Full wwPDB X-ray Structure Validation Report (i)

Sep 12, 2023 – 07:33 PM EDT

PDB ID	:	4N4D
Title	:	Structure of ThiT with AV-38 bound
Authors	:	Swier, L.J.Y.M.; Guskov, A.; Slotboom, D.J.
Deposited on	:	2013-10-08
Resolution	:	2.40 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 (i) 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 (i)) were used in the production of this report:

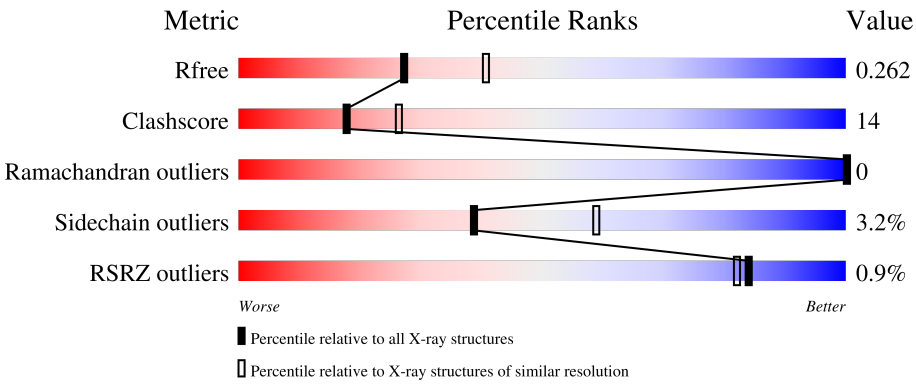
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.40 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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	182	% 79% 18% • •
1	B	182	% 86% 10% • •

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	BNG	B	203	-	-	X	-
5	PEG	A	210	-	-	X	-
5	PEG	A	212	-	-	X	-
5	PEG	B	206	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 3165 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.

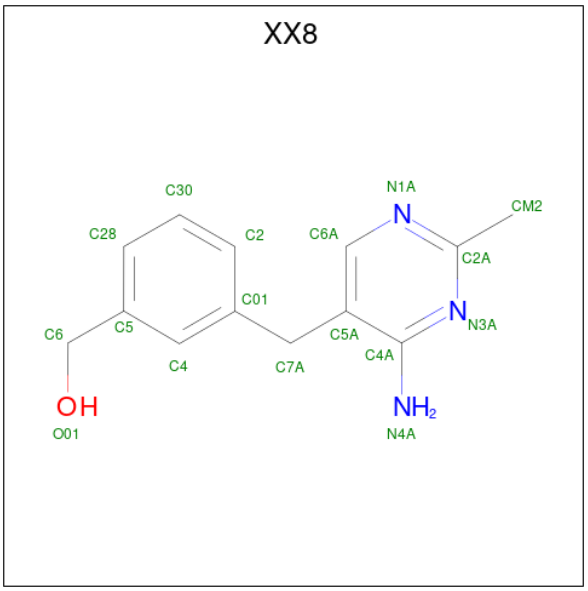
- Molecule 1 is a protein called thiamine binding protein ThiT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	176	1366	936	213	214	3	0	0	0
1	B	176	1366	936	213	214	3	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

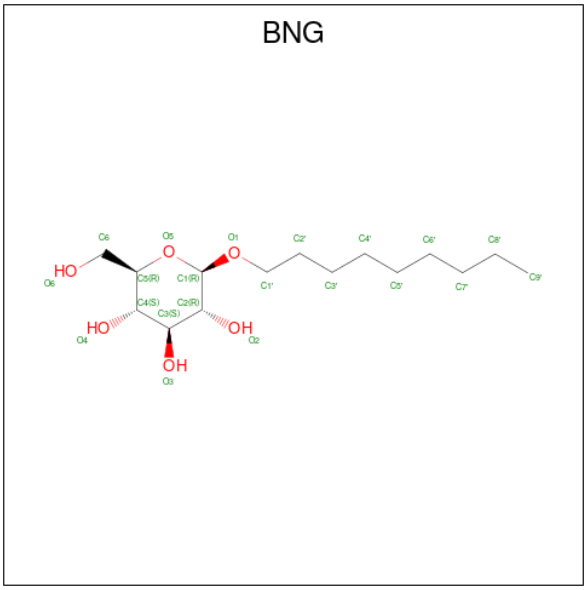
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP D8KFM5
A	2	SER	-	expression tag	UNP D8KFM5
A	3	ASN	-	expression tag	UNP D8KFM5
A	4	SER	-	expression tag	UNP D8KFM5
A	5	LYS	-	expression tag	UNP D8KFM5
A	6	PHE	-	expression tag	UNP D8KFM5
B	1	MET	-	expression tag	UNP D8KFM5
B	2	SER	-	expression tag	UNP D8KFM5
B	3	ASN	-	expression tag	UNP D8KFM5
B	4	SER	-	expression tag	UNP D8KFM5
B	5	LYS	-	expression tag	UNP D8KFM5
B	6	PHE	-	expression tag	UNP D8KFM5

- Molecule 2 is {3-[(4-amino-2-methylpyrimidin-5-yl)methyl]phenyl}methanol (three-letter code: XX8) (formula: $C_{13}H_{15}N_3O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	17	13	3	1	0	0
2	B	1	17	13	3	1	0	0

- Molecule 3 is nonyl beta-D-glucopyranoside (three-letter code: BNG) (formula: $C_{15}H_{30}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
3	A	1	21	15	6		0	0
3	A	1	21	15	6		0	0

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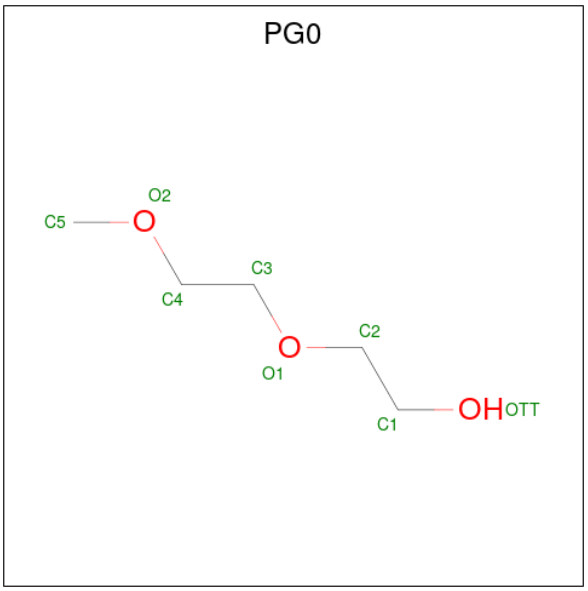
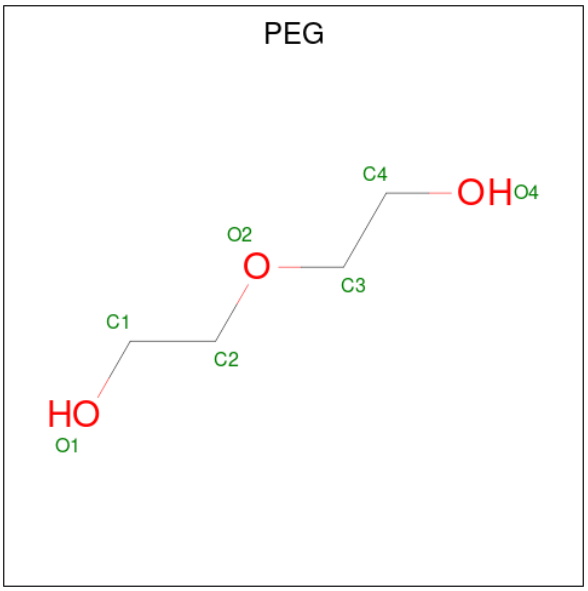
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	21	15	6	0	0
			Total	C	O		
3	B	1	21	15	6	0	0
			Total	C	O		
3	B	1	21	15	6	0	0

- Molecule 4 is 2-(2-METHOXYETHOXY)ETHANOL (three-letter code: PG0) (formula: $C_5H_{12}O_3$).



