



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 02:39 PM BST

PDB ID : 4MHW
Title : Crystal structure of ThiT with small molecule BAT-25
Authors : Swier, L.J.Y.M.; Guskov, A.; Slotboom, D.J.
Deposited on : 2013-08-30
Resolution : 2.50 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.13.1
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) : 2.13.1

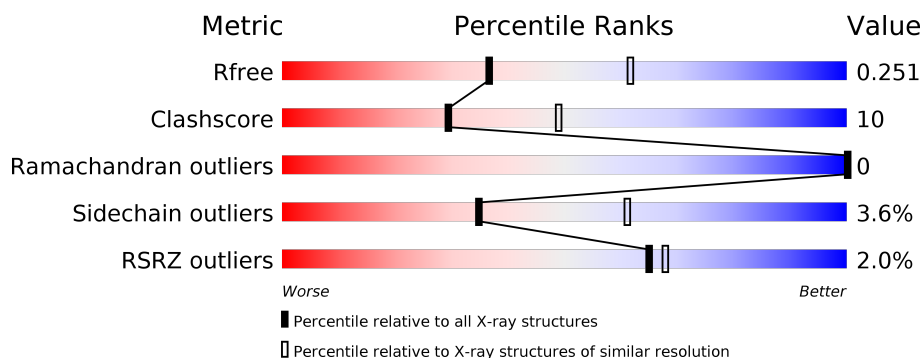
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on 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	192	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>12%</div> <div>8%</div> </div> </div>
1	B	192	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>10%</div> <div>8%</div> </div> </div>

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	P6G	A	204	-	-	X	-
6	PEG	B	209	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 3207 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.

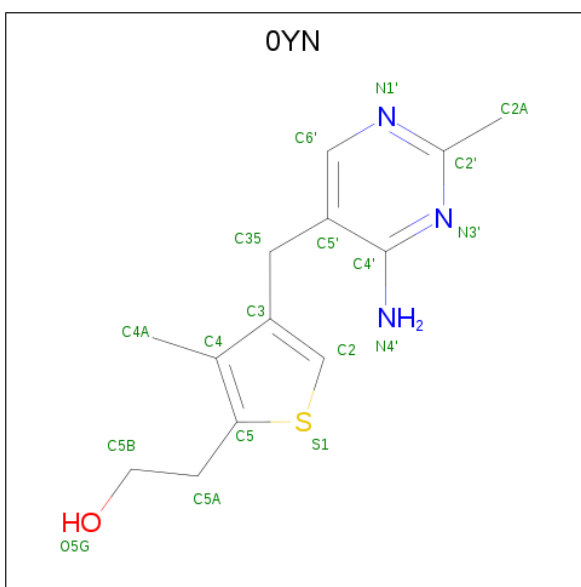
- Molecule 1 is a protein called Thiamine transporter ThiT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	177	Total	C	N	O	S	0	0	0
			1377	945	214	215	3			
1	B	176	Total	C	N	O	S	0	0	0
			1366	936	213	214	3			

There are 20 discrepancies between the modelled and reference sequences:

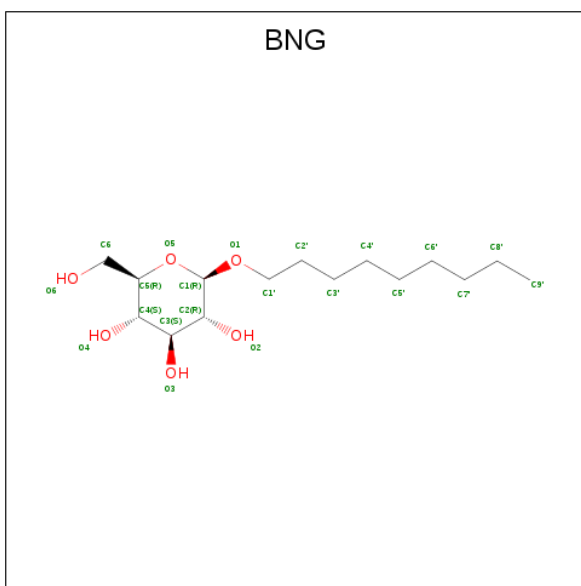
Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	expression tag	UNP D8KFM5
A	-8	HIS	-	expression tag	UNP D8KFM5
A	-7	HIS	-	expression tag	UNP D8KFM5
A	-6	HIS	-	expression tag	UNP D8KFM5
A	-5	HIS	-	expression tag	UNP D8KFM5
A	-4	HIS	-	expression tag	UNP D8KFM5
A	-3	HIS	-	expression tag	UNP D8KFM5
A	-2	HIS	-	expression tag	UNP D8KFM5
A	-1	HIS	-	expression tag	UNP D8KFM5
A	0	ALA	-	expression tag	UNP D8KFM5
B	-9	MET	-	expression tag	UNP D8KFM5
B	-8	HIS	-	expression tag	UNP D8KFM5
B	-7	HIS	-	expression tag	UNP D8KFM5
B	-6	HIS	-	expression tag	UNP D8KFM5
B	-5	HIS	-	expression tag	UNP D8KFM5
B	-4	HIS	-	expression tag	UNP D8KFM5
B	-3	HIS	-	expression tag	UNP D8KFM5
B	-2	HIS	-	expression tag	UNP D8KFM5
B	-1	HIS	-	expression tag	UNP D8KFM5
B	0	ALA	-	expression tag	UNP D8KFM5

