Full wwPDB X-ray Structure Validation Report ⓘ

Nov 9, 2024 – 12:57 pm GMT

PDB ID	:	8P3K
Title	:	Fusion hSlp2-a_Rab27A non-covalent complex with compound IMP-2505
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	:	2.58 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:

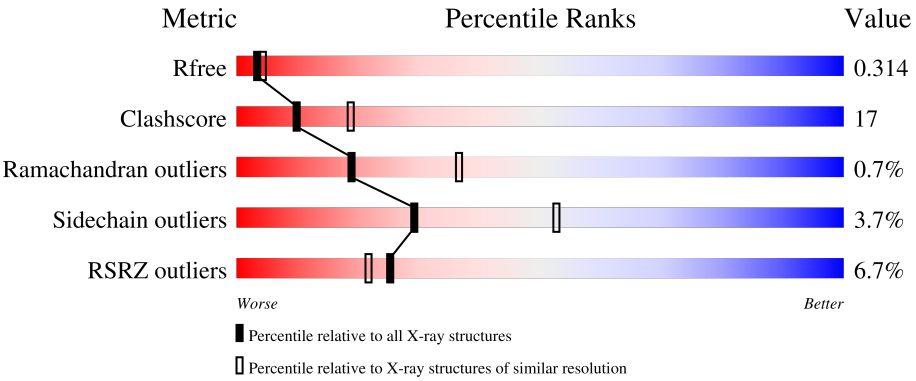
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.58 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}	164625	4456 (2.60-2.56)
Clashscore	180529	4905 (2.60-2.56)
Ramachandran outliers	177936	4847 (2.60-2.56)
Sidechain outliers	177891	4847 (2.60-2.56)
RSRZ outliers	164620	4456 (2.60-2.56)

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 <=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	3% 63% 27% · 8%
1	B	230	9% 55% 34% · 9%

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	WTB	A	302	-	X	-	-
3	WTB	B	201	-	X	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3565 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	0	0
			1683	1064	290	321	8			
1	B	209	Total	C	N	O	S	0	0	0
			1657	1048	284	318	7			

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

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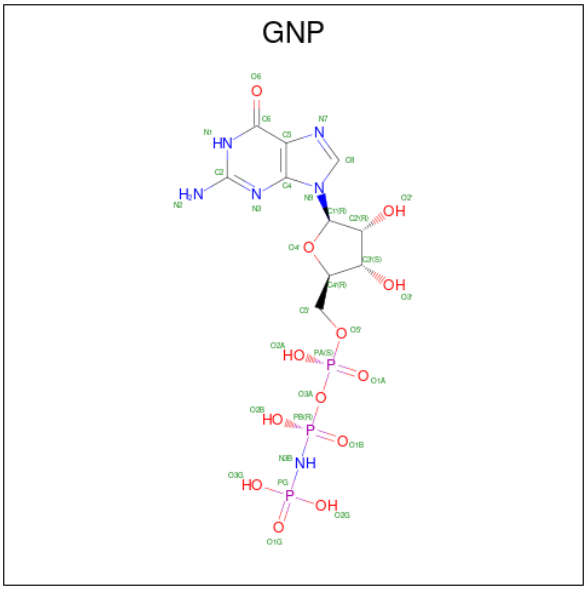
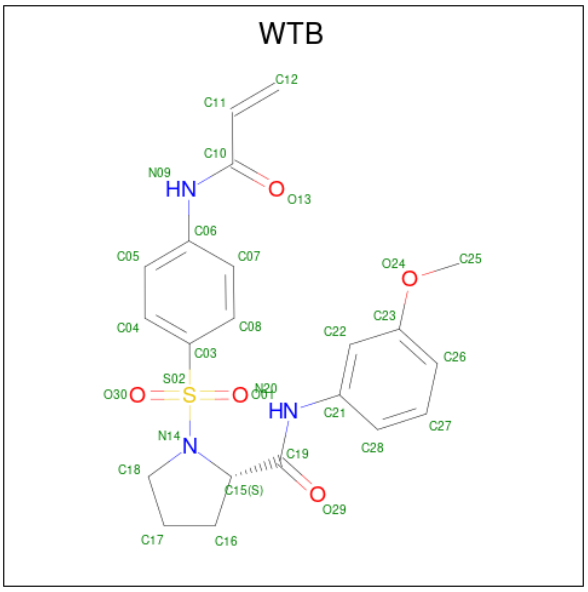
Chain	Residue	Modelled	Actual	Comment	Reference
B	188	SER	CYS	engineered mutation	UNP P51159

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



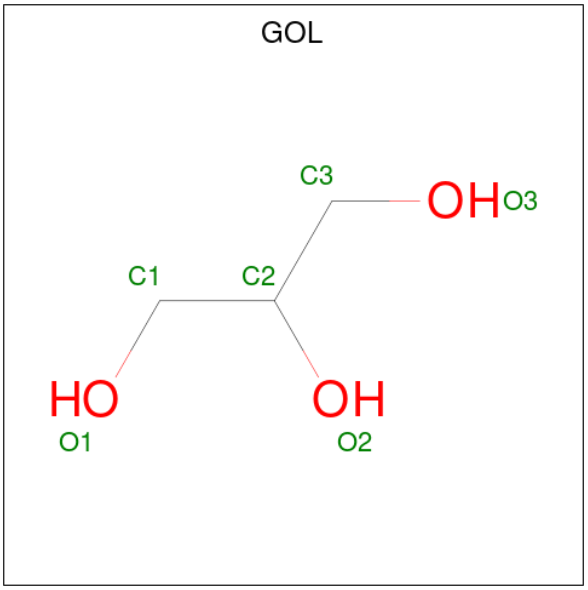
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
2	B	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 3 is (2 {S})- {N}-(3-methoxyphenyl)-1-[4-(prop-2-enoylamino)phenyl]sulfonyl-pyrrolidine-2-carboxamide (three-letter code: WTB) (formula: $C_{21}H_{23}N_3O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			30	21	3	5	1		
3	B	1	Total	C	N	O	S	0	0
			30	21	3	5	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 5 is MAGNESIUM ION (three-letter code: 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.