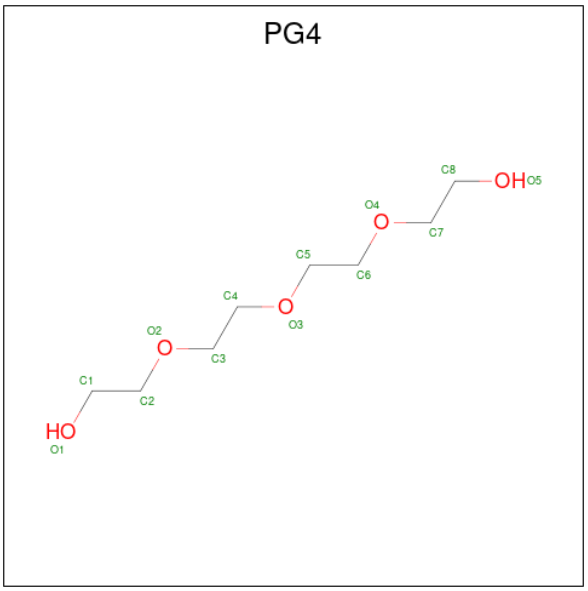
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	8	5	3	0	0
			Total	C	O		
4	A	1	8	5	3	0	0
			Total	C	O		
4	B	1	8	5	3	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



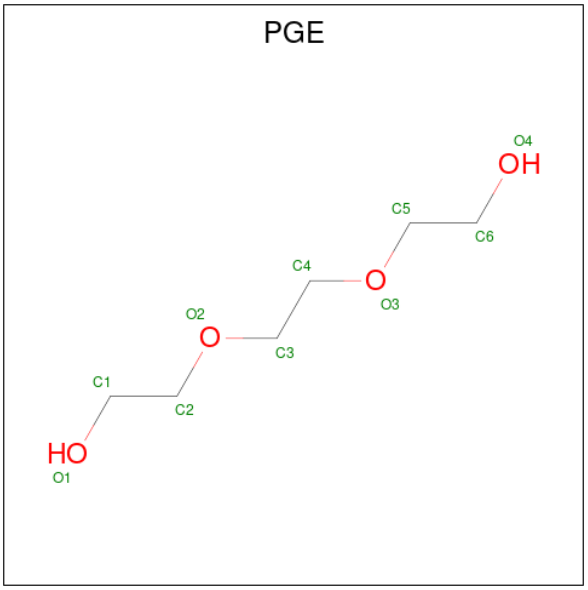
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
5	A	1	7	4	3		0	0
5	A	1	7	4	3		0	0
5	A	1	7	4	3		0	0
5	A	1	7	4	3		0	0
5	A	1	7	4	3		0	0
5	A	1	7	4	3		0	0
5	B	1	7	4	3		0	0
5	B	1	7	4	3		0	0

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	13	8	5	0	0
			Total	C	O		
6	B	1	13	8	5	0	0

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	10	6	4	0	0
			Total	C	O		
7	A	1	20	12	8	0	1

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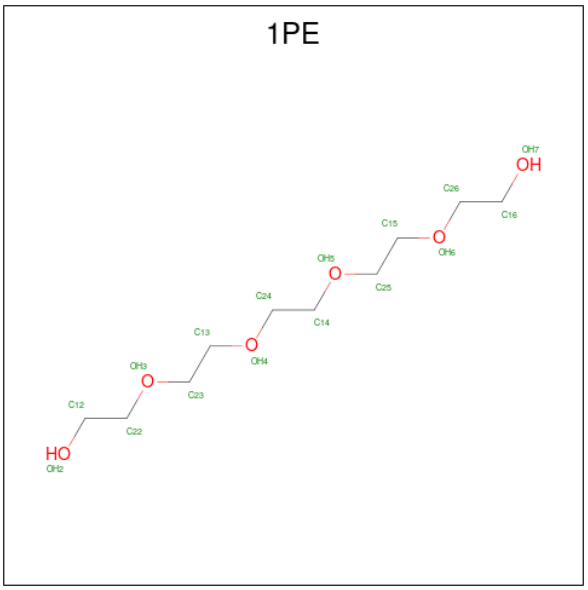
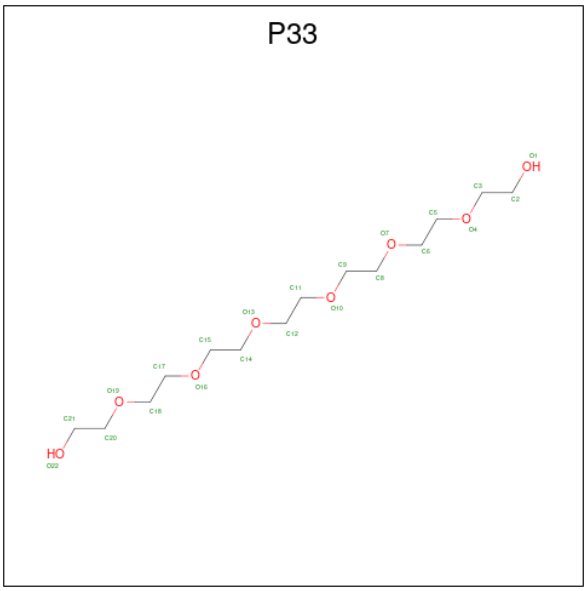
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	10	6	4	0	0
			Total	C	O		
7	A	1	10	6	4	0	0
			Total	C	O		
7	B	1	10	6	4	0	0
			Total	C	O		
7	B	1	10	6	4	0	0

- Molecule 8 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	32	20	12	0	1
			Total	C	O		
8	B	1	16	10	6	0	0

- Molecule 9 is 3,6,9,12,15,18-HEXAOXAICOSANE-1,20-DIOL (three-letter code: P33) (formula: $C_{14}H_{30}O_8$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	B	1	22	14	8	0	0

- Molecule 10 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
10	B	1	1	1	0	0

- Molecule 11 is water.

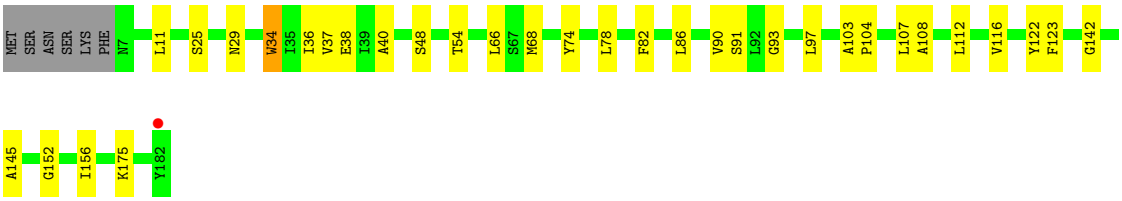
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	20	21	21	0	1
			Total	O		
11	B	26	26	26	0	0

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.

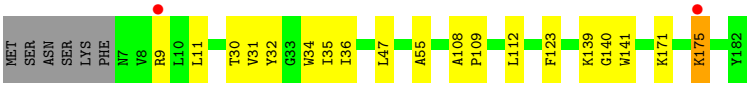
• Molecule 1: thiamine binding protein ThiT

Chain A:



• Molecule 1: thiamine binding protein ThiT

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	63.16Å 84.26Å 127.25Å 90.00° 94.17° 90.00°	Depositor
Resolution (Å)	42.30 – 2.40 47.85 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (42.30-2.40) 99.3 (47.85-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.204 , 0.257 0.208 , 0.262	Depositor DCC
R_{free} test set	1297 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	46.4	Xtriage
Anisotropy	0.374	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 48.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	3165	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.51% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, XX8, PEG, PG4, PG0, 1PE, PGE, BNG, P33

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	0.64	0/1404	0.67	0/1914
1	B	0.65	0/1404	0.65	0/1914
All	All	0.65	0/2808	0.66	0/3828

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 (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	1366	0	1462	46	0
1	B	1366	0	1462	23	0
2	A	17	0	15	4	0
2	B	17	0	15	0	0
3	A	63	0	90	7	0
3	B	42	0	60	16	0
4	A	16	0	24	4	0
4	B	8	0	12	0	0
5	A	42	0	54	20	0
5	B	14	0	18	5	0
6	A	13	0	18	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	13	0	18	4	0
7	A	50	0	70	6	0
7	B	20	0	28	3	0
8	A	32	0	44	8	0
8	B	16	0	22	6	0
9	B	22	0	30	0	0
10	B	1	0	0	0	0
11	A	21	0	0	1	0
11	B	26	0	0	1	0
All	All	3165	0	3442	89	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 14.