- Molecule 2 is 2-{4-[(4-amino-2-methylpyrimidin-5-yl)methyl]-3-methylthiophen-2-yl}ethanol (three-letter code: 0YN) (formula: C₁₃H₁₇N₃OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			18	13	3	1	1		
2	B	1	Total	C	N	O	S	0	0
			18	13	3	1	1		

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



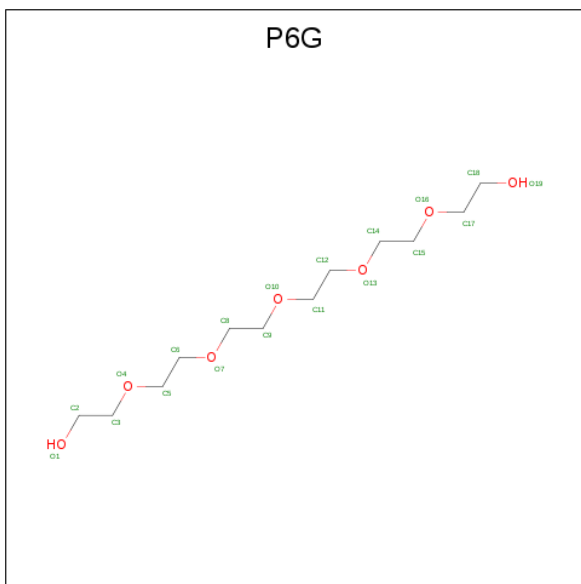
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	15	6		
3	B	1	Total	C	O	0	0
			21	15	6		

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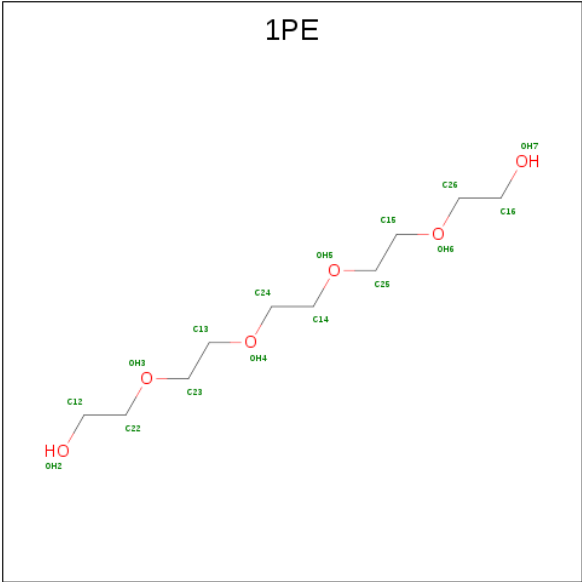
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			21	15	6		