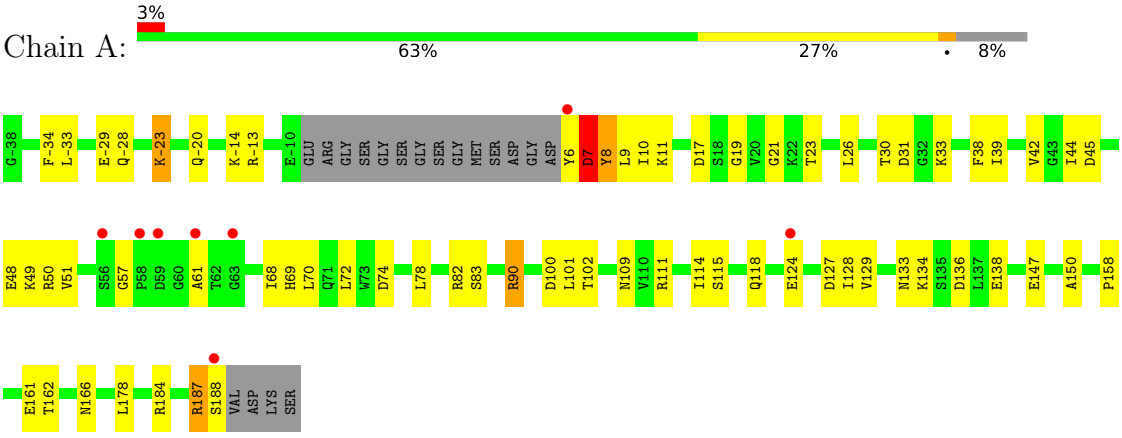
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	25	Total O 25 25	0	0
6	B	14	Total O 14 14	0	0

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.

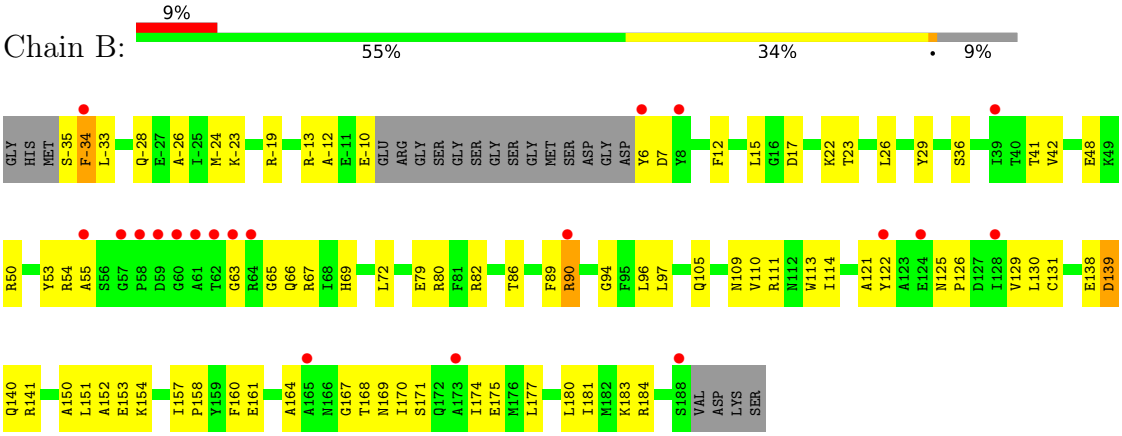
• Molecule 1: Synaptotagmin-like protein 2,Ras-related protein Rab-27A

Chain A:



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

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	60.90Å 76.54Å 117.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.09 – 2.58 54.09 – 2.58	Depositor EDS
% Data completeness (in resolution range)	98.8 (54.09-2.58) 98.9 (54.09-2.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.20 (at 2.58Å)	Xtriage
Refinement program	PHENIX (1.17_3644: ???)	Depositor
R, R_{free}	0.238 , 0.315 0.241 , 0.314	Depositor DCC
R_{free} test set	870 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	41.9	Xtriage
Anisotropy	0.712	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 44.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	3565	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.00% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, WTB, 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	0/1710	0.61	0/2301
1	B	0.48	0/1683	0.61	0/2267
All	All	0.47	0/3393	0.61	0/4568

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1683	0	1655	52	0
1	B	1657	0	1624	80	0
2	A	32	0	13	3	0
2	B	32	0	13	3	0
3	A	30	0	0	1	0
3	B	30	0	0	2	0
4	A	24	0	31	3	0
4	B	36	0	47	5	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	25	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	14	0	0	2	0
All	All	3565	0	3383	119	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 17.

