WTO	O23-C22-C21	5.81	121.28	110.89
4	B	203	WTO	C14-C17-S18	5.24	124.94	119.73
4	A	205	WTO	C12-N11-C10	-5.11	118.48	127.52
4	B	203	WTO	C09-C10-N11	4.88	127.27	114.65
4	A	205	WTO	C28-N20-C21	-4.64	104.89	111.25
4	B	203	WTO	O19-S18-C17	4.53	113.73	108.10
2	A	201	GNP	O1G-PG-N3B	-4.33	105.39	111.77
4	A	205	WTO	O23-C22-C21	4.29	118.56	110.89
4	B	203	WTO	O29-S18-C17	3.86	112.91	108.10
4	A	205	WTO	C28-N20-S18	3.61	127.27	119.00
4	A	205	WTO	C21-N20-S18	3.54	127.79	119.77
4	B	203	WTO	C21-N20-S18	3.50	127.71	119.77
4	B	203	WTO	C28-N20-C21	-3.43	106.55	111.25
4	A	205	WTO	C14-C17-S18	3.38	123.09	119.73
4	A	205	WTO	O19-S18-N20	3.32	112.77	106.97
4	B	203	WTO	C26-C21-N20	3.22	107.20	102.91
2	A	201	GNP	O2G-PG-O3G	3.20	116.18	107.59
4	B	203	WTO	O30-C10-C09	-3.08	113.82	122.13
4	B	203	WTO	O19-S18-N20	2.84	111.94	106.97
4	B	203	WTO	C28-N20-S18	2.83	125.48	119.00
4	B	203	WTO	O25-C22-C21	-2.79	118.30	124.46
4	A	205	WTO	O30-C10-N11	-2.72	118.76	123.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	GNP	O2G-PG-O1G	-2.68	106.72	113.45
4	A	205	WTO	O23-C22-O25	-2.67	118.65	123.85
4	A	205	WTO	O29-S18-C17	2.64	111.39	108.10
4	B	203	WTO	O30-C10-N11	-2.64	118.91	123.64
3	A	202	GOL	C3-C2-C1	-2.58	102.32	111.80
4	B	203	WTO	C16-C17-C14	-2.43	117.30	120.47
4	A	205	WTO	C09-C10-N11	2.39	120.83	114.65
4	A	205	WTO	C15-C16-C17	2.36	121.73	119.44
2	B	201	GNP	O1G-PG-N3B	-2.34	108.32	111.77
4	B	203	WTO	C27-C28-N20	2.25	107.17	103.32
2	B	201	GNP	O2A-PA-O5'	2.25	117.77	107.57
4	B	203	WTO	C15-C16-C17	2.15	121.53	119.44
3	B	202	GOL	C3-C2-C1	-2.11	104.06	111.80

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	GNP	C5'-O5'-PA-O3A
2	A	201	GNP	C5'-O5'-PA-O2A
2	B	201	GNP	PB-N3B-PG-O1G
2	B	201	GNP	PA-O3A-PB-O1B
2	B	201	GNP	PA-O3A-PB-O2B
3	A	203	GOL	O1-C1-C2-C3
3	A	204	GOL	O1-C1-C2-C3
4	A	205	WTO	C21-C22-O23-C24
4	A	205	WTO	O25-C22-O23-C24
4	B	203	WTO	C21-C22-O23-C24
4	B	203	WTO	O30-C10-N11-C12
4	B	203	WTO	O25-C22-O23-C24
4	B	203	WTO	C09-C10-N11-C12
4	B	203	WTO	C16-C17-S18-N20
4	B	203	WTO	C14-C17-S18-N20
4	A	205	WTO	C28-N20-S18-O29
2	A	201	GNP	O4'-C4'-C5'-O5'
3	A	203	GOL	O1-C1-C2-O2
3	A	204	GOL	O1-C1-C2-O2
2	A	201	GNP	C3'-C4'-C5'-O5'
4	B	203	WTO	C21-N20-S18-O19
3	A	204	GOL	C1-C2-C3-O3
4	A	205	WTO	C14-C17-S18-N20
4	A	205	WTO	C28-N20-S18-C17