- Molecule 4 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



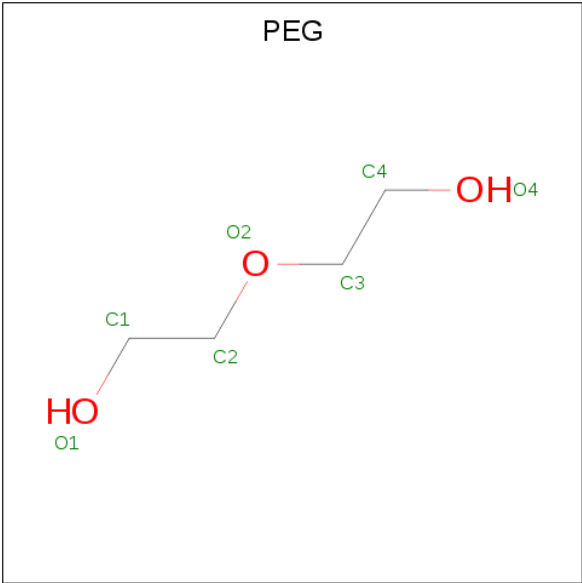
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			19	12	7		
4	A	1	Total	C	O	0	0
			19	12	7		

- Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			16	10	6		
5	B	1	Total	C	O	0	0
			16	10	6		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



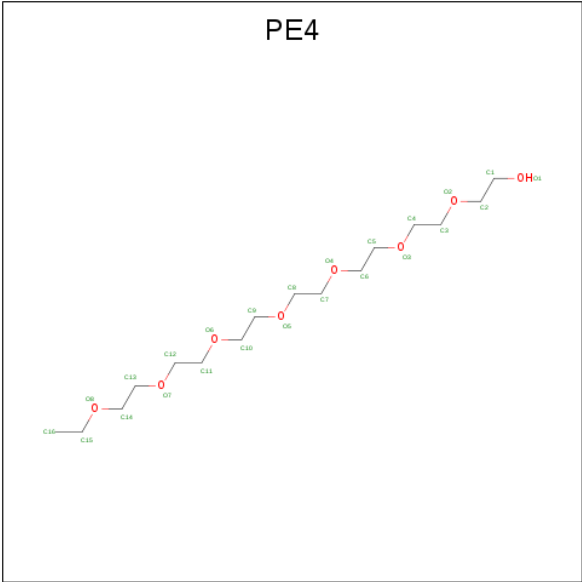
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		

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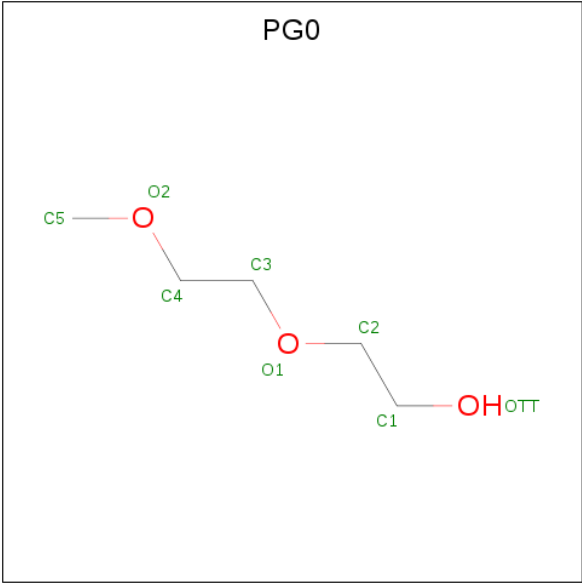
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total	C	O	0	0
			7	4	3		
6	B	1	Total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

- Molecule 7 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: C₁₆H₃₄O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			24	16	8		

- Molecule 8 is 2-(2-METHOXYETHOXY)ETHANOL (three-letter code: PG0) (formula: C₅H₁₂O₃).



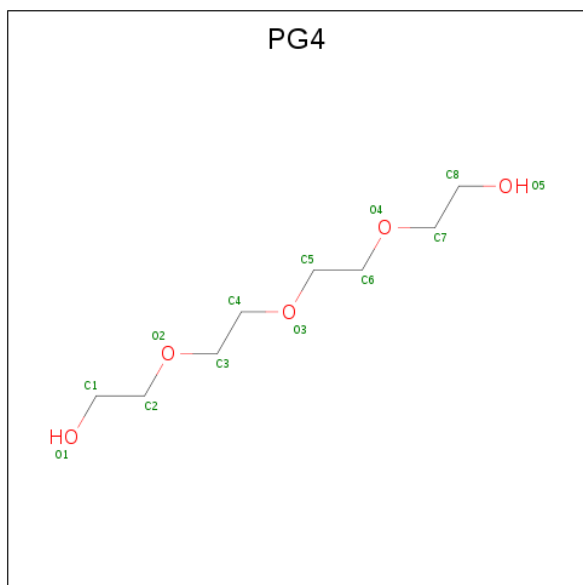
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			8	5	3		
8	B	1	Total	C	O	0	0
			8	5	3		