All (89) 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:38:GLU:HG3	5:A:212:PEG:H41	1.38	1.03
8:A:218[A]:1PE:H142	8:B:211:1PE:H131	1.55	0.89
1:A:25:SER:HB2	5:A:212:PEG:H32	1.62	0.81
1:A:91:SER:CB	5:A:210:PEG:H11	2.15	0.77
1:B:32:TYR:HB2	3:B:203:BNG:H8'2	1.67	0.76
1:A:40:ALA:HB3	5:A:212:PEG:H42	1.67	0.74
1:A:36:ILE:HG21	5:A:209:PEG:H42	1.71	0.71
1:B:36:ILE:HG21	5:B:206:PEG:H31	1.73	0.70
1:B:36:ILE:CG2	5:B:206:PEG:H31	2.22	0.70
1:A:78:LEU:CD2	4:A:206:PG0:H32	2.24	0.68
1:A:91:SER:HB3	5:A:210:PEG:H11	1.76	0.67
1:A:25:SER:CB	5:A:212:PEG:H32	2.26	0.65
1:B:32:TYR:CB	3:B:203:BNG:H8'2	2.27	0.64
1:A:38:GLU:CG	5:A:212:PEG:H41	2.21	0.64
3:A:203:BNG:C5'	3:A:203:BNG:H9'3	2.28	0.63
8:A:218[B]:1PE:H251	8:B:211:1PE:H131	1.81	0.63
1:A:142:GLY:H	7:A:214:PGE:H22	1.65	0.61
1:B:141:TRP:CD1	3:B:202:BNG:H1'1	2.35	0.61
1:A:91:SER:HA	5:A:210:PEG:H22	1.83	0.61
1:A:90:VAL:HG11	5:A:211:PEG:H22	1.83	0.60
1:A:78:LEU:HD23	4:A:206:PG0:H32	1.83	0.60
1:B:35:ILE:CD1	3:B:203:BNG:H5'2	2.32	0.59
1:B:11:LEU:HD21	7:B:210:PGE:H5	1.86	0.58
1:B:30:THR:OG1	5:B:206:PEG:H42	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:203:BNG:H9'3	3:A:203:BNG:H5'1	1.86	0.57
1:A:74:TYR:OH	5:A:209:PEG:H32	2.04	0.57
1:B:35:ILE:HD12	3:B:203:BNG:H5'2	1.86	0.57
1:A:29:ASN:HD21	5:A:212:PEG:H21	1.73	0.54
6:B:207:PG4:H52	6:B:207:PG4:C8	2.38	0.53
1:A:25:SER:HB2	5:A:212:PEG:C3	2.37	0.53
1:A:97:LEU:CD1	3:A:202:BNG:H4'2	2.39	0.52
1:A:145:ALA:CB	7:A:214:PGE:H2	2.39	0.52
1:A:122:TYR:CE2	2:A:201:XX8:H8	2.46	0.51
8:B:211:1PE:C25	8:B:211:1PE:H132	2.42	0.50
1:A:108:ALA:HA	3:B:203:BNG:H6'2	1.93	0.50
1:A:68:MET:HB3	5:A:207:PEG:H31	1.94	0.49
7:B:209:PGE:H3	7:B:209:PGE:H5	1.62	0.49
1:B:35:ILE:HD12	3:B:203:BNG:C3'	2.42	0.48
8:A:218[A]:1PE:H251	8:A:218[A]:1PE:H242	1.58	0.47
1:A:107:LEU:HD23	3:B:203:BNG:H9'3	1.96	0.47
2:A:201:XX8:H15	11:A:309:HOH:O	2.14	0.47
5:B:205:PEG:H42	5:B:205:PEG:H21	1.64	0.47
1:B:175:LYS:HD3	1:B:175:LYS:H	1.80	0.47
1:A:40:ALA:CB	5:A:212:PEG:H42	2.41	0.47
6:B:207:PG4:H52	6:B:207:PG4:H82	1.96	0.47
5:A:210:PEG:H21	5:A:211:PEG:H12	1.97	0.46
1:A:156:ILE:HG12	8:A:218[B]:1PE:H261	1.96	0.46
1:B:141:TRP:CE2	3:B:202:BNG:H3'2	2.51	0.46
1:A:78:LEU:HD22	4:A:206:PG0:H32	1.97	0.46
1:A:116:VAL:HG22	3:B:202:BNG:H9'3	1.98	0.46
8:A:218[A]:1PE:H142	8:B:211:1PE:C13	2.38	0.46
1:A:25:SER:HA	5:A:212:PEG:H32	1.98	0.45
1:A:122:TYR:HE2	2:A:201:XX8:C6	2.30	0.45
1:A:152:GLY:HA3	8:A:218[B]:1PE:H241	1.97	0.45
1:A:38:GLU:HG3	5:A:212:PEG:C4	2.28	0.45
1:A:97:LEU:HD12	3:A:202:BNG:H4'2	1.99	0.45
7:B:210:PGE:H1	11:B:324:HOH:O	2.15	0.45
6:B:207:PG4:H82	6:B:207:PG4:C5	2.46	0.45
1:A:48:SER:OG	1:A:93:GLY:HA2	2.17	0.45
1:B:108:ALA:HB3	1:B:109:PRO:HD3	1.98	0.44
1:A:54:THR:CG2	7:A:217:PGE:H2	2.47	0.44
1:A:29:ASN:HA	6:A:213:PG4:H82	1.98	0.44
1:B:47:LEU:HD21	1:B:55:ALA:O	2.17	0.44
3:A:203:BNG:H9'2	3:A:203:BNG:H6'2	1.52	0.43
1:A:112:LEU:HB2	3:B:203:BNG:H2'2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:GLY:O	3:B:202:BNG:H1'2	2.19	0.43
1:B:175:LYS:H	1:B:175:LYS:CD	2.31	0.43
1:A:91:SER:HB2	5:A:210:PEG:H11	1.97	0.43
1:B:123:PHE:CE1	8:B:211:1PE:H221	2.53	0.43
6:B:207:PG4:C8	6:B:207:PG4:C5	2.97	0.43
1:A:145:ALA:HB3	7:A:214:PGE:H2	2.00	0.42
4:A:205:PG0:C5	1:B:32:TYR:CD2	3.02	0.42
3:A:202:BNG:H9'2	3:B:202:BNG:H6'1	2.01	0.42
1:B:31:VAL:HG22	3:B:203:BNG:H8'1	2.01	0.42
1:B:35:ILE:HD13	3:B:203:BNG:H5'2	2.02	0.42
1:B:123:PHE:HD1	8:B:211:1PE:H232	1.84	0.42
1:A:25:SER:CA	5:A:212:PEG:H32	2.50	0.42
1:A:156:ILE:CG1	8:A:218[B]:1PE:H261	2.50	0.42
1:A:103:ALA:HB1	1:A:104:PRO:HA	2.01	0.42
1:A:97:LEU:HD13	3:A:202:BNG:H4'2	2.01	0.42
1:A:37:VAL:HB	6:A:213:PG4:H81	2.01	0.41
1:B:34:TRP:CZ3	5:B:206:PEG:H21	2.55	0.41
1:A:34:TRP:CZ2	1:A:74:TYR:CD2	3.08	0.40
1:B:35:ILE:CD1	3:B:203:BNG:C3'	2.99	0.40
1:A:34:TRP:CE2	2:A:201:XX8:H13	2.56	0.40
1:A:82:PHE:CD1	1:A:86:LEU:HD12	2.56	0.40
8:A:218[A]:1PE:C24	8:A:218[A]:1PE:H152	2.52	0.40
7:A:215[A]:PGE:H22	7:A:215[A]:PGE:H4	1.19	0.40
1:A:123:PHE:HD1	7:A:215[A]:PGE:H32	1.87	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	174/182 (96%)	169 (97%)	5 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	174/182 (96%)	168 (97%)	6 (3%)	0	100	100
All	All	348/364 (96%)	337 (97%)	11 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	140/146 (96%)	136 (97%)	4 (3%)	42	62
1	B	140/146 (96%)	135 (96%)	5 (4%)	35	54
All	All	280/292 (96%)	271 (97%)	9 (3%)	39	59