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Mol	Chain	Res	Type	Atoms
4	A	205	WTO	C16-C17-S18-O19
4	A	205	WTO	C14-C17-S18-O19
4	A	205	WTO	C13-C12-N11-C10
4	B	203	WTO	C13-C12-N11-C10
4	A	205	WTO	C16-C17-S18-N20
4	A	205	WTO	C28-N20-S18-O19
4	A	205	WTO	C15-C12-N11-C10
4	B	203	WTO	C21-N20-S18-O29
4	B	203	WTO	C14-C17-S18-O29
4	B	203	WTO	C16-C17-S18-O29
4	B	203	WTO	C21-N20-S18-C17
3	A	204	GOL	O2-C2-C3-O3
4	B	203	WTO	C15-C12-N11-C10
2	A	201	GNP	C5'-O5'-PA-O1A
4	A	205	WTO	C21-N20-S18-O29
4	B	203	WTO	C26-C21-C22-O23
4	B	203	WTO	C26-C21-C22-O25
3	B	202	GOL	O2-C2-C3-O3

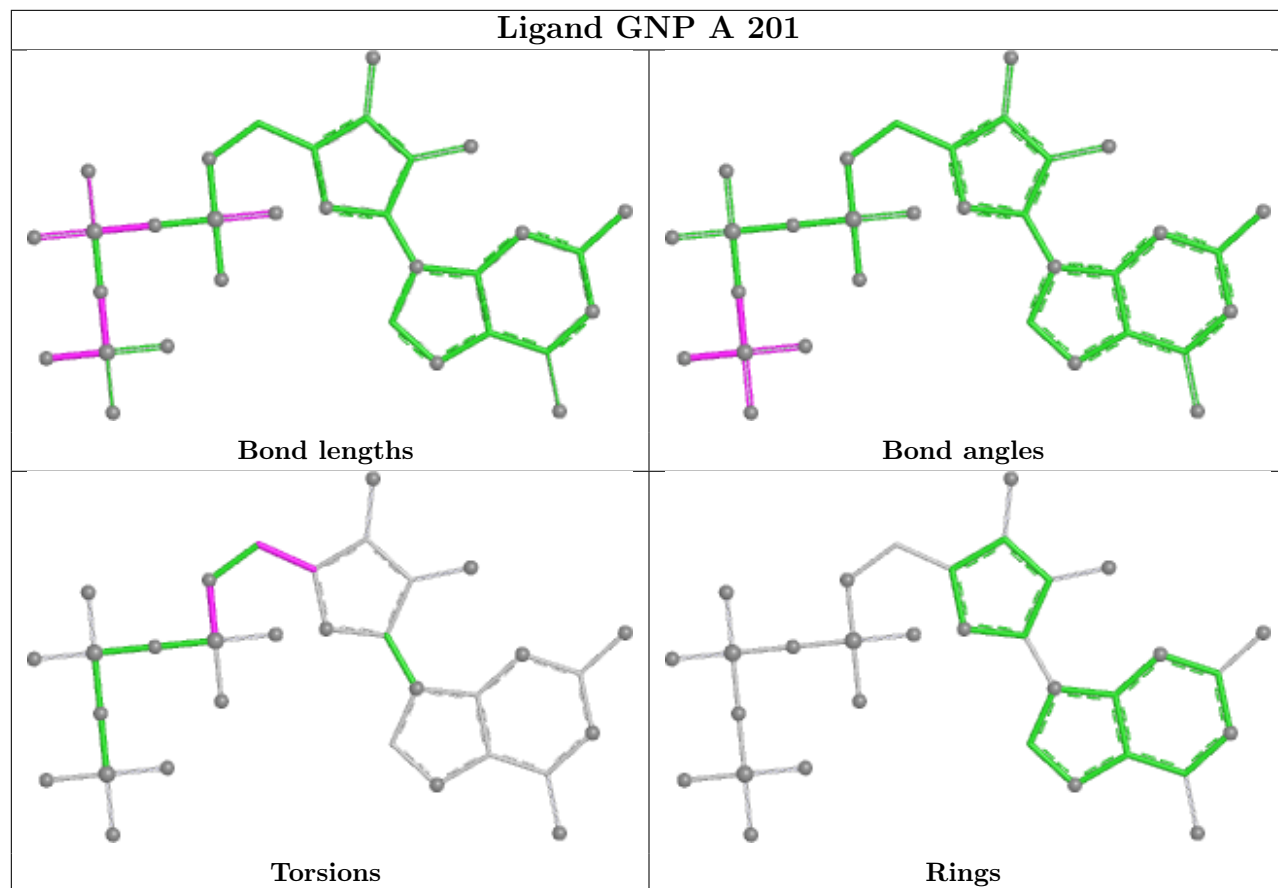
There are no ring outliers.