All (119) 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:124:GLU:HG3	1:B:-13:ARG:CD	1.32	1.56
1:A:124:GLU:OE2	1:B:-13:ARG:NH1	1.71	1.21
1:A:124:GLU:CG	1:B:-13:ARG:HD3	1.71	1.20
1:A:124:GLU:CG	1:B:-13:ARG:CD	2.20	1.18
1:A:124:GLU:HG3	1:B:-13:ARG:HD2	1.36	1.05
2:A:301:GNP:HN22	4:A:306:GOL:H11	1.35	0.92
1:B:-23:LYS:NZ	1:B:-19:ARG:HH11	1.70	0.89
1:B:-23:LYS:HZ2	1:B:-19:ARG:HH11	1.18	0.85
1:B:82:ARG:NH2	6:B:301:HOH:O	2.09	0.85
1:A:19:GLY:H	2:A:301:GNP:HNB3	1.24	0.84
1:A:124:GLU:CG	1:B:-13:ARG:HD2	1.97	0.80
1:A:124:GLU:HG3	1:B:-13:ARG:HD3	0.80	0.79
1:B:-23:LYS:NZ	1:B:-19:ARG:NH1	2.33	0.77
1:A:124:GLU:CD	1:B:-13:ARG:HD2	2.11	0.71
1:A:101:LEU:HD11	1:A:161:GLU:HG2	1.74	0.70
1:B:129:VAL:HG23	1:B:177:LEU:HD13	1.74	0.69
1:B:167:GLY:HA2	1:B:170:ILE:HG13	1.74	0.69
1:A:124:GLU:CD	1:B:-13:ARG:HH11	1.92	0.69
1:A:26:LEU:HD22	1:A:72:LEU:HD23	1.76	0.68
1:B:94:GLY:HA3	1:B:181:ILE:HD11	1.78	0.66
1:A:57:GLY:HA3	1:A:61:ALA:HB3	1.77	0.66
1:B:-23:LYS:HZ2	1:B:-19:ARG:NH1	1.91	0.64
1:A:23:THR:OG1	1:A:74:ASP:OD2	2.16	0.64
1:B:111:ARG:NH1	4:B:207:GOL:O1	2.31	0.63
1:B:125:ASN:O	1:B:184:ARG:NH2	2.29	0.63
1:A:129:VAL:HG22	1:A:158:PRO:HB2	1.81	0.62
1:A:30:THR:HA	1:A:49:LYS:HD2	1.83	0.61
1:A:90:ARG:HE	1:B:90:ARG:HD2	1.66	0.61
1:B:125:ASN:OD1	4:B:208:GOL:H2	2.01	0.60
1:B:111:ARG:HA	1:B:114:ILE:HD12	1.84	0.59
1:B:96:LEU:HD11	1:B:174:ILE:HG22	1.83	0.59
1:A:-14:LYS:HE3	1:A:11:LYS:HD3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ASP:OD2	1:A:109:ASN:ND2	2.32	0.57
1:B:171:SER:O	1:B:175:GLU:HG3	2.04	0.57
1:B:-23:LYS:HZ1	1:B:-19:ARG:NH1	2.01	0.57
1:B:17:ASP:O	1:B:22:LYS:NZ	2.36	0.57
1:A:38:PHE:HB2	4:A:304:GOL:H11	1.86	0.57
1:A:187:ARG:HD3	1:A:188:SER:H	1.69	0.57
1:B:141:ARG:NH2	1:B:161:GLU:OE2	2.30	0.57
1:B:164:ALA:HB3	2:B:202:GNP:N7	2.20	0.57
1:A:7:ASP:OD1	1:A:50:ARG:NH2	2.38	0.57
1:A:31:ASP:O	1:A:33:LYS:HG3	2.04	0.57
1:B:158:PRO:HA	4:B:203:GOL:H32	1.87	0.56
1:B:105:GLN:NE2	1:B:109:ASN:OD1	2.34	0.55
1:A:39:ILE:HB	4:A:305:GOL:H11	1.89	0.54
1:A:-13:ARG:NH1	1:B:121:ALA:O	2.41	0.54
1:B:150:ALA:O	1:B:153:GLU:HG2	2.08	0.54
1:B:6:TYR:N	1:B:50:ARG:HH22	2.07	0.53
1:B:126:PRO:HB3	3:B:201:WTB:C12	2.39	0.53
1:B:90:ARG:HB2	1:B:122:TYR:CZ	2.44	0.53
1:B:42:VAL:HG13	1:B:42:VAL:O	2.09	0.52
1:A:100:ASP:OD1	1:A:102:THR:N	2.36	0.52
1:B:130:LEU:HB2	1:B:157:ILE:HD12	1.92	0.52
1:B:54:ARG:HA	1:B:65:GLY:HA3	1.91	0.52
1:B:82:ARG:O	1:B:86:THR:OG1	2.21	0.51
1:A:21:GLY:HA2	2:A:301:GNP:O1A	2.11	0.51
1:B:41:THR:N	6:B:302:HOH:O	2.43	0.51
1:B:-35:SER:OG	1:B:-34:PHE:N	2.43	0.51
1:B:129:VAL:HG13	1:B:158:PRO:HB2	1.93	0.51
1:A:10:ILE:HG21	1:A:178:LEU:HD12	1.93	0.51
1:B:7:ASP:HB3	1:B:67:ARG:O	2.11	0.50
1:A:138:GLU:N	1:A:138:GLU:OE2	2.45	0.49
1:B:17:ASP:OD1	1:B:113:TRP:NE1	2.36	0.49
1:A:128:ILE:N	3:A:302:WTB:O13	2.36	0.49
1:B:164:ALA:HB3	2:B:202:GNP:C5	2.43	0.49
1:A:9:LEU:HD12	1:A:10:ILE:N	2.28	0.49
1:A:187:ARG:HD3	1:A:188:SER:N	2.27	0.49
1:B:6:TYR:O	1:B:67:ARG:NH1	2.46	0.49
1:B:154:LYS:NZ	4:B:207:GOL:H32	2.28	0.49
1:A:114:ILE:O	1:A:118:GLN:HG2	2.13	0.49
1:B:90:ARG:NH1	1:B:122:TYR:OH	2.45	0.48
1:B:-28:GLN:O	1:B:-24:MET:HG2	2.13	0.48
1:B:138:GLU:OE2	1:B:138:GLU:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:VAL:HG12	1:B:114:ILE:HD11	1.96	0.47
1:A:118:GLN:OE1	6:A:401:HOH:O	2.20	0.47
1:B:22:LYS:O	1:B:26:LEU:HG	2.14	0.47
1:A:184:ARG:NH1	1:A:184:ARG:HG3	2.31	0.45
1:B:79:GLU:CD	1:B:80:ARG:HG3	2.36	0.45
1:A:44:ILE:HG13	1:A:45:ASP:N	2.30	0.45
1:A:70:LEU:HD11	1:A:178:LEU:HD13	1.98	0.45
1:B:150:ALA:O	1:B:154:LYS:HG3	2.16	0.45
1:A:51:VAL:CG1	1:A:68:ILE:HB	2.46	0.45
1:B:7:ASP:OD1	1:B:66:GLN:NE2	2.50	0.45
1:B:53:TYR:O	1:B:66:GLN:N	2.49	0.45
1:A:78:LEU:HD23	1:A:78:LEU:HA	1.77	0.44
1:B:-12:ALA:O	1:B:-10:GLU:N	2.48	0.44
1:A:-29:GLU:HG2	1:A:42:VAL:HG13	1.98	0.44
1:B:36:SER:HA	2:B:202:GNP:O2'	2.16	0.44
1:A:133:ASN:HA	1:A:162:THR:OG1	2.17	0.44
1:A:124:GLU:OE2	1:B:-13:ARG:HD2	2.17	0.44
1:B:86:THR:HA	1:B:89:PHE:CE1	2.53	0.44
1:A:147:GLU:O	1:A:150:ALA:HB3	2.18	0.44
1:A:-33:LEU:CB	1:A:-28:GLN:HG3	2.48	0.44
1:A:9:LEU:O	1:A:10:ILE:HD13	2.18	0.43
1:A:127:ASP:OD2	1:A:184:ARG:NE	2.50	0.43
1:A:83:SER:HB3	1:B:-28:GLN:HG3	2.00	0.43
1:B:12:PHE:CE2	1:B:72:LEU:HD23	2.53	0.43
1:B:-26:ALA:O	1:B:-23:LYS:HB3	2.18	0.43
1:B:15:LEU:HA	1:B:22:LYS:HD3	2.01	0.42
1:A:136:ASP:HB3	1:A:166:ASN:ND2	2.34	0.42
1:B:151:LEU:HA	1:B:154:LYS:HE2	2.02	0.42
1:B:79:GLU:HG2	1:B:80:ARG:N	2.34	0.42
1:A:-34:PHE:CE2	1:B:-33:LEU:HB2	2.55	0.42
1:A:48:GLU:HA	1:A:70:LEU:O	2.19	0.41
1:B:23:THR:HG22	4:B:205:GOL:H31	2.02	0.41
1:B:55:ALA:CB	1:B:63:GLY:H	2.33	0.41
1:B:126:PRO:HA	3:B:201:WTB:O13	2.20	0.41
1:B:168:THR:HG22	1:B:169:ASN:OD1	2.20	0.41
1:B:48:GLU:OE2	1:B:69:HIS:NE2	2.54	0.41
1:B:89:PHE:N	1:B:89:PHE:CD1	2.87	0.41
1:A:6:TYR:O	1:A:7:ASP:HB2	2.21	0.41
1:B:29:TYR:OH	1:B:174:ILE:HD11	2.20	0.41
1:B:131:CYS:HA	1:B:160:PHE:O	2.20	0.41
1:B:97:LEU:HD12	1:B:97:LEU:HA	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:ALA:HB1	1:B:157:ILE:O	2.21	0.41
1:B:180:LEU:HD23	1:B:180:LEU:HA	1.85	0.40
1:B:139:ASP:O	1:B:140:GLN:HG3	2.21	0.40
1:A:-23:LYS:HE2	1:A:-20:GLN:CD	2.42	0.40
1:B:80:ARG:HG3	1:B:80:ARG:H	1.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	208/230 (90%)	187 (90%)	19 (9%)	2 (1%)	13	27
1	B	205/230 (89%)	189 (92%)	15 (7%)	1 (0%)	25	45
All	All	413/460 (90%)	376 (91%)	34 (8%)	3 (1%)	19	36