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	34	TRP
1	A	66	LEU
1	A	175	LYS
1	B	9	ARG
1	B	112	LEU
1	B	139	LYS
1	B	171	LYS
1	B	175	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	72	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 32 ligands modelled in this entry, 1 is monoatomic - leaving 31 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	$\#\|Z\| > 2$
7	PGE	A	216	-	9,9,9	0.40	0	8,8,8	0.42	0
3	BNG	B	203	-	21,21,21	0.92	1 (4%)	26,26,26	1.58	4 (15%)
5	PEG	A	208	-	6,6,6	0.62	0	5,5,5	0.65	0
8	1PE	A	218[B]	-	15,15,15	0.76	0	14,14,14	0.35	0
5	PEG	A	212	-	6,6,6	0.67	0	5,5,5	0.85	0
3	BNG	A	203	-	21,21,21	0.88	0	26,26,26	1.69	5 (19%)
7	PGE	A	215[B]	-	9,9,9	0.35	0	8,8,8	0.27	0
7	PGE	A	217	-	9,9,9	0.32	0	8,8,8	0.48	0
5	PEG	B	205	-	6,6,6	0.63	0	5,5,5	0.27	0
9	P33	B	208	-	21,21,21	0.96	0	20,20,20	0.49	0
6	PG4	A	213	-	12,12,12	0.72	0	11,11,11	0.43	0
3	BNG	A	204	-	21,21,21	0.78	0	26,26,26	0.93	1 (3%)
4	PG0	B	204	-	7,7,7	0.40	0	6,6,6	0.51	0
7	PGE	B	209	-	9,9,9	0.36	0	8,8,8	0.39	0
2	XX8	B	201	-	18,18,18	1.91	4 (22%)	24,24,24	1.52	4 (16%)
3	BNG	B	202	-	21,21,21	0.93	1 (4%)	26,26,26	1.56	5 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	PGE	A	214	-	9,9,9	0.34	0	8,8,8	0.34	0
4	PG0	A	205	-	7,7,7	0.32	0	6,6,6	0.46	0
8	1PE	A	218[A]	-	15,15,15	0.72	0	14,14,14	0.46	0
4	PG0	A	206	-	7,7,7	0.34	0	6,6,6	0.21	0
7	PGE	B	210	-	9,9,9	0.33	0	8,8,8	0.46	0
7	PGE	A	215[A]	-	9,9,9	0.27	0	8,8,8	0.52	0
5	PEG	A	207	-	6,6,6	0.56	0	5,5,5	0.43	0
5	PEG	A	209	-	6,6,6	0.65	0	5,5,5	0.42	0
5	PEG	A	211	-	6,6,6	0.59	0	5,5,5	0.38	0
6	PG4	B	207	-	12,12,12	0.80	0	11,11,11	0.45	0
5	PEG	A	210	-	6,6,6	0.57	0	5,5,5	0.38	0
5	PEG	B	206	-	6,6,6	0.68	0	5,5,5	0.45	0
2	XX8	A	201	-	18,18,18	1.94	6 (33%)	24,24,24	1.52	4 (16%)
3	BNG	A	202	-	21,21,21	0.81	0	26,26,26	1.34	2 (7%)
8	1PE	B	211	-	15,15,15	0.77	0	14,14,14	0.30	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
7	PGE	A	216	-	-	6/7/7/7	-
3	BNG	B	203	-	-	6/12/32/32	0/1/1/1
5	PEG	A	208	-	-	1/4/4/4	-
8	1PE	A	218[B]	-	-	6/13/13/13	-
5	PEG	A	212	-	-	3/4/4/4	-
3	BNG	A	203	-	-	6/12/32/32	0/1/1/1
7	PGE	A	215[B]	-	-	4/7/7/7	-
7	PGE	A	217	-	-	2/7/7/7	-
5	PEG	B	205	-	-	3/4/4/4	-
9	P33	B	208	-	-	12/19/19/19	-
6	PG4	A	213	-	-	5/10/10/10	-
3	BNG	A	204	-	-	7/12/32/32	0/1/1/1
4	PG0	B	204	-	-	4/5/5/5	-
7	PGE	B	209	-	-	4/7/7/7	-
2	XX8	B	201	-	-	2/6/6/6	0/2/2/2
3	BNG	B	202	-	-	8/12/32/32	0/1/1/1
7	PGE	A	214	-	-	3/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PG0	A	205	-	-	2/5/5/5	-
8	1PE	A	218[A]	-	-	10/13/13/13	-
4	PG0	A	206	-	-	1/5/5/5	-
7	PGE	B	210	-	-	3/7/7/7	-
7	PGE	A	215[A]	-	-	4/7/7/7	-
5	PEG	A	207	-	-	3/4/4/4	-
5	PEG	A	209	-	-	3/4/4/4	-
5	PEG	A	211	-	-	2/4/4/4	-
6	PG4	B	207	-	-	4/10/10/10	-
5	PEG	A	210	-	-	3/4/4/4	-
5	PEG	B	206	-	-	0/4/4/4	-
2	XX8	A	201	-	-	0/6/6/6	0/2/2/2
3	BNG	A	202	-	-	10/12/32/32	0/1/1/1
8	1PE	B	211	-	-	7/13/13/13	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	XX8	C4A-N4A	4.41	1.45	1.34
2	B	201	XX8	C4A-N4A	4.24	1.44	1.34
2	B	201	XX8	C4-C01	3.85	1.45	1.39
2	A	201	XX8	C4A-N3A	3.49	1.40	1.35
2	B	201	XX8	C4A-N3A	2.77	1.39	1.35
2	A	201	XX8	C4-C01	2.71	1.43	1.39
2	B	201	XX8	C30-C28	2.66	1.44	1.38
2	A	201	XX8	C6A-C5A	2.34	1.42	1.37
2	A	201	XX8	C30-C28	2.29	1.43	1.38
3	B	202	BNG	O1-C1	2.20	1.43	1.40
3	B	203	BNG	O1-C1	2.14	1.43	1.40
2	A	201	XX8	O01-C6	2.10	1.50	1.41

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	202	BNG	C1-O5-C5	-4.42	105.01	113.69
3	A	202	BNG	O1-C1-C2	4.31	115.04	108.30
3	B	203	BNG	C3-C4-C5	3.97	117.31	110.24
3	A	203	BNG	O1-C1-C2	3.94	114.45	108.30
2	A	201	XX8	C6A-N1A-C2A	3.75	122.35	115.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	203	BNG	O1-C1-C2	3.61	113.94	108.30
3	A	202	BNG	C1-O5-C5	-3.40	107.01	113.69
2	B	201	XX8	C6A-N1A-C2A	3.40	121.74	115.96
3	A	203	BNG	C1-O5-C5	-3.30	107.22	113.69
3	B	202	BNG	C3-C4-C5	-3.26	104.43	110.24
3	A	203	BNG	O5-C1-C2	-3.25	103.47	110.35
3	A	203	BNG	C3-C4-C5	3.23	116.00	110.24
2	A	201	XX8	N1A-C2A-N3A	-2.93	120.50	125.54
3	B	203	BNG	C6-C5-C4	-2.82	106.40	113.00
2	B	201	XX8	C5A-C6A-N1A	-2.64	119.42	123.82
3	B	203	BNG	O3-C3-C4	-2.56	104.42	110.35
3	B	202	BNG	O5-C5-C6	2.55	112.78	106.44
2	B	201	XX8	C01-C4-C5	-2.54	118.10	121.23
3	B	202	BNG	C1'-O1-C1	2.52	118.01	113.84
3	A	204	BNG	C1-O5-C5	-2.47	108.84	113.69
2	A	201	XX8	C5A-C6A-N1A	-2.46	119.72	123.82
3	B	202	BNG	O5-C5-C4	-2.44	105.26	109.69
2	B	201	XX8	N1A-C2A-N3A	-2.20	121.76	125.54
2	A	201	XX8	C2A-N3A-C4A	2.13	121.41	118.08
3	A	203	BNG	C1'-O1-C1	-2.03	110.48	113.84

There are no chirality outliers.

All (134) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	202	BNG	C2-C1-O1-C1'
3	A	202	BNG	O5-C1-O1-C1'
3	A	202	BNG	C2'-C1'-O1-C1
8	A	218[A]	1PE	C25-C15-OH6-C26
9	B	208	P33	C8-C9-O10-C11
9	B	208	P33	C17-C18-O19-C20
7	A	215[A]	PGE	C4-C3-O2-C2
8	A	218[A]	1PE	C24-C14-OH5-C25
3	A	204	BNG	C1'-C2'-C3'-C4'
8	B	211	1PE	C14-C24-OH4-C13
3	A	202	BNG	O5-C5-C6-O6
3	B	202	BNG	O5-C5-C6-O6
4	A	206	PG0	O1-C3-C4-O2
7	A	217	PGE	O2-C3-C4-O3
8	B	211	1PE	OH5-C14-C24-OH4
3	B	203	BNG	O5-C5-C6-O6
3	A	203	BNG	O5-C1-O1-C1'