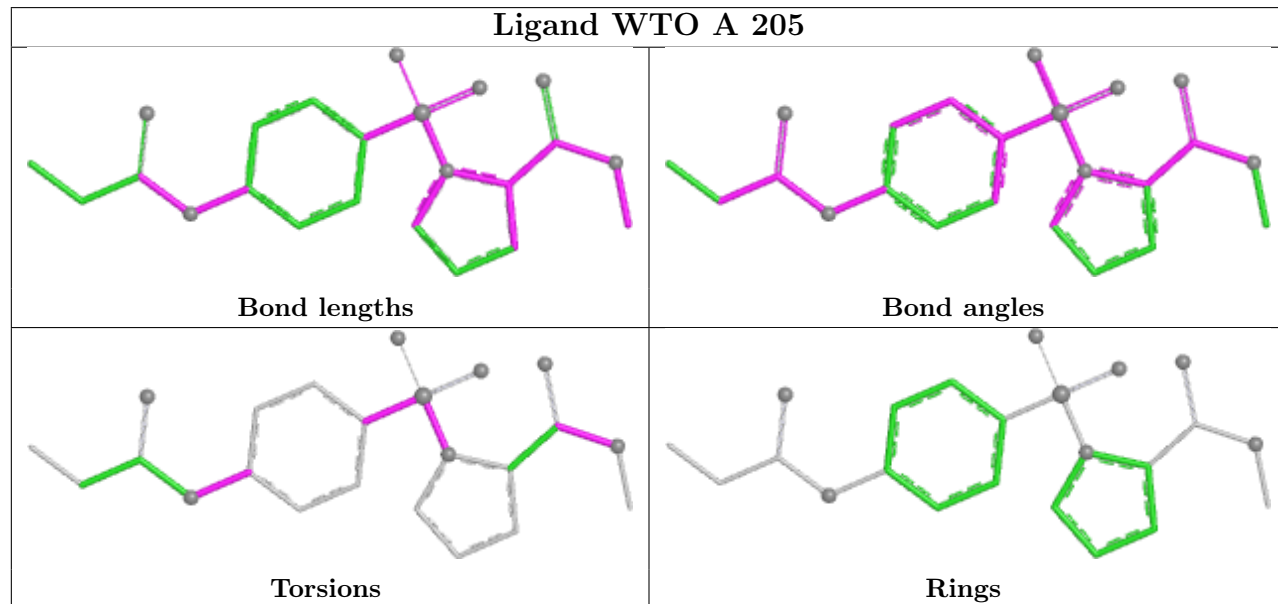
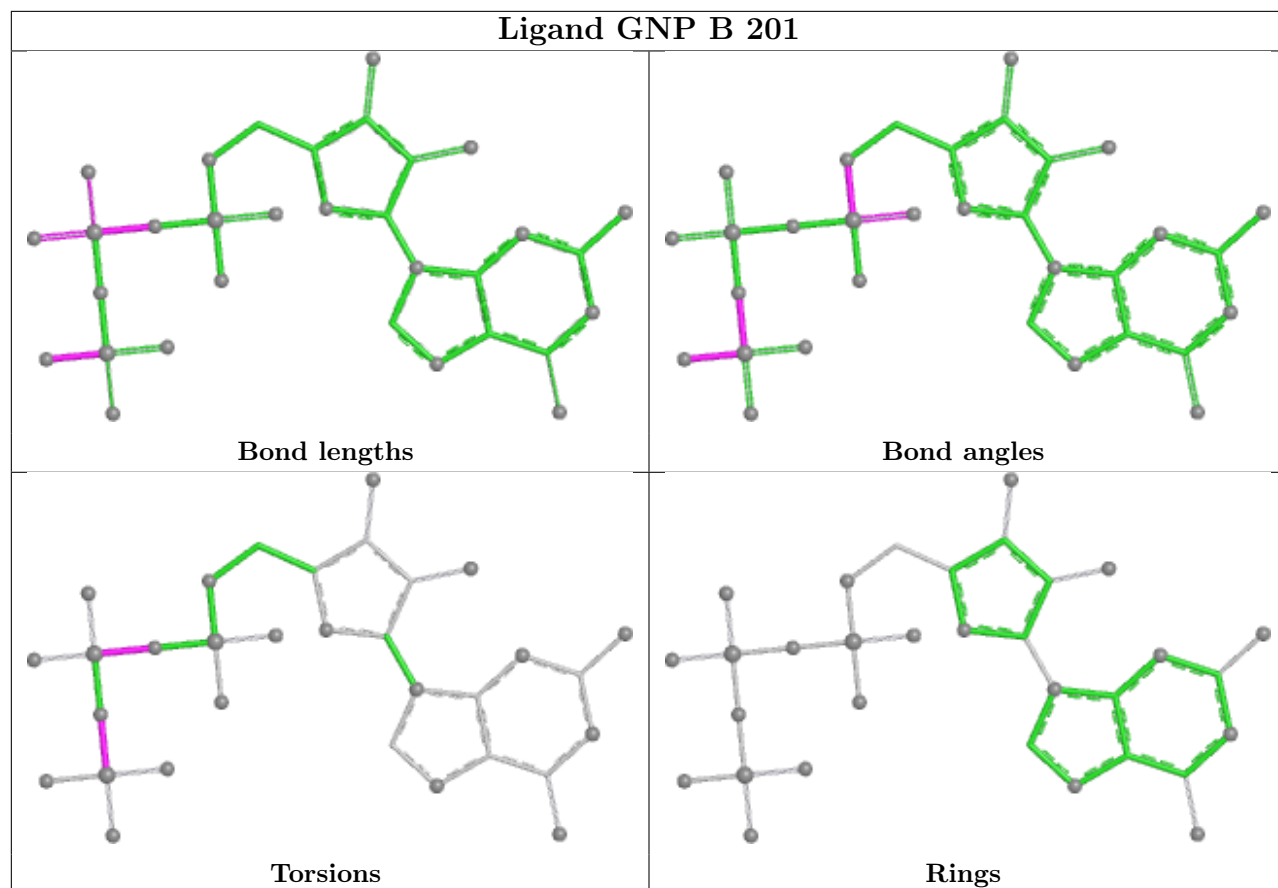
7 monomers are involved in 11 short contacts:

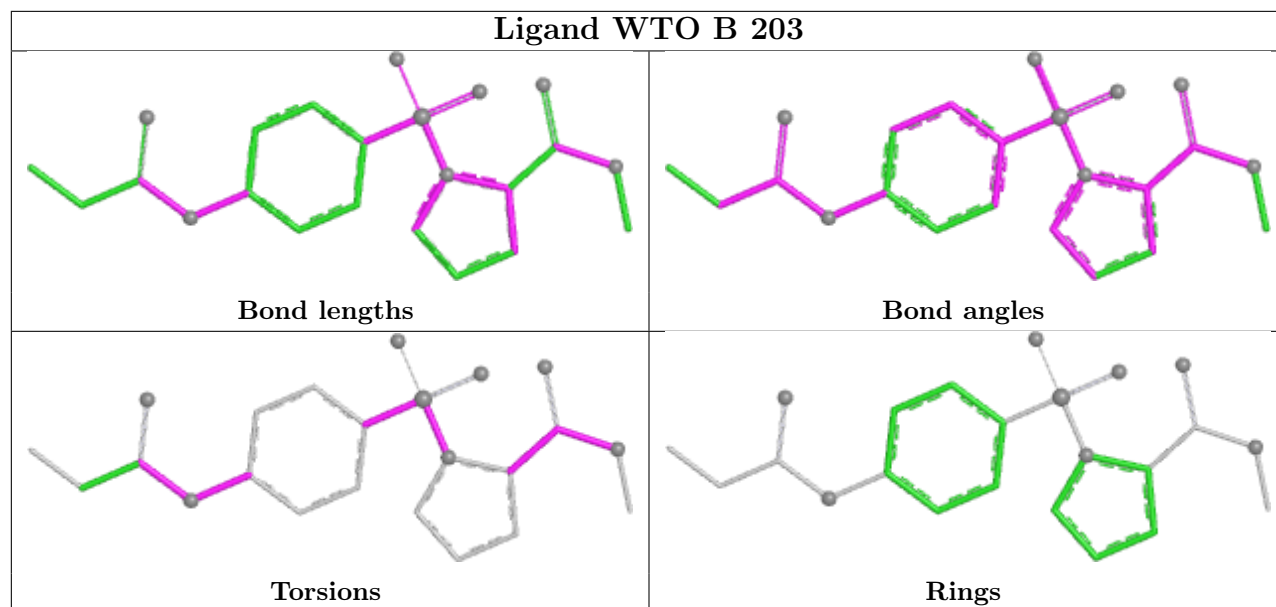
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	GNP	4	0
3	A	204	GOL	1	0
2	B	201	GNP	1	0
4	A	205	WTO	1	0
3	A	202	GOL	2	0
3	B	202	GOL	1	0
4	B	203	WTO	2	0