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	TYR
1	B	-34	PHE
1	A	7	ASP

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	176/192 (92%)	166 (94%)	10 (6%)	17 35
1	B	173/192 (90%)	170 (98%)	3 (2%)	56 76
All	All	349/384 (91%)	336 (96%)	13 (4%)	29 53

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-23	LYS
1	A	7	ASP
1	A	8	TYR
1	A	69	HIS
1	A	82	ARG
1	A	90	ARG
1	A	111	ARG
1	A	115	SER
1	A	134	LYS
1	A	187	ARG
1	B	90	ARG
1	B	139	ASP
1	B	183	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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	203	-	5,5,5	1.25	1 (20%)	5,5,5	0.68	0
4	GOL	B	207	-	5,5,5	1.04	0	5,5,5	1.11	0
2	GNP	B	202	5	29,34,34	1.78	7 (24%)	33,54,54	2.31	6 (18%)
4	GOL	B	205	-	5,5,5	0.74	0	5,5,5	0.98	0
4	GOL	A	304	-	5,5,5	1.20	0	5,5,5	0.80	0
3	WTB	B	201	-	32,32,32	4.49	13 (40%)	44,45,45	3.48	17 (38%)
3	WTB	A	302	-	32,32,32	4.58	13 (40%)	44,45,45	3.46	14 (31%)
4	GOL	B	208	-	5,5,5	1.37	1 (20%)	5,5,5	1.12	0
4	GOL	B	206	-	5,5,5	1.05	0	5,5,5	0.88	0
4	GOL	B	204	-	5,5,5	1.11	0	5,5,5	0.94	0
4	GOL	A	303	-	5,5,5	1.27	0	5,5,5	0.67	0
4	GOL	A	305	-	5,5,5	0.73	0	5,5,5	1.18	1 (20%)
4	GOL	A	306	-	5,5,5	1.43	1 (20%)	5,5,5	1.16	0
2	GNP	A	301	5	29,34,34	1.70	7 (24%)	33,54,54	2.39	8 (24%)

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	203	-	-	4/4/4/4	-
4	GOL	B	207	-	-	0/4/4/4	-
2	GNP	B	202	5	-	7/14/38/38	0/3/3/3
4	GOL	B	205	-	-	1/4/4/4	-
4	GOL	A	304	-	-	4/4/4/4	-
3	WTB	B	201	-	-	20/28/38/38	0/3/3/3
3	WTB	A	302	-	-	22/28/38/38	0/3/3/3
4	GOL	B	208	-	-	3/4/4/4	-
4	GOL	B	206	-	-	4/4/4/4	-
4	GOL	B	204	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	303	-	-	0/4/4/4	-
4	GOL	A	305	-	-	0/4/4/4	-
4	GOL	A	306	-	-	4/4/4/4	-
2	GNP	A	301	5	-	4/14/38/38	0/3/3/3

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	WTB	C18-N14	-11.67	1.31	1.48
3	B	201	WTB	C18-N14	-11.33	1.31	1.48
3	A	302	WTB	C15-N14	11.32	1.65	1.48
3	B	201	WTB	C15-N14	11.29	1.65	1.48
3	B	201	WTB	C16-C15	-9.46	1.31	1.53
3	A	302	WTB	C16-C15	-9.33	1.31	1.53
3	A	302	WTB	C10-N09	8.55	1.50	1.35
3	B	201	WTB	S02-N14	8.42	1.76	1.63
3	A	302	WTB	S02-N14	8.40	1.76	1.63
3	B	201	WTB	C03-S02	7.57	1.87	1.76
3	B	201	WTB	C10-N09	7.36	1.48	1.35
3	A	302	WTB	C19-N20	6.87	1.51	1.35
3	A	302	WTB	C03-S02	6.75	1.85	1.76
3	B	201	WTB	C19-N20	6.46	1.50	1.35
2	A	301	GNP	PB-O3A	5.56	1.66	1.59
2	B	202	GNP	PB-O3A	4.90	1.65	1.59
3	A	302	WTB	O24-C23	4.40	1.46	1.37
3	B	201	WTB	O24-C23	4.20	1.46	1.37
3	A	302	WTB	C04-C03	3.80	1.44	1.38
2	B	202	GNP	O6-C6	3.61	1.33	1.24
2	B	202	GNP	C6-N1	3.45	1.39	1.33
3	B	201	WTB	C11-C10	3.42	1.53	1.48
3	B	201	WTB	C04-C03	3.31	1.44	1.38
3	A	302	WTB	C11-C10	3.24	1.53	1.48
2	A	301	GNP	PB-O1B	3.10	1.51	1.46
2	B	202	GNP	PB-O1B	2.94	1.50	1.46
4	A	306	GOL	O2-C2	-2.93	1.34	1.43
2	A	301	GNP	C6-N1	2.88	1.38	1.33
2	B	202	GNP	PG-N3B	2.84	1.70	1.63
4	B	208	GOL	O2-C2	-2.79	1.35	1.43
2	A	301	GNP	PG-O1G	2.78	1.50	1.46
2	B	202	GNP	PG-O1G	2.77	1.50	1.46
2	A	301	GNP	PG-N3B	2.73	1.70	1.63
3	B	201	WTB	C08-C07	2.60	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	202	GNP	C5-C6	2.45	1.45	1.41
3	A	302	WTB	C08-C03	-2.45	1.35	1.38
2	A	301	GNP	C5-C6	2.43	1.45	1.41
3	B	201	WTB	C21-N20	2.42	1.46	1.41
3	A	302	WTB	C21-N20	2.35	1.46	1.41
4	B	203	GOL	C3-C2	2.06	1.60	1.51
3	B	201	WTB	C15-C19	2.03	1.57	1.52
2	A	301	GNP	PB-O2B	-2.01	1.51	1.56
3	A	302	WTB	C15-C19	2.00	1.57	1.52