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

- Molecule 9 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	29	Total	O	0	1
			30	30		

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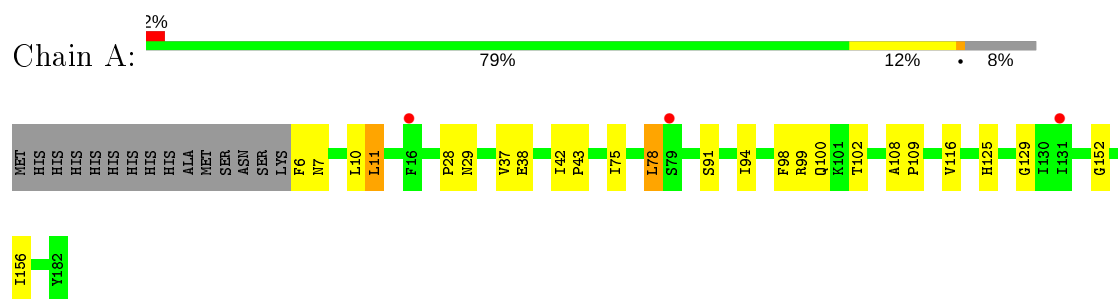
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	22	Total	O	0	2
			24	24		

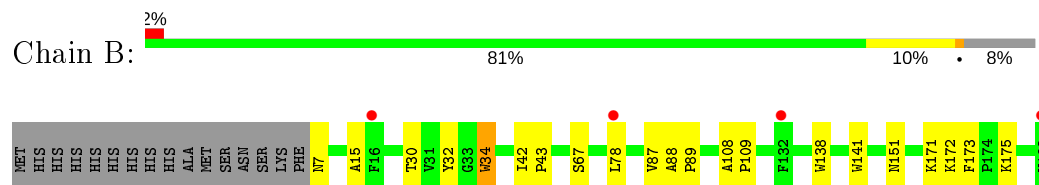
3 Residue-property plots [i](#)

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 transporter ThiT



- Molecule 1: Thiamine transporter ThiT



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	63.73Å 84.09Å 128.81Å 90.00° 94.58° 90.00°	Depositor
Resolution (Å)	42.80 – 2.50 48.21 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (42.80-2.50) 99.6 (48.21-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.188 , 0.250 0.192 , 0.251	Depositor DCC
R_{free} test set	1174 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	45.1	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 81.6	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	3207	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.27% 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: 0YN, PE4, 1PE, PG4, P6G, PG0, PEG, BNG

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	0.67	0/1416	0.69	0/1930
1	B	0.61	0/1404	0.68	0/1914
All	All	0.64	0/2820	0.69	0/3844

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	1377	0	1471	25	0
1	B	1366	0	1462	15	0
2	A	18	0	17	1	0
2	B	18	0	17	0	0
3	A	21	0	30	2	0
3	B	42	0	60	5	0
4	A	38	0	52	18	0
5	A	16	0	22	2	0
5	B	16	0	22	4	0
6	A	42	0	54	4	0
6	B	70	0	91	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	24	0	34	0	0
8	A	8	0	12	2	0
8	B	32	0	48	3	0
9	A	39	0	54	9	0
9	B	26	0	36	4	0
10	A	30	0	0	0	0
10	B	24	0	0	1	0
All	All	3207	0	3482	63	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 10.