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.







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	206/230 (89%)	0.51	10 (4%) 35 34	25, 60, 91, 110	1 (0%)
1	B	203/230 (88%)	0.68	18 (8%) 15 15	42, 62, 96, 107	0
All	All	409/460 (88%)	0.59	28 (6%) 23 23	25, 60, 94, 110	1 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-8	TYR	3.8
1	A	-2	PHE	3.5
1	A	43	ALA	3.4
1	A	30	ILE	3.3
1	B	74	PHE	3.2
1	B	63	LEU	3.1
1	A	-8	TYR	3.0
1	B	96	LEU	2.9
1	A	42	SER	2.9
1	A	164	MET	2.9
1	B	-34	PHE	2.9
1	B	42	GLY	2.8
1	B	75	LEU	2.8
1	A	-35	SER	2.5
1	B	125	GLU	2.4
1	B	-33	LEU	2.3
1	B	-27	GLU	2.2
1	B	44	GLY	2.2
1	B	-32	THR	2.1
1	B	102	CYS	2.1
1	A	155	ALA	2.1
1	A	124	VAL	2.1
1	B	38	VAL	2.1
1	B	41	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	167	MET	2.0
1	B	121	VAL	2.0
1	B	-6	TYR	2.0
1	B	134	TYR	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](#)