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	302	WTB	C11-C10-N09	15.27	123.90	113.84
3	B	201	WTB	O30-S02-O01	-12.53	99.22	119.52
3	A	302	WTB	O30-S02-O01	-10.53	102.46	119.52
3	B	201	WTB	C11-C10-N09	10.16	120.53	113.84
2	B	202	GNP	C5-C6-N1	-9.43	110.54	123.43
2	A	301	GNP	C5-C6-N1	-8.35	112.00	123.43
3	B	201	WTB	C06-N09-C10	-6.86	117.91	128.26
3	B	201	WTB	C15-C19-N20	6.61	130.51	114.12
2	B	202	GNP	C2-N1-C6	6.37	126.05	115.93
2	A	301	GNP	C2-N1-C6	5.76	125.09	115.93
3	B	201	WTB	O29-C19-N20	-5.76	111.54	123.93
2	A	301	GNP	O1G-PG-N3B	-5.43	103.78	111.77
3	B	201	WTB	C21-N20-C19	5.18	139.81	127.40
3	A	302	WTB	C15-C19-N20	4.65	125.65	114.12
3	A	302	WTB	C06-N09-C10	-4.52	121.43	128.26
3	A	302	WTB	C15-N14-S02	4.36	128.98	119.60
3	A	302	WTB	C18-N14-C15	-4.09	105.63	111.25
3	B	201	WTB	C18-N14-C15	-3.99	105.77	111.25
3	B	201	WTB	C15-N14-S02	3.93	128.05	119.60
3	A	302	WTB	O13-C10-C11	-3.81	116.62	122.72
3	A	302	WTB	C04-C03-S02	3.36	123.30	119.76
3	A	302	WTB	O01-S02-N14	3.32	113.02	106.97
3	B	201	WTB	O13-C10-N09	-3.31	119.26	123.05
3	A	302	WTB	C08-C03-S02	-3.29	116.29	119.76
3	B	201	WTB	O01-S02-N14	3.14	112.70	106.97
3	A	302	WTB	O29-C19-N20	-3.13	117.20	123.93
3	A	302	WTB	O13-C10-N09	-3.12	119.47	123.05
2	A	301	GNP	O2B-PB-O3A	3.02	114.72	104.64
3	B	201	WTB	C18-N14-S02	2.87	126.03	119.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	GNP	N3-C2-N1	-2.82	123.45	127.22
3	B	201	WTB	O30-S02-C03	2.66	111.41	108.05
2	A	301	GNP	C4-C5-C6	-2.61	118.31	120.80
2	B	202	GNP	N3-C2-N1	-2.53	123.85	127.22
2	B	202	GNP	C2-N3-C4	-2.53	112.47	115.36
3	A	302	WTB	C18-N14-S02	2.52	125.19	119.16
3	A	302	WTB	O01-S02-C03	2.51	111.22	108.05
2	B	202	GNP	O1G-PG-N3B	-2.40	108.24	111.77
2	B	202	GNP	O1B-PB-N3B	-2.37	108.28	111.77
3	B	201	WTB	C28-C21-N20	-2.35	112.51	120.40
3	B	201	WTB	C03-S02-N14	2.34	111.52	107.36
3	B	201	WTB	C22-C21-N20	2.30	127.68	120.18
2	A	301	GNP	O1B-PB-N3B	2.22	115.04	111.77
3	B	201	WTB	O01-S02-C03	2.18	110.80	108.05
4	A	305	GOL	C3-C2-C1	-2.09	103.59	111.70
2	A	301	GNP	O3G-PG-O1G	-2.09	108.21	113.45
3	B	201	WTB	O30-S02-N14	2.00	110.62	106.97

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	GNP	PB-N3B-PG-O1G
2	B	202	GNP	PB-N3B-PG-O1G
2	B	202	GNP	PG-N3B-PB-O1B
2	B	202	GNP	C5'-O5'-PA-O3A
2	B	202	GNP	C5'-O5'-PA-O1A
3	A	302	WTB	N09-C10-C11-C12
3	A	302	WTB	O13-C10-C11-C12
3	A	302	WTB	C11-C10-N09-C06
3	A	302	WTB	O13-C10-N09-C06
3	A	302	WTB	C16-C15-C19-N20
3	A	302	WTB	C16-C15-C19-O29
3	A	302	WTB	C15-C19-N20-C21
3	B	201	WTB	N09-C10-C11-C12
3	B	201	WTB	O13-C10-C11-C12
3	B	201	WTB	C11-C10-N09-C06
3	B	201	WTB	O13-C10-N09-C06
3	B	201	WTB	C15-C19-N20-C21
3	B	201	WTB	C18-N14-S02-C03
4	A	304	GOL	O1-C1-C2-C3
4	B	206	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	A	302	WTB	O29-C19-N20-C21
3	B	201	WTB	O29-C19-N20-C21
3	A	302	WTB	C26-C23-O24-C25
3	A	302	WTB	C22-C23-O24-C25
3	A	302	WTB	C08-C03-S02-N14
3	A	302	WTB	C04-C03-S02-N14
3	B	201	WTB	C18-N14-S02-O01
2	A	301	GNP	O4'-C4'-C5'-O5'
3	A	302	WTB	C22-C21-N20-C19
3	A	302	WTB	C28-C21-N20-C19
3	B	201	WTB	C04-C03-S02-N14
4	A	304	GOL	O2-C2-C3-O3
3	A	302	WTB	C18-N14-S02-O30
3	B	201	WTB	C05-C06-N09-C10
3	B	201	WTB	C08-C03-S02-N14
3	B	201	WTB	C07-C06-N09-C10
3	B	201	WTB	C15-N14-S02-O01
4	A	304	GOL	C1-C2-C3-O3
4	A	306	GOL	O1-C1-C2-C3
4	A	306	GOL	C1-C2-C3-O3
4	B	203	GOL	C1-C2-C3-O3
4	B	204	GOL	O1-C1-C2-C3
4	B	206	GOL	C1-C2-C3-O3
4	B	208	GOL	O1-C1-C2-C3
4	B	208	GOL	C1-C2-C3-O3
4	A	306	GOL	O1-C1-C2-O2
4	B	206	GOL	O1-C1-C2-O2
4	B	208	GOL	O2-C2-C3-O3
3	B	201	WTB	C16-C15-C19-O29
3	B	201	WTB	C08-C03-S02-O30
3	B	201	WTB	C04-C03-S02-O30
3	B	201	WTB	C15-N14-S02-C03
3	A	302	WTB	C15-N14-S02-O30
3	A	302	WTB	C08-C03-S02-O30
3	A	302	WTB	C04-C03-S02-O30
4	B	203	GOL	O2-C2-C3-O3
3	A	302	WTB	C18-N14-S02-C03
3	A	302	WTB	C18-N14-S02-O01
3	B	201	WTB	C18-N14-S02-O30
2	A	301	GNP	C3'-C4'-C5'-O5'
3	B	201	WTB	C16-C15-C19-N20
4	A	304	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	B	204	GOL	O1-C1-C2-O2
2	B	202	GNP	O4'-C4'-C5'-O5'
3	A	302	WTB	C05-C06-N09-C10
4	B	203	GOL	O1-C1-C2-O2
2	B	202	GNP	C5'-O5'-PA-O2A
3	A	302	WTB	C07-C06-N09-C10
2	B	202	GNP	C3'-C4'-C5'-O5'
3	B	201	WTB	N14-C15-C19-O29
4	A	306	GOL	O2-C2-C3-O3
4	B	206	GOL	O2-C2-C3-O3
4	B	203	GOL	O1-C1-C2-C3
4	B	205	GOL	C1-C2-C3-O3
2	A	301	GNP	PG-N3B-PB-O3A

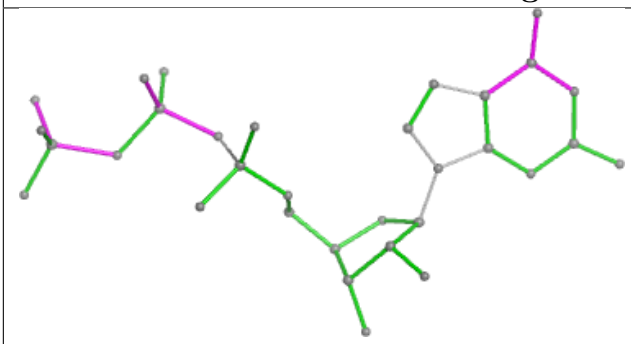
There are no ring outliers.