All (63) 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)
4:A:204:P6G:H121	9:B:220:PG4:H12	1.17	1.10
1:A:94:ILE:HD11	4:A:203:P6G:H92	1.47	0.92
1:B:30:THR:OG1	8:B:216:PG0:H12	1.80	0.81
1:A:152:GLY:HA3	4:A:204:P6G:H91	1.64	0.79
9:A:214:PG4:H32	9:A:215:PG4:H41	1.66	0.77
4:A:204:P6G:H61	4:A:204:P6G:C11	2.19	0.73
4:A:204:P6G:H121	9:B:220:PG4:C1	2.10	0.71
1:A:116:VAL:CG1	4:A:203:P6G:H81	2.26	0.66
1:A:94:ILE:CD1	4:A:203:P6G:H92	2.26	0.63
1:A:75:ILE:HG21	9:A:214:PG4:H41	1.81	0.62
4:A:204:P6G:C14	6:B:209:PEG:H41	2.31	0.61
1:B:87:VAL:HG13	8:B:215:PG0:H51	1.83	0.60
1:A:156:ILE:HG13	4:A:204:P6G:H171	1.85	0.59
1:B:138:TRP:CZ2	6:B:207:PEG:H42	2.39	0.57
1:A:28:PRO:HB2	5:A:205:1PE:H122	1.86	0.57
1:B:141:TRP:CE2	5:B:204:1PE:H242	2.40	0.56
1:A:91:SER:HA	6:A:207:PEG:H31	1.88	0.55
4:A:204:P6G:H142	6:B:209:PEG:H41	1.88	0.55
5:B:204:1PE:H162	5:B:204:1PE:H251	1.88	0.54
1:A:78:LEU:HD13	9:A:214:PG4:H21	1.89	0.54
5:B:204:1PE:C16	5:B:204:1PE:H251	2.38	0.53
4:A:204:P6G:H141	6:B:209:PEG:H41	1.91	0.52
1:B:15:ALA:HB1	3:B:203:BNG:H5	1.91	0.52
3:B:203:BNG:O4	3:B:203:BNG:O6	2.18	0.52
6:A:211:PEG:C4	9:A:216:PG4:H41	2.41	0.51
3:A:202:BNG:H1	3:A:202:BNG:H3'2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:GLY:CA	4:A:204:P6G:H91	2.41	0.49
1:A:116:VAL:HG11	4:A:203:P6G:H81	1.94	0.48
1:A:116:VAL:HG13	4:A:203:P6G:H51	1.97	0.47
1:B:32:TYR:CE1	6:B:207:PEG:H31	2.49	0.47
4:A:204:P6G:H61	4:A:204:P6G:H111	1.96	0.47
1:B:172:LYS:HD2	1:B:173:PHE:CE2	2.49	0.47
1:B:15:ALA:HB1	3:B:203:BNG:H3	1.97	0.46
1:A:78:LEU:HD13	9:A:214:PG4:C2	2.47	0.45
3:A:202:BNG:H3'2	3:A:202:BNG:C1	2.48	0.44
1:B:34:TRP:CZ3	8:B:216:PG0:H21	2.52	0.44
6:A:211:PEG:H42	9:A:216:PG4:H41	1.99	0.44
1:A:78:LEU:CD1	9:A:214:PG4:H21	2.47	0.44
1:A:38:GLU:OE2	2:A:201:OYN:H13	2.17	0.44
4:A:204:P6G:H61	4:A:204:P6G:H112	1.96	0.43
3:B:202:BNG:H6'1	3:B:202:BNG:H9'3	1.74	0.43
1:B:141:TRP:NE1	5:B:204:1PE:H242	2.34	0.43
1:B:42:ILE:HB	1:B:43:PRO:HD3	2.01	0.43
6:A:211:PEG:H41	9:A:216:PG4:H41	2.00	0.42
5:A:205:1PE:H132	9:A:216:PG4:H61	2.01	0.42
1:A:108:ALA:HB3	1:A:109:PRO:HD3	2.02	0.42
1:A:116:VAL:HG13	4:A:203:P6G:H81	2.01	0.42
1:B:108:ALA:HB3	1:B:109:PRO:HD3	2.01	0.42
1:A:10:LEU:HD21	8:A:213:PG0:H32	2.01	0.42
1:A:29:ASN:HB2	1:A:37:VAL:O	2.20	0.42
6:B:213:PEG:O4	6:B:214:PEG:H42	2.20	0.42
1:A:125:HIS:O	1:A:129:GLY:N	2.49	0.41
1:A:10:LEU:HD21	8:A:213:PG0:C3	2.51	0.41
1:A:6:PHE:CD2	1:A:11:LEU:HD11	2.55	0.41
1:B:15:ALA:CB	3:B:203:BNG:H5	2.51	0.41
6:B:213:PEG:O4	6:B:214:PEG:H31	2.20	0.41
1:B:88:ALA:HB3	1:B:89:PRO:HD3	2.03	0.41
1:B:151:ASN:ND2	10:B:301:HOH:O	2.53	0.41
6:B:209:PEG:C3	9:B:220:PG4:H11	2.50	0.41
9:B:219:PG4:H62	9:B:219:PG4:H81	1.78	0.40
1:A:42:ILE:HB	1:A:43:PRO:HD3	2.03	0.40
1:A:98:PHE:CZ	4:A:203:P6G:H121	2.56	0.40
1:A:99:ARG:HG3	1:A:100:GLN:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	175/192 (91%)	172 (98%)	3 (2%)	0	100	100
1	B	174/192 (91%)	168 (97%)	6 (3%)	0	100	100
All	All	349/384 (91%)	340 (97%)	9 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	141/155 (91%)	137 (97%)	4 (3%)	43	70
1	B	140/155 (90%)	134 (96%)	6 (4%)	29	53
All	All	281/310 (91%)	271 (96%)	10 (4%)	35	61