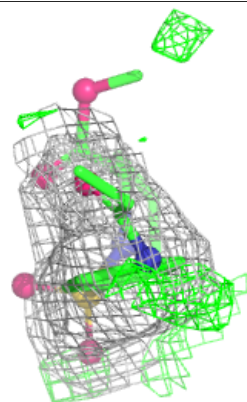
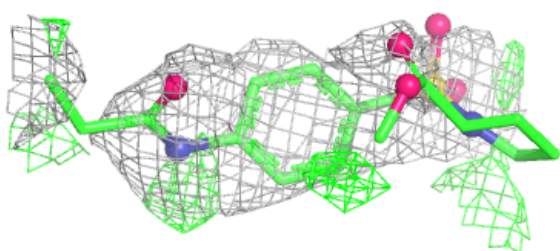
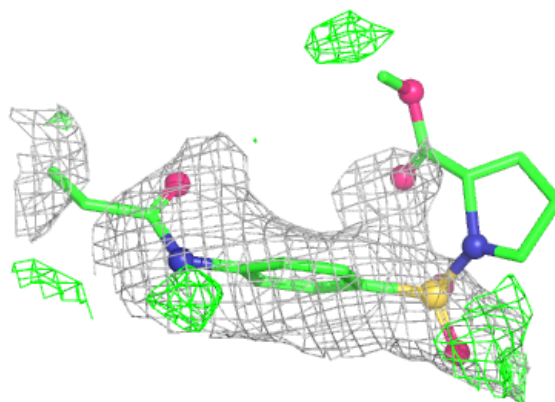
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	WTO	A	205	23/23	0.66	0.21	70,84,97,100	5
4	WTO	B	203	23/23	0.76	0.19	62,73,81,81	13
3	GOL	A	203	6/6	0.83	0.13	60,62,65,76	0
3	GOL	B	202	6/6	0.86	0.11	48,53,58,61	0
3	GOL	A	204	6/6	0.89	0.12	50,51,54,61	0
3	GOL	A	202	6/6	0.94	0.09	49,58,60,63	0
2	GNP	A	201	32/32	0.97	0.07	39,49,54,57	0
2	GNP	B	201	32/32	0.97	0.06	43,49,55,59	0
5	MG	A	206	1/1	0.99	0.07	47,47,47,47	0
5	MG	B	204	1/1	1.00	0.07	43,43,43,43	0

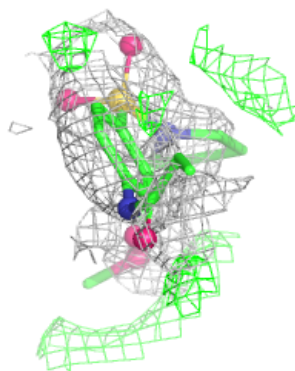
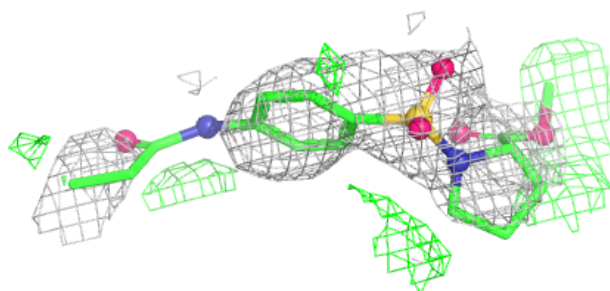
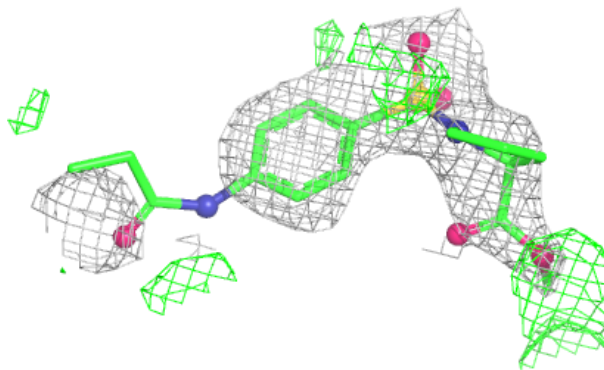
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around WTO A 205:

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

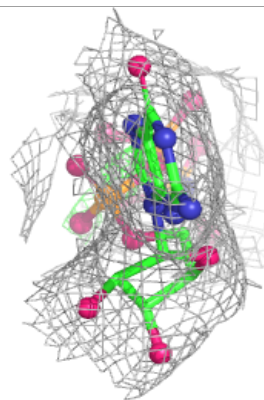
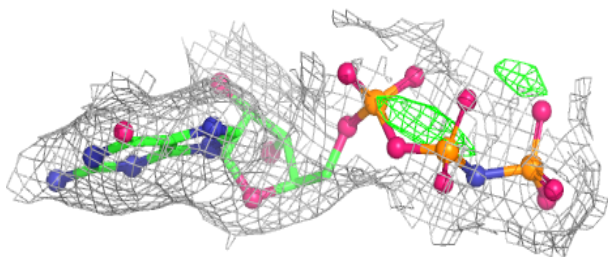
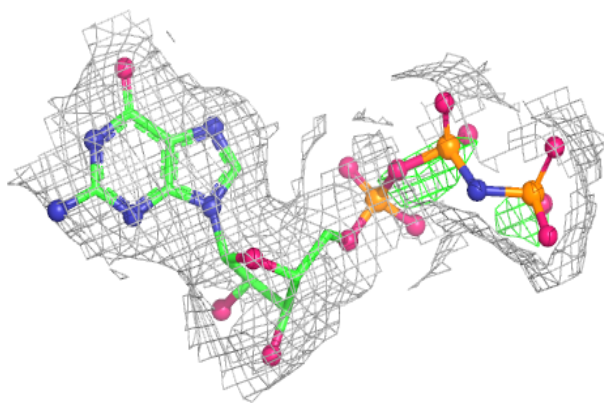
**Electron density around WTO B 203:**

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

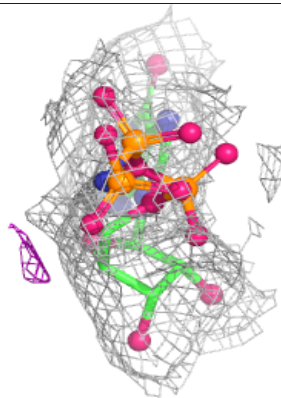
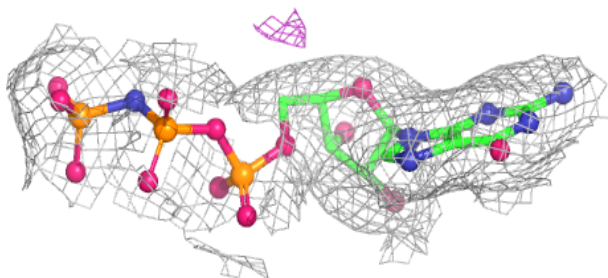
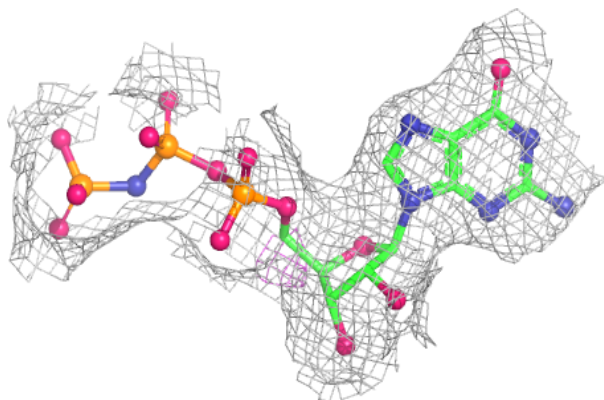


Electron density around GNP A 201:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.