11 monomers are involved in 16 short contacts:

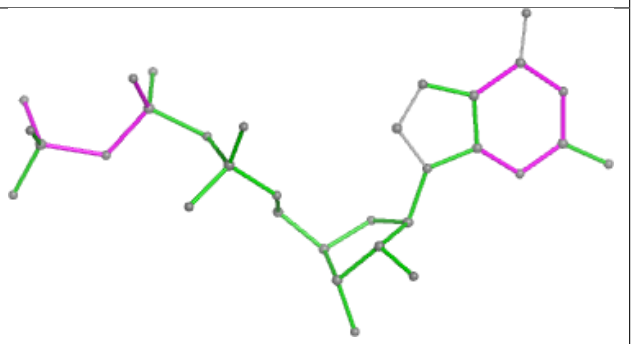
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	203	GOL	1	0
4	B	207	GOL	2	0
2	B	202	GNP	3	0
4	B	205	GOL	1	0
4	A	304	GOL	1	0
3	B	201	WTB	2	0
3	A	302	WTB	1	0
4	B	208	GOL	1	0
4	A	305	GOL	1	0
4	A	306	GOL	1	0
2	A	301	GNP	3	0

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 then 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.

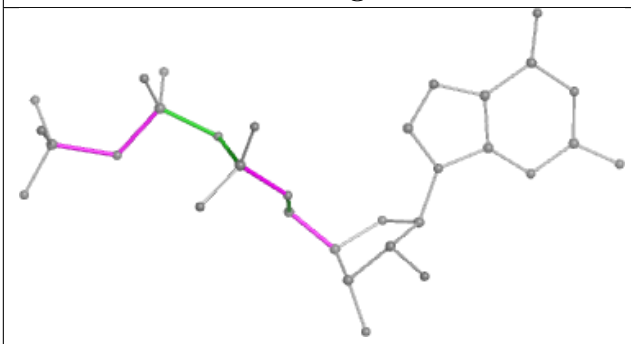
Ligand GNP B 202



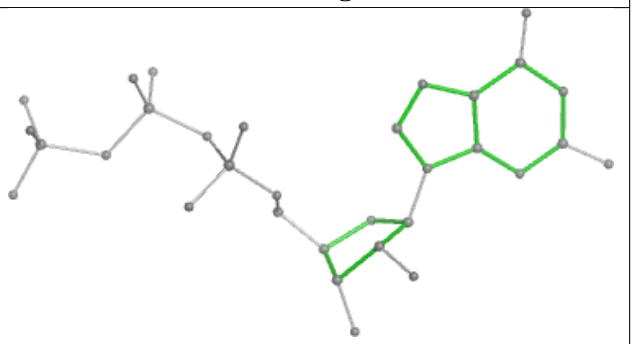
Bond lengths



Bond angles

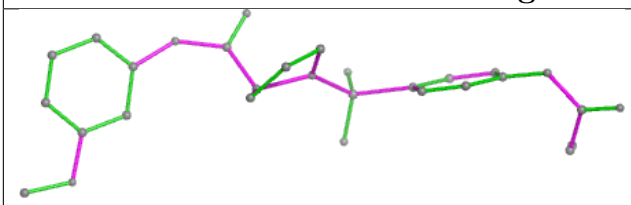


Torsions

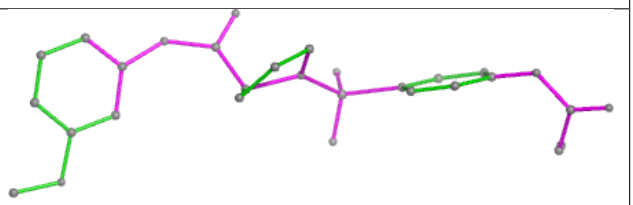


Rings

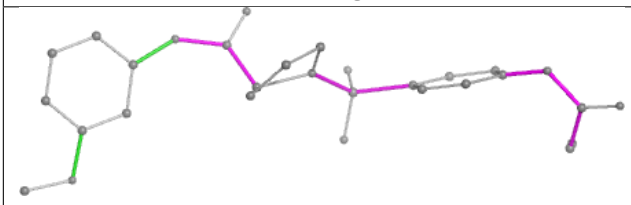
Ligand WTB B 201



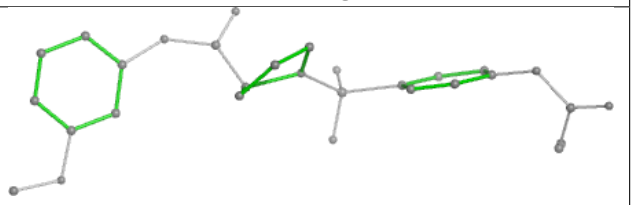
Bond lengths



Bond angles

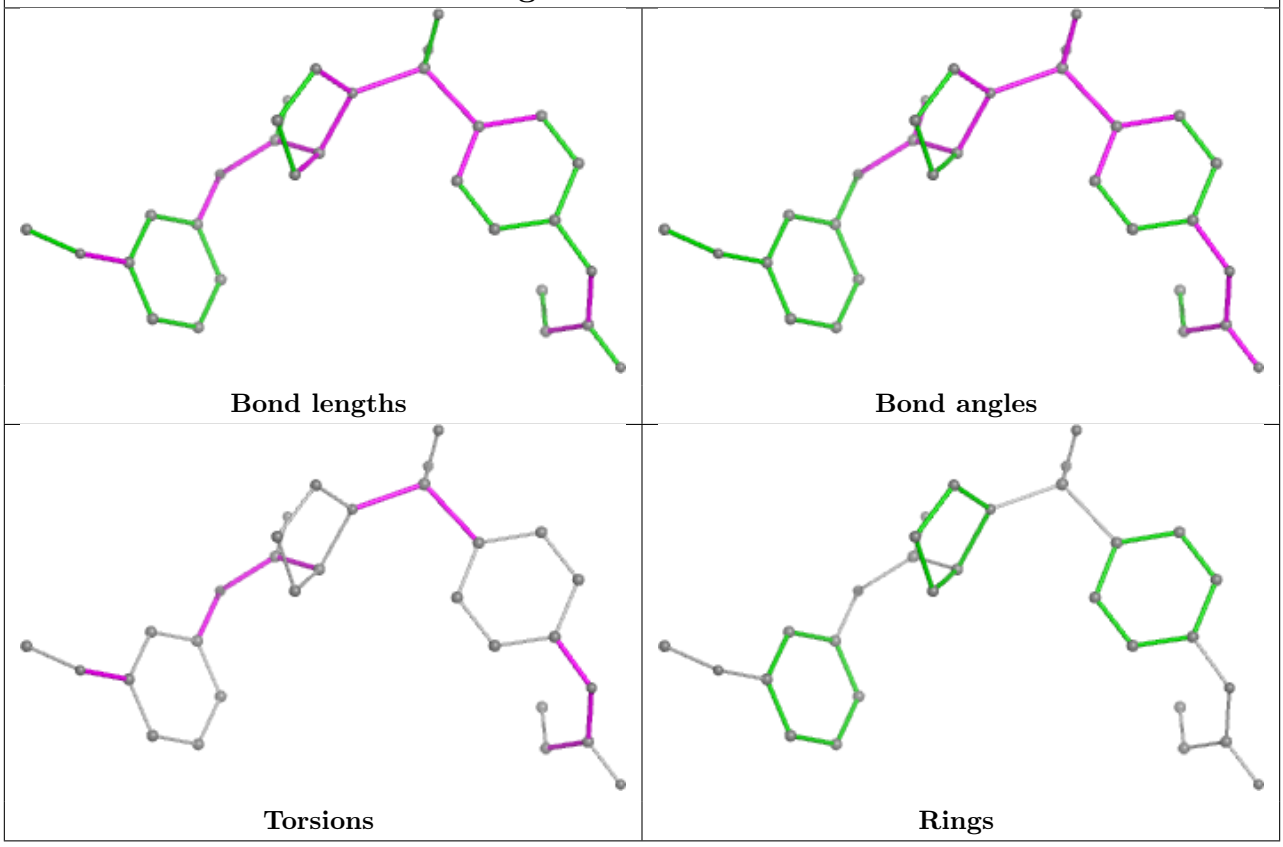


Torsions

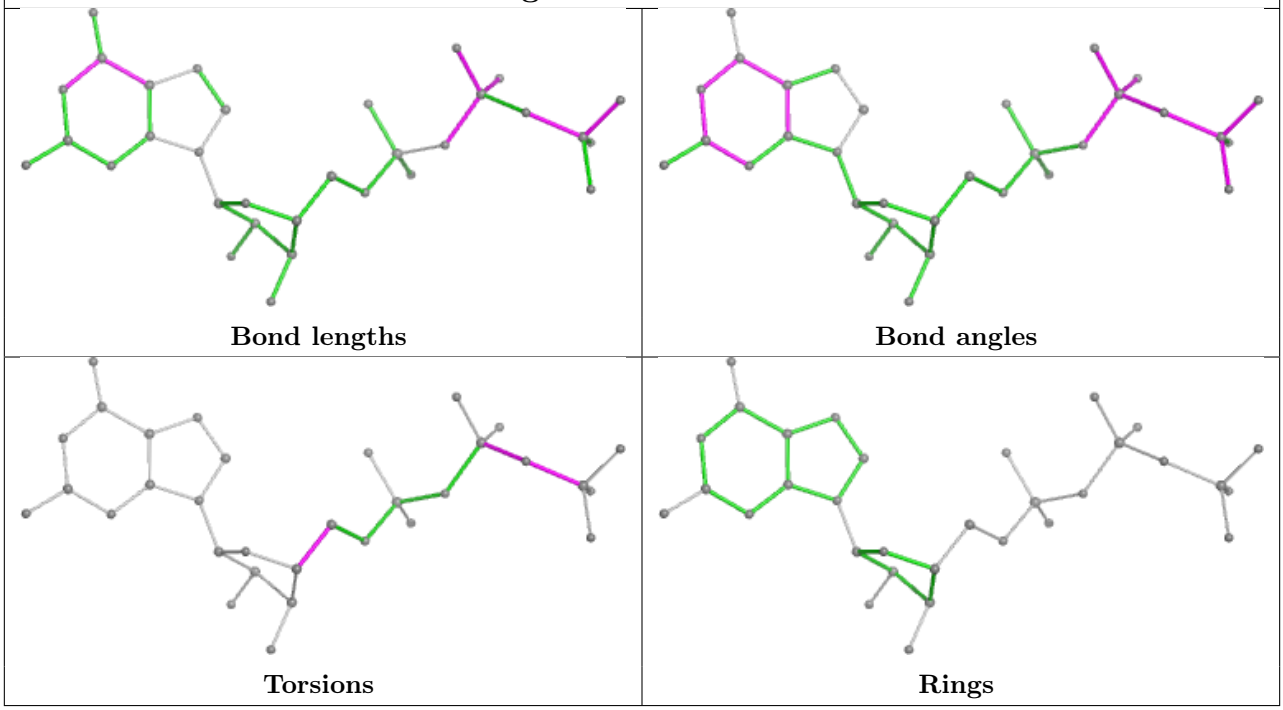


Rings

Ligand WTB A 302



Ligand GNP A 301