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Mol	Chain	Res	Type	Atoms
7	A	215[B]	PGE	O2-C3-C4-O3
3	A	202	BNG	C4-C5-C6-O6
8	A	218[A]	1PE	OH5-C14-C24-OH4
5	A	210	PEG	O1-C1-C2-O2
3	B	202	BNG	C4-C5-C6-O6
4	A	205	PG0	O1-C3-C4-O2
9	B	208	P33	O4-C5-C6-O7
3	B	203	BNG	C4-C5-C6-O6
7	B	210	PGE	O2-C3-C4-O3
9	B	208	P33	O10-C11-C12-O13
3	B	203	BNG	O1-C1'-C2'-C3'
5	A	207	PEG	O2-C3-C4-O4
9	B	208	P33	O19-C20-C21-O22
9	B	208	P33	O7-C8-C9-O10
7	A	215[A]	PGE	O2-C3-C4-O3
8	A	218[B]	1PE	OH4-C13-C23-OH3
3	A	203	BNG	C6'-C7'-C8'-C9'
3	A	203	BNG	O1-C1'-C2'-C3'
5	A	207	PEG	O1-C1-C2-O2
5	A	209	PEG	O1-C1-C2-O2
5	A	210	PEG	O2-C3-C4-O4
5	A	212	PEG	O1-C1-C2-O2
7	B	209	PGE	O3-C5-C6-O4
7	B	210	PGE	O3-C5-C6-O4
8	A	218[B]	1PE	OH2-C12-C22-OH3
3	A	202	BNG	O1-C1'-C2'-C3'
3	B	202	BNG	O1-C1'-C2'-C3'
3	A	202	BNG	C2'-C3'-C4'-C5'
6	B	207	PG4	O4-C7-C8-O5
3	A	202	BNG	C4'-C5'-C6'-C7'
3	A	204	BNG	C3'-C4'-C5'-C6'
3	A	204	BNG	C2'-C1'-O1-C1
7	B	209	PGE	C3-C4-O3-C5
3	B	203	BNG	C3'-C4'-C5'-C6'
3	A	202	BNG	C1'-C2'-C3'-C4'
7	A	215[B]	PGE	O3-C5-C6-O4
6	A	213	PG4	O3-C5-C6-O4
5	B	205	PEG	C4-C3-O2-C2
3	B	202	BNG	C2-C1-O1-C1'
3	B	202	BNG	C5'-C6'-C7'-C8'
4	B	204	PG0	OTT-C1-C2-O1
7	A	214	PGE	O3-C5-C6-O4

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Mol	Chain	Res	Type	Atoms
7	B	209	PGE	O2-C3-C4-O3
3	A	204	BNG	C6'-C7'-C8'-C9'
9	B	208	P33	O1-C2-C3-O4
3	A	203	BNG	C2'-C1'-O1-C1
3	B	203	BNG	C2'-C3'-C4'-C5'
7	A	215[B]	PGE	C6-C5-O3-C4
7	A	216	PGE	O1-C1-C2-O2
7	B	209	PGE	O1-C1-C2-O2
7	A	216	PGE	O2-C3-C4-O3
4	B	204	PG0	C3-C4-O2-C5
3	A	204	BNG	C5'-C6'-C7'-C8'
5	B	205	PEG	O1-C1-C2-O2
5	B	205	PEG	O2-C3-C4-O4
8	A	218[A]	1PE	C15-C25-OH5-C14
3	A	204	BNG	C4'-C5'-C6'-C7'
5	A	208	PEG	O2-C3-C4-O4
7	A	216	PGE	O3-C5-C6-O4
9	B	208	P33	C18-C17-O16-C15
9	B	208	P33	C11-C12-O13-C14
3	A	203	BNG	C2'-C3'-C4'-C5'
3	B	203	BNG	C5'-C6'-C7'-C8'
5	A	211	PEG	C4-C3-O2-C2
8	A	218[A]	1PE	C13-C23-OH3-C22
8	A	218[B]	1PE	C14-C24-OH4-C13
9	B	208	P33	C14-C15-O16-C17
5	A	211	PEG	C1-C2-O2-C3
7	A	216	PGE	C3-C4-O3-C5
3	A	202	BNG	C3'-C4'-C5'-C6'
8	B	211	1PE	C24-C14-OH5-C25
8	A	218[A]	1PE	OH2-C12-C22-OH3
6	B	207	PG4	O2-C3-C4-O3
5	A	207	PEG	C4-C3-O2-C2
7	B	210	PGE	C3-C4-O3-C5
3	A	203	BNG	C5'-C6'-C7'-C8'
7	A	215[A]	PGE	C3-C4-O3-C5
8	B	211	1PE	C23-C13-OH4-C24
4	A	205	PG0	C3-C4-O2-C5
7	A	216	PGE	C1-C2-O2-C3
5	A	209	PEG	O2-C3-C4-O4
8	B	211	1PE	C12-C22-OH3-C23
3	B	202	BNG	O5-C1-O1-C1'
5	A	210	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
4	B	204	PG0	C4-C3-O1-C2
8	B	211	1PE	C16-C26-OH6-C15
7	A	214	PGE	C3-C4-O3-C5
6	A	213	PG4	C8-C7-O4-C6
8	A	218[A]	1PE	C23-C13-OH4-C24
2	B	201	XX8	C4-C01-C7A-C5A
7	A	215[A]	PGE	O3-C5-C6-O4
8	A	218[A]	1PE	OH4-C13-C23-OH3
4	B	204	PG0	O1-C3-C4-O2
6	A	213	PG4	O2-C3-C4-O3
6	B	207	PG4	C8-C7-O4-C6
8	B	211	1PE	C25-C15-OH6-C26
2	B	201	XX8	C2-C01-C7A-C5A
5	A	212	PEG	C1-C2-O2-C3
7	A	215[B]	PGE	C1-C2-O2-C3
3	B	202	BNG	C2'-C3'-C4'-C5'
6	A	213	PG4	C1-C2-O2-C3
8	A	218[B]	1PE	C23-C13-OH4-C24
9	B	208	P33	C2-C3-O4-C5
5	A	209	PEG	C1-C2-O2-C3
7	A	216	PGE	C6-C5-O3-C4
6	B	207	PG4	O3-C5-C6-O4
3	B	202	BNG	C4'-C5'-C6'-C7'
8	A	218[B]	1PE	C15-C25-OH5-C14
7	A	217	PGE	C6-C5-O3-C4
5	A	212	PEG	C4-C3-O2-C2
8	A	218[A]	1PE	C14-C24-OH4-C13
6	A	213	PG4	C3-C4-O3-C5
3	A	204	BNG	C2-C1-O1-C1'
8	A	218[B]	1PE	OH5-C14-C24-OH4
9	B	208	P33	O16-C17-C18-O19
7	A	214	PGE	C1-C2-O2-C3
8	A	218[A]	1PE	OH6-C15-C25-OH5

There are no ring outliers.

24 monomers are involved in 81 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	203	BNG	11	0
8	A	218[B]	1PE	4	0
5	A	212	PEG	11	0
3	A	203	BNG	3	0

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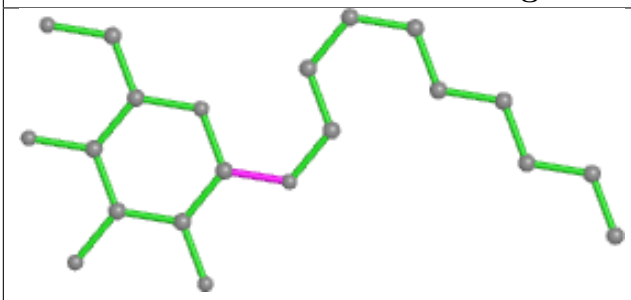
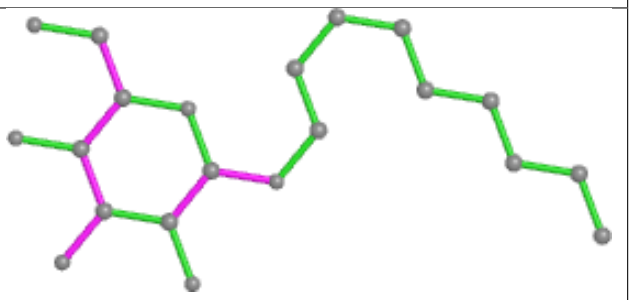
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	217	PGE	1	0
5	B	205	PEG	1	0
6	A	213	PG4	2	0
7	B	209	PGE	1	0
3	B	202	BNG	5	0
7	A	214	PGE	3	0
4	A	205	PG0	1	0
8	A	218[A]	1PE	4	0
4	A	206	PG0	3	0
7	B	210	PGE	2	0
7	A	215[A]	PGE	2	0
5	A	207	PEG	1	0
5	A	209	PEG	2	0
5	A	211	PEG	2	0
6	B	207	PG4	4	0
5	A	210	PEG	5	0
5	B	206	PEG	4	0
2	A	201	XX8	4	0
3	A	202	BNG	4	0
8	B	211	1PE	6	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.