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	11	LEU
1	A	78	LEU
1	A	102	THR
1	B	7	ASN
1	B	34	TRP
1	B	67	SER
1	B	78	LEU

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Mol	Chain	Res	Type
1	B	171	LYS
1	B	175	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	ASN
1	B	151	ASN

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](#)

36 ligands are modelled in this entry.

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	$\# Z > 2$
6	PEG	B	212	-	6,6,6	0.56	0	5,5,5	0.47	0
6	PEG	A	209	-	6,6,6	0.58	0	5,5,5	0.28	0
6	PEG	B	208	-	6,6,6	0.62	0	5,5,5	0.55	0
6	PEG	B	206	-	6,6,6	0.65	0	5,5,5	0.50	0
6	PEG	B	207	-	6,6,6	0.56	0	5,5,5	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BNG	A	202	-	21,21,21	0.83	0	26,26,26	1.05	0
2	OYN	B	201	-	17,19,19	2.85	3 (17%)	21,26,26	2.20	9 (42%)
7	PE4	A	212	-	23,23,23	0.80	0	22,22,22	0.34	0
2	OYN	A	201	-	17,19,19	2.27	4 (23%)	21,26,26	2.71	11 (52%)
6	PEG	A	207	-	6,6,6	0.65	0	5,5,5	0.52	0
9	PG4	A	216	-	12,12,12	0.74	0	11,11,11	0.36	0
4	P6G	A	204	-	18,18,18	0.72	0	17,17,17	0.50	0
3	BNG	B	203	-	21,21,21	0.88	0	26,26,26	0.99	1 (3%)
6	PEG	B	214	-	6,6,6	0.60	0	5,5,5	0.52	0
5	1PE	B	204	-	15,15,15	0.77	0	14,14,14	0.36	0
8	PG0	B	215	-	7,7,7	0.33	0	6,6,6	0.25	0
9	PG4	A	215	-	12,12,12	0.76	0	11,11,11	0.33	0
6	PEG	A	206	-	6,6,6	0.53	0	5,5,5	0.70	0
6	PEG	A	208	-	6,6,6	0.59	0	5,5,5	0.40	0
6	PEG	B	205	-	6,6,6	0.57	0	5,5,5	0.40	0
6	PEG	B	213	-	6,6,6	0.52	0	5,5,5	0.60	0
9	PG4	A	214	-	12,12,12	0.75	0	11,11,11	0.61	0
9	PG4	B	219	-	12,12,12	0.77	0	11,11,11	0.34	0
6	PEG	B	210	-	6,6,6	0.62	0	5,5,5	0.40	0
8	PG0	B	216	-	7,7,7	0.50	0	6,6,6	0.48	0
8	PG0	B	218	-	7,7,7	0.40	0	6,6,6	0.45	0
6	PEG	A	210	-	6,6,6	0.53	0	5,5,5	1.03	0
6	PEG	B	211	-	6,6,6	0.62	0	5,5,5	0.25	0
6	PEG	B	209	-	6,6,6	0.64	0	5,5,5	0.41	0
8	PG0	B	217	-	7,7,7	0.36	0	6,6,6	0.48	0
8	PG0	A	213	-	7,7,7	0.25	0	6,6,6	0.17	0
9	PG4	B	220	-	12,12,12	0.81	0	11,11,11	0.48	0
4	P6G	A	203	-	18,18,18	0.79	0	17,17,17	0.39	0
6	PEG	A	211	-	6,6,6	0.59	0	5,5,5	0.36	0
5	1PE	A	205	-	15,15,15	0.81	0	14,14,14	0.43	0
3	BNG	B	202	-	21,21,21	0.85	0	26,26,26	1.39	2 (7%)