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, 95^{th} 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%)	0.33	8 (3%)	44	40	27, 41, 69, 116	0
1	B	209/230 (90%)	0.68	20 (9%)	15	13	32, 45, 84, 107	0
All	All	421/460 (91%)	0.50	28 (6%)	25	22	27, 43, 81, 116	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	60	GLY	4.6
1	B	59	ASP	4.5
1	B	58	PRO	4.4
1	B	63	GLY	4.4
1	B	61	ALA	4.2
1	A	58	PRO	4.0
1	B	6	TYR	3.6
1	B	55	ALA	3.5
1	A	188	SER	3.5
1	B	8	TYR	3.4
1	B	124	GLU	3.1
1	B	188	SER	3.0
1	B	173	ALA	2.7
1	B	62	THR	2.6
1	A	124	GLU	2.6
1	A	61	ALA	2.5
1	A	63	GLY	2.5
1	A	6	TYR	2.4
1	B	122	TYR	2.4
1	B	64	ARG	2.3
1	B	128	ILE	2.3
1	B	57	GLY	2.2
1	A	56	SER	2.2
1	B	39	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	165	ALA	2.1
1	B	90	ARG	2.1
1	B	-34	PHE	2.1
1	A	59	ASP	2.1

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 monosaccharides 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, 95^{th} 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.