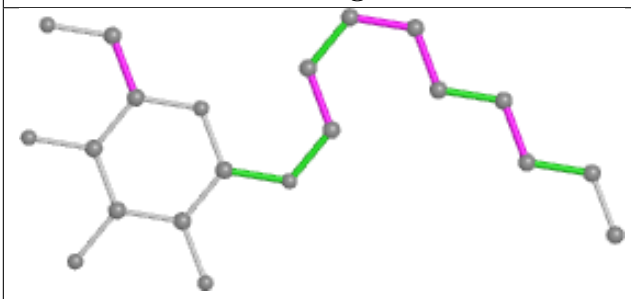
Ligand BNG B 203



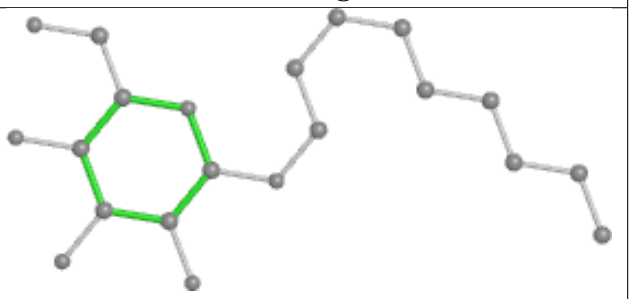
Bond lengths



Bond angles

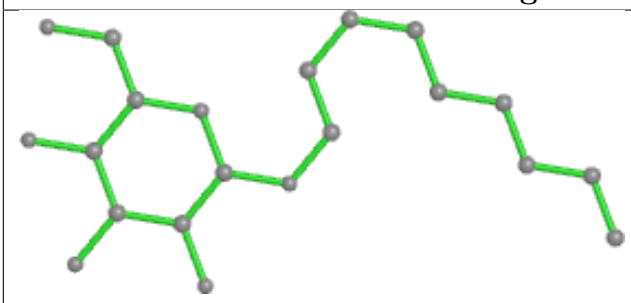


Torsions

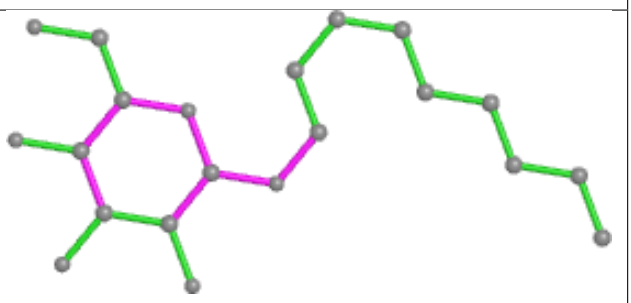


Rings

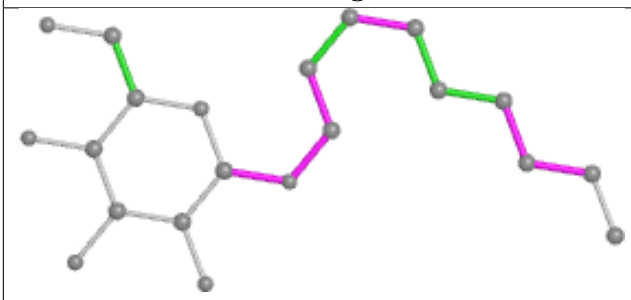
Ligand BNG A 203



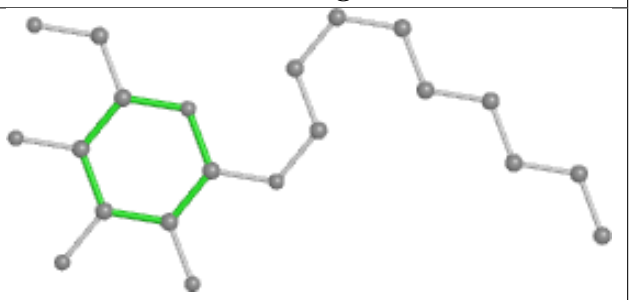
Bond lengths



Bond angles



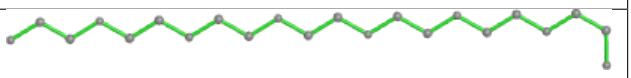
Torsions



Rings

Ligand P33 B 208

Bond lengths

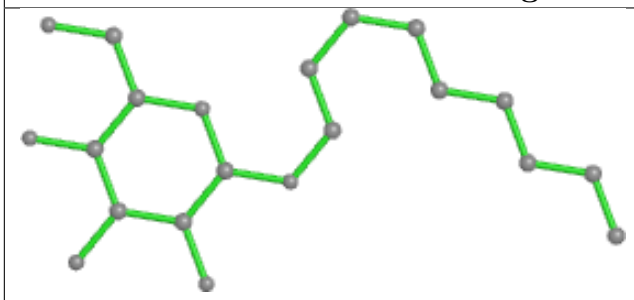


Bond angles

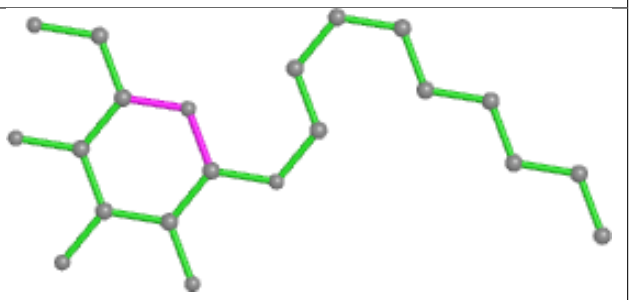
Torsions

Rings

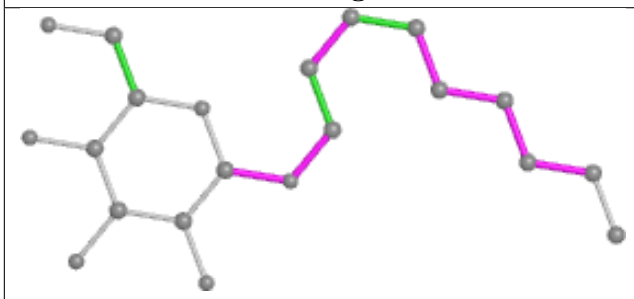
Ligand BNG A 204



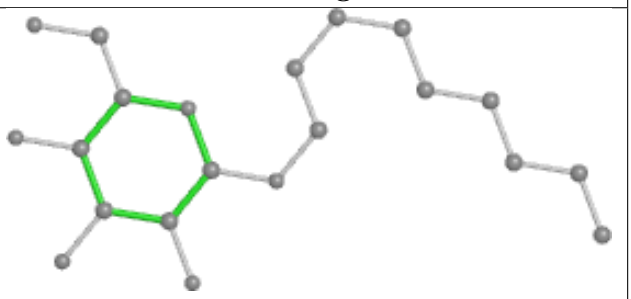
Bond lengths



Bond angles

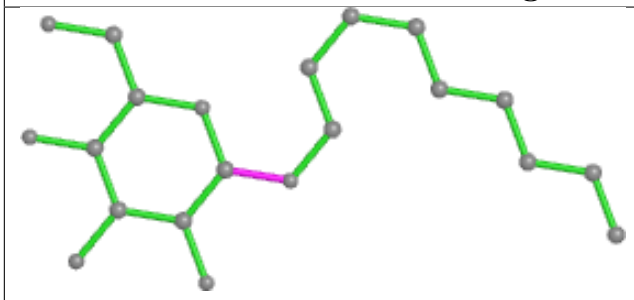


Torsions

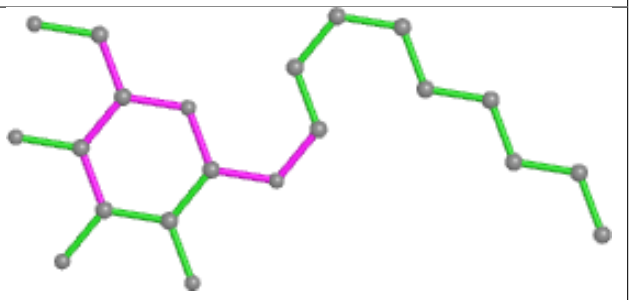


Rings

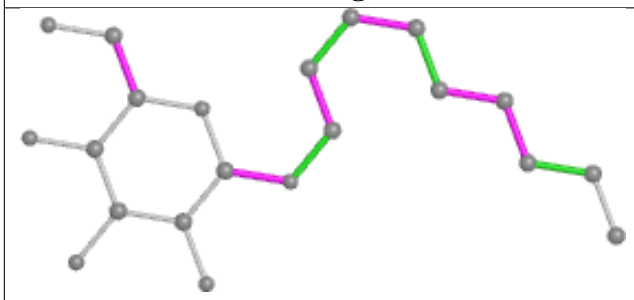
Ligand BNG B 202



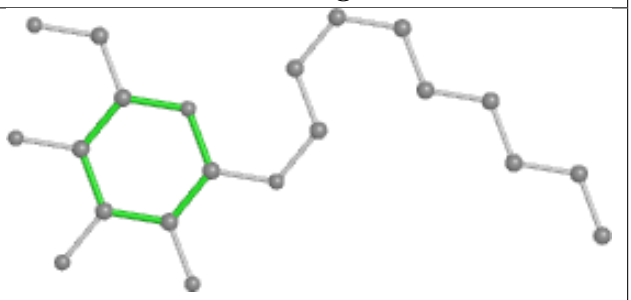
Bond lengths



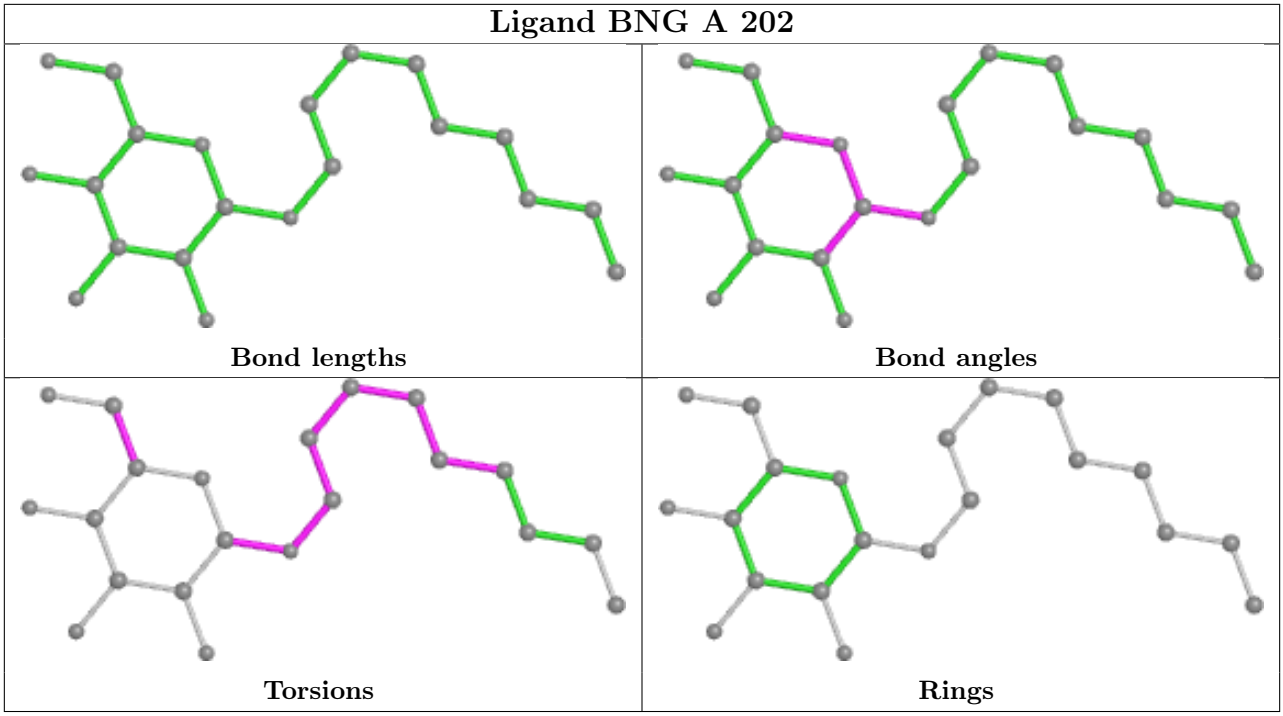
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	176/182 (96%)	-0.63	1 (0%)	89	88	33, 50, 80, 126	0
1	B	176/182 (96%)	-0.51	2 (1%)	80	79	34, 52, 87, 119	0
All	All	352/364 (96%)	-0.57	3 (0%)	84	82	33, 51, 86, 126	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	9	ARG	2.7
1	B	175	LYS	2.2
1	A	182	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 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	PGE	A	216	10/10	0.72	0.27	76,90,95,95	0
5	PEG	B	206	7/7	0.79	0.16	61,76,87,87	0

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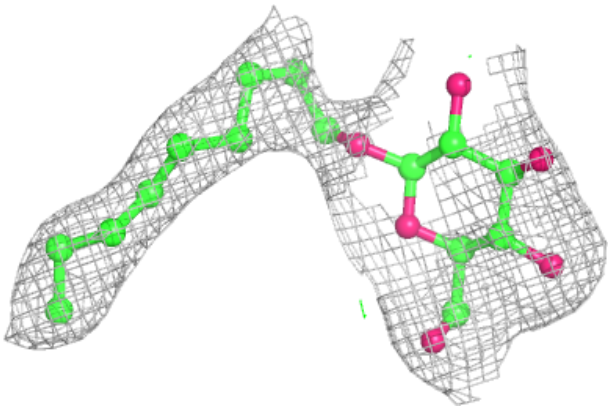