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
6	PEG	B	212	-	-	3/4/4/4	-
6	PEG	A	209	-	-	2/4/4/4	-
6	PEG	B	208	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PEG	B	206	-	-	2/4/4/4	-
6	PEG	B	207	-	-	3/4/4/4	-
3	BNG	A	202	-	-	8/12/32/32	0/1/1/1
2	0YN	B	201	-	-	3/6/7/7	0/2/2/2
7	PE4	A	212	-	-	11/21/21/21	-
2	0YN	A	201	-	-	2/6/7/7	0/2/2/2
6	PEG	A	207	-	-	3/4/4/4	-
9	PG4	A	216	-	-	4/10/10/10	-
4	P6G	A	204	-	-	8/16/16/16	-
3	BNG	B	203	-	-	4/12/32/32	0/1/1/1
6	PEG	B	214	-	-	3/4/4/4	-
5	1PE	B	204	-	-	7/13/13/13	-
8	PG0	B	215	-	-	1/5/5/5	-
9	PG4	A	215	-	-	4/10/10/10	-
6	PEG	A	206	-	-	3/4/4/4	-
6	PEG	A	208	-	-	4/4/4/4	-
6	PEG	B	205	-	-	2/4/4/4	-
6	PEG	B	213	-	-	1/4/4/4	-
9	PG4	A	214	-	-	7/10/10/10	-
9	PG4	B	219	-	-	4/10/10/10	-
6	PEG	B	210	-	-	1/4/4/4	-
8	PG0	B	216	-	-	5/5/5/5	-
8	PG0	B	218	-	-	3/5/5/5	-
6	PEG	A	210	-	-	4/4/4/4	-
6	PEG	B	211	-	-	3/4/4/4	-
6	PEG	B	209	-	-	0/4/4/4	-
8	PG0	B	217	-	-	1/5/5/5	-
8	PG0	A	213	-	-	3/5/5/5	-
9	PG4	B	220	-	-	8/10/10/10	-
4	P6G	A	203	-	-	10/16/16/16	-
6	PEG	A	211	-	-	1/4/4/4	-
5	1PE	A	205	-	-	5/13/13/13	-
3	BNG	B	202	-	-	5/12/32/32	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	0YN	C2-C3	10.56	1.43	1.37
2	A	201	0YN	C2-C3	7.14	1.41	1.37
2	A	201	0YN	C4'-N4'	4.02	1.44	1.34
2	B	201	0YN	C5A-C5	3.30	1.52	1.50
2	B	201	0YN	C4'-N4'	3.10	1.41	1.34
2	A	201	0YN	C5A-C5	2.84	1.52	1.50
2	A	201	0YN	C2'-N1'	-2.24	1.30	1.34

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	0YN	C3-C2-S1	-7.81	103.94	112.26
2	B	201	0YN	C3-C2-S1	-4.69	107.27	112.26
3	B	202	BNG	C3-C4-C5	-4.37	102.45	110.24
2	A	201	0YN	C2'-N3'-C4'	3.71	123.87	118.08
2	B	201	0YN	C35-C3-C4	-3.63	120.00	126.49
2	A	201	0YN	C35-C3-C4	-3.62	120.03	126.49
2	B	201	0YN	C6'-N1'-C2'	3.47	121.87	115.96
2	A	201	0YN	C5'-C4'-N3'	-3.24	116.15	121.24
2	A	201	0YN	C6'-N1'-C2'	3.15	121.32	115.96
2	A	201	0YN	C2A-C2'-N3'	2.86	121.61	117.15
2	B	201	0YN	C5'-C6'-N1'	-2.85	119.07	123.82
2	A	201	0YN	C5'-C6'-N1'	-2.82	119.13	123.82
2	A	201	0YN	N1'-C2'-N3'	-2.77	120.78	125.54
2	B	201	0YN	C5A-C5-C4	-2.72	120.32	127.45
2	B	201	0YN	N1'-C2'-N3'	-2.66	120.95	125.54
2	B	201	0YN	C35-C5'-C6'	-2.32	118.53	121.73
2	B	201	0YN	C2'-N3'-C4'	2.26	121.61	118.08
3	B	203	BNG	O5-C1-C2	2.26	115.14	110.35
2	A	201	0YN	N4'-C4'-N3'	2.21	120.16	117.03
2	A	201	0YN	C35-C5'-C6'	-2.20	118.68	121.73
2	A	201	0YN	C6'-C5'-C4'	2.17	118.67	115.72
2	B	201	0YN	C2A-C2'-N3'	2.02	120.31	117.15
3	B	202	BNG	C4-C3-C2	-2.02	107.30	110.82

There are no chirality outliers.