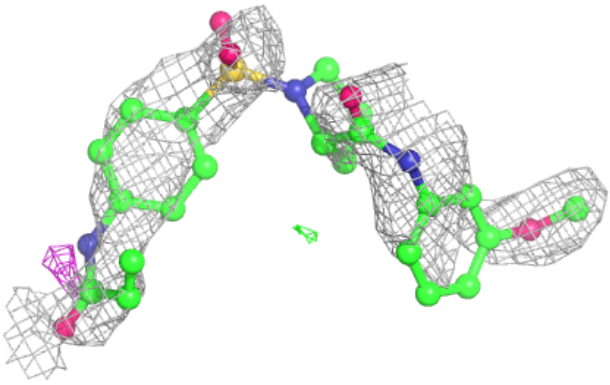
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	WTB	A	302	30/30	0.62	0.21	37,70,95,106	30
4	GOL	B	204	6/6	0.70	0.16	57,60,64,64	0
4	GOL	A	304	6/6	0.71	0.19	48,52,54,59	0
3	WTB	B	201	30/30	0.73	0.22	45,53,62,62	30
4	GOL	B	208	6/6	0.77	0.21	52,58,61,68	0
4	GOL	A	306	6/6	0.81	0.18	39,46,52,54	0
4	GOL	B	203	6/6	0.84	0.13	39,47,53,57	0
4	GOL	A	305	6/6	0.84	0.17	34,39,45,46	0
4	GOL	A	303	6/6	0.84	0.10	37,41,46,47	0
4	GOL	B	207	6/6	0.86	0.12	45,55,59,59	0
4	GOL	B	206	6/6	0.88	0.10	40,48,54,55	0
4	GOL	B	205	6/6	0.89	0.12	36,38,43,48	0
2	GNP	B	202	32/32	0.95	0.07	32,40,49,52	0
2	GNP	A	301	32/32	0.96	0.07	26,35,39,42	0
5	MG	A	307	1/1	0.97	0.05	30,30,30,30	0
5	MG	B	209	1/1	0.98	0.05	42,42,42,42	0

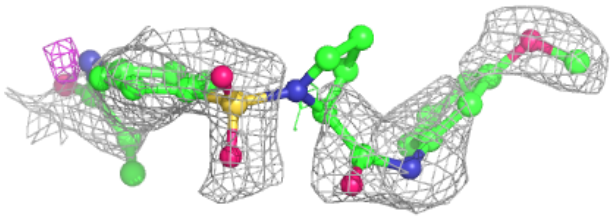
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

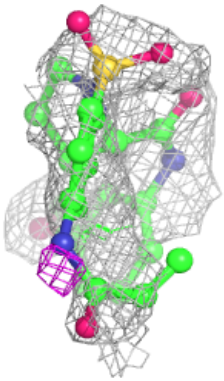
as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around WTB A 302:

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

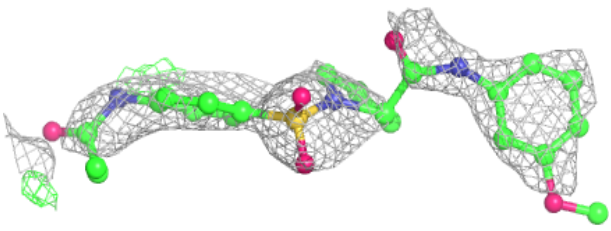


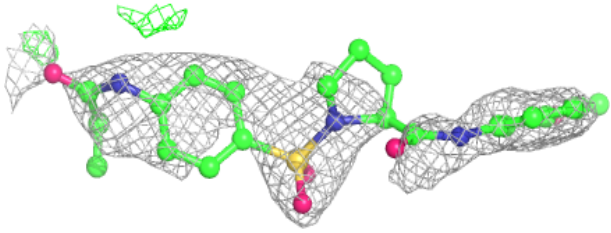


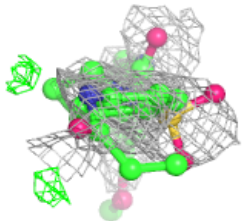


Electron density around WTB B 201:

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

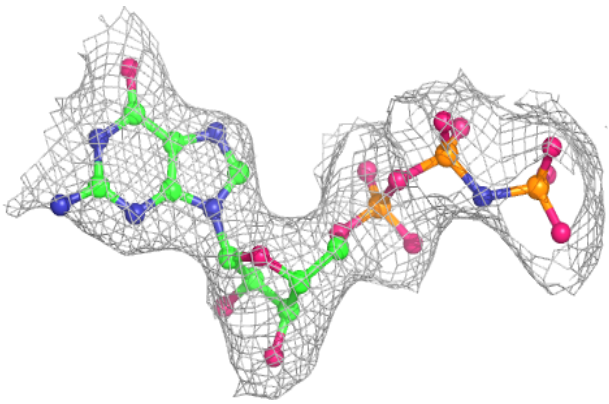


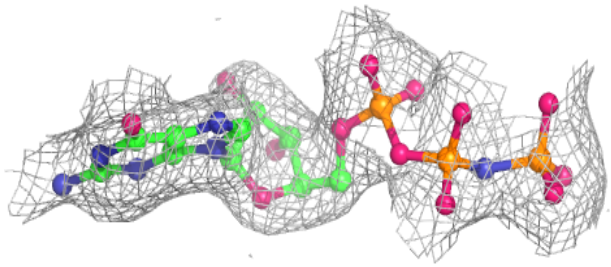


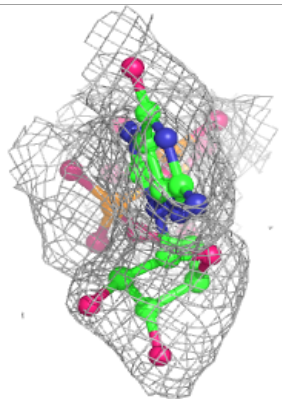


Electron density around GNP B 202:

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

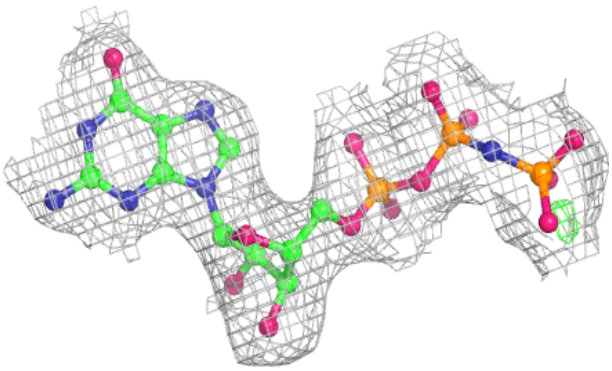


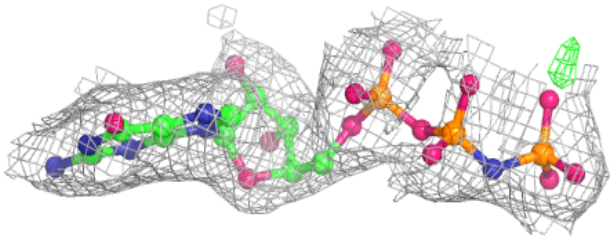


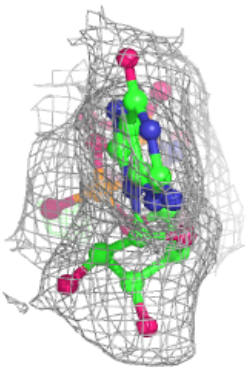


Electron density around GNP A 301:

$2mF_o$-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.