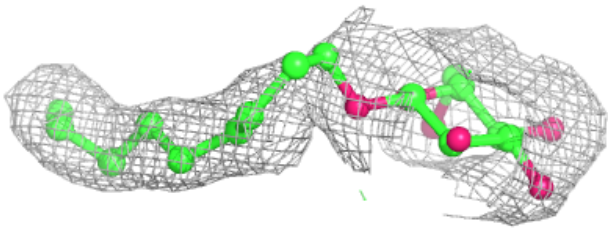
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	PGE	B	210	10/10	0.79	0.22	87,95,99,100	0
4	PG0	B	204	8/8	0.80	0.33	65,78,88,91	0
5	PEG	A	211	7/7	0.81	0.31	68,84,92,92	0
3	BNG	A	204	21/21	0.82	0.18	47,95,116,118	0
3	BNG	A	202	21/21	0.84	0.19	42,73,103,106	0
7	PGE	A	217	10/10	0.84	0.25	81,93,100,101	0
7	PGE	B	209	10/10	0.84	0.12	71,77,89,92	0
7	PGE	A	214	10/10	0.84	0.11	81,88,102,102	0
6	PG4	B	207	13/13	0.85	0.16	67,75,92,92	0
5	PEG	A	212	7/7	0.86	0.16	66,84,88,89	0
5	PEG	A	209	7/7	0.87	0.21	64,68,70,75	0
6	PG4	A	213	13/13	0.88	0.12	78,88,96,100	0
8	1PE	A	218[A]	16/16	0.88	0.21	48,58,61,61	16
8	1PE	A	218[B]	16/16	0.88	0.21	38,53,59,60	16
4	PG0	A	205	8/8	0.89	0.11	49,69,77,78	0
9	P33	B	208	22/22	0.89	0.17	40,53,61,68	22
5	PEG	B	205	7/7	0.90	0.26	64,73,96,102	0
3	BNG	A	203	21/21	0.90	0.17	28,57,69,71	21
4	PG0	A	206	8/8	0.91	0.25	73,76,82,82	0
3	BNG	B	202	21/21	0.92	0.17	51,76,94,103	0
7	PGE	A	215[A]	10/10	0.94	0.24	51,59,69,69	10
7	PGE	A	215[B]	10/10	0.94	0.24	43,64,73,75	10
8	1PE	B	211	16/16	0.94	0.18	49,74,80,82	0
5	PEG	A	207	7/7	0.94	0.22	73,76,79,79	0
5	PEG	A	210	7/7	0.95	0.29	75,77,90,90	0
3	BNG	B	203	21/21	0.95	0.21	41,57,64,67	0
5	PEG	A	208	7/7	0.96	0.17	70,73,76,76	0
10	CL	B	212	1/1	0.97	0.11	76,76,76,76	0
2	XX8	A	201	17/17	0.98	0.10	30,42,54,55	0
2	XX8	B	201	17/17	0.98	0.12	35,40,49,54	0

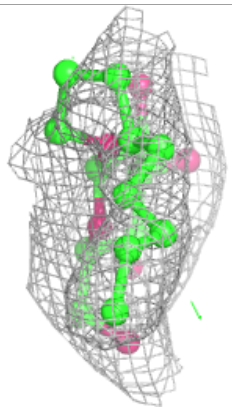
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BNG A 204:

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

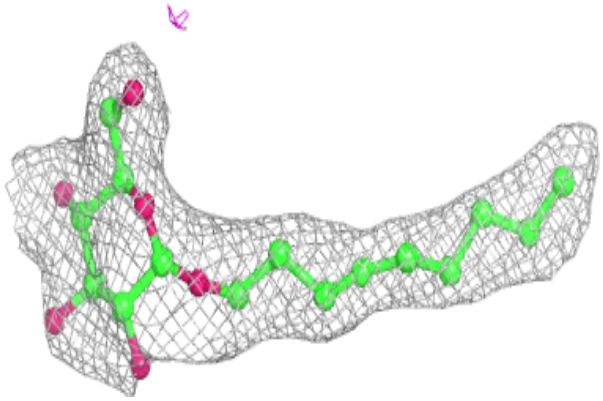


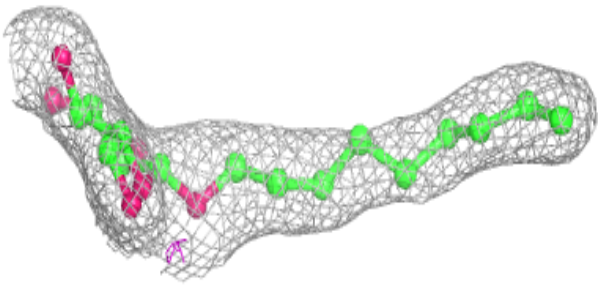


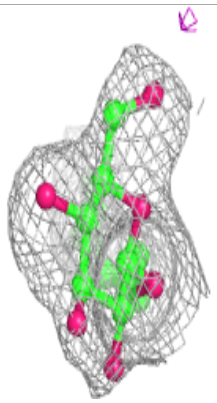


Electron density around BNG A 202:

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

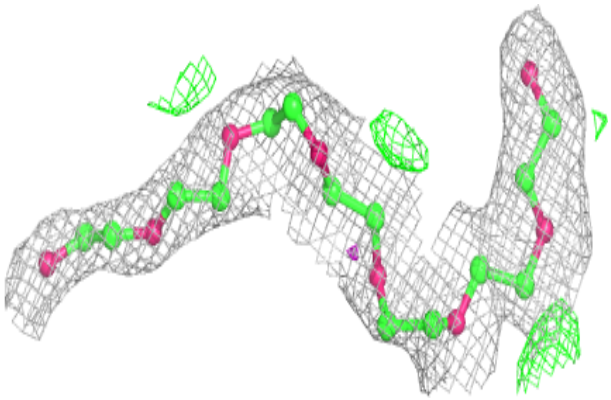


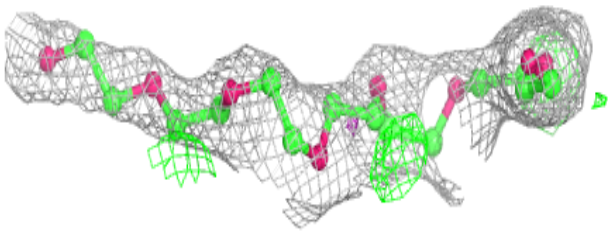


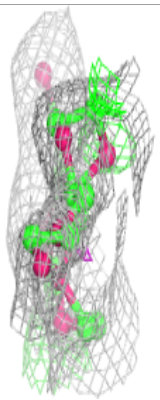


Electron density around P33 B 208:

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

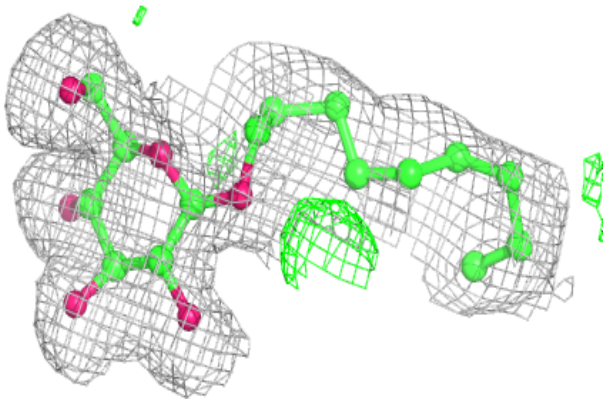


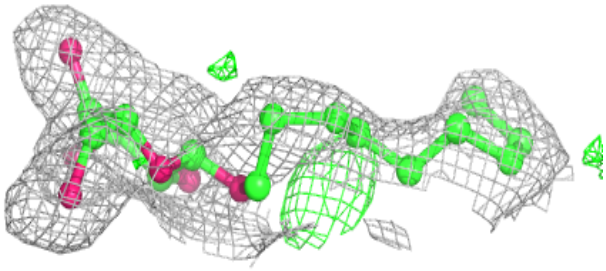


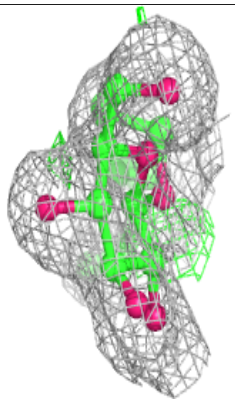


Electron density around BNG A 203:

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

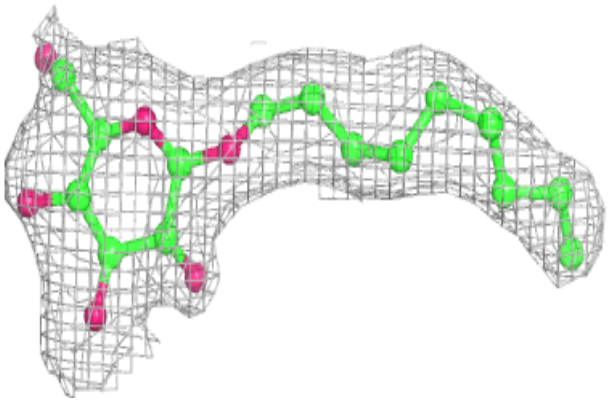


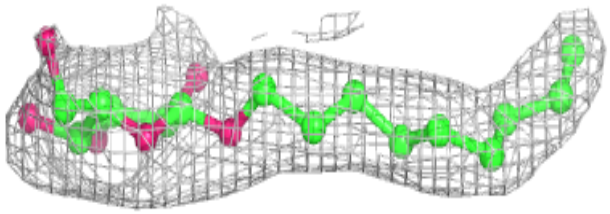


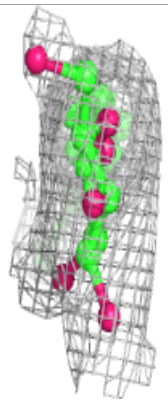


Electron density around BNG B 202:

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

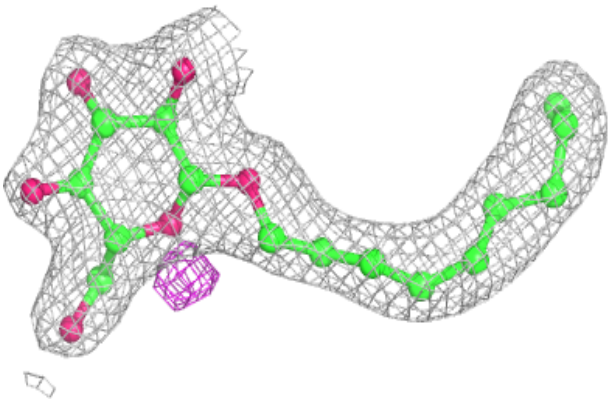


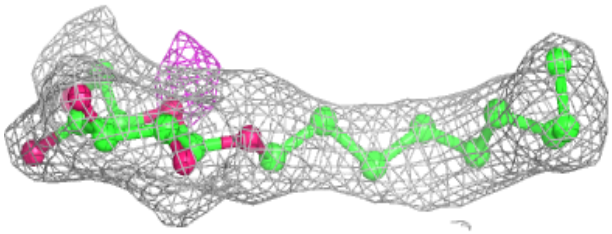


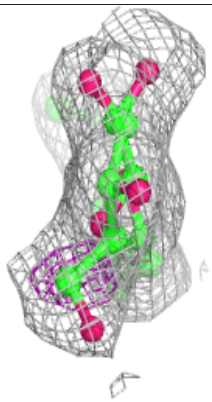


Electron density around BNG B 203:

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







6.5 Other polymers (i)

There are no such residues in this entry.