All (139) 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'
2	B	201	0YN	C4-C5-C5A-C5B

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Mol	Chain	Res	Type	Atoms
2	B	201	0YN	C5-C5A-C5B-O5G
2	A	201	0YN	C5-C5A-C5B-O5G
7	A	212	PE4	C12-C11-O6-C10
9	B	220	PG4	C3-C4-O3-C5
9	A	214	PG4	C5-C6-O4-C7
7	A	212	PE4	C7-C8-O5-C9
5	B	204	1PE	OH7-C16-C26-OH6
4	A	203	P6G	O16-C17-C18-O19
9	A	214	PG4	C6-C5-O3-C4
5	B	204	1PE	OH6-C15-C25-OH5
8	B	216	PG0	O1-C3-C4-O2
8	B	217	PG0	O1-C3-C4-O2
4	A	203	P6G	O4-C5-C6-O7
7	A	212	PE4	O6-C11-C12-O7
4	A	203	P6G	O10-C11-C12-O13
4	A	203	P6G	O13-C14-C15-O16
9	B	220	PG4	O2-C3-C4-O3
4	A	203	P6G	O7-C8-C9-O10
9	A	216	PG4	O2-C3-C4-O3
5	A	205	1PE	OH6-C15-C25-OH5
9	A	216	PG4	O3-C5-C6-O4
6	B	207	PEG	O2-C3-C4-O4
7	A	212	PE4	O2-C3-C4-O3
3	B	203	BNG	O5-C5-C6-O6
9	B	220	PG4	O3-C5-C6-O4
4	A	204	P6G	O4-C5-C6-O7
6	A	207	PEG	O2-C3-C4-O4
9	B	220	PG4	O4-C7-C8-O5
5	A	205	1PE	OH7-C16-C26-OH6
6	A	209	PEG	O1-C1-C2-O2
7	A	212	PE4	O1-C1-C2-O2
6	A	207	PEG	O1-C1-C2-O2
9	A	215	PG4	O1-C1-C2-O2
6	A	210	PEG	O2-C3-C4-O4
9	B	220	PG4	O1-C1-C2-O2
4	A	203	P6G	O1-C2-C3-O4
2	B	201	0YN	C4-C3-C35-C5'
2	A	201	0YN	C4-C3-C35-C5'
8	B	218	PG0	C3-C4-O2-C5
9	A	214	PG4	O2-C3-C4-O3
8	A	213	PG0	O1-C3-C4-O2
3	A	202	BNG	C2'-C3'-C4'-C5'

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Mol	Chain	Res	Type	Atoms
6	B	207	PEG	O1-C1-C2-O2
6	B	211	PEG	O1-C1-C2-O2
6	A	210	PEG	O1-C1-C2-O2
6	A	211	PEG	O1-C1-C2-O2
3	B	203	BNG	C5'-C6'-C7'-C8'
3	A	202	BNG	C2'-C1'-O1-C1
3	A	202	BNG	C1'-C2'-C3'-C4'
9	B	219	PG4	O2-C3-C4-O3
4	A	204	P6G	O7-C8-C9-O10
8	B	218	PG0	O1-C3-C4-O2
9	A	214	PG4	O4-C7-C8-O5
8	B	216	PG0	C4-C3-O1-C2
8	B	216	PG0	C3-C4-O2-C5
3	B	202	BNG	C2-C1-O1-C1'
6	B	212	PEG	O1-C1-C2-O2
6	A	208	PEG	O1-C1-C2-O2
6	B	205	PEG	O2-C3-C4-O4
8	B	216	PG0	OTT-C1-C2-O1
3	A	202	BNG	C5'-C6'-C7'-C8'
6	B	214	PEG	C4-C3-O2-C2
6	B	214	PEG	O2-C3-C4-O4
3	B	202	BNG	C4'-C5'-C6'-C7'
4	A	204	P6G	O10-C11-C12-O13
6	A	208	PEG	O2-C3-C4-O4
9	A	215	PG4	O3-C5-C6-O4
3	A	202	BNG	C6'-C7'-C8'-C9'
9	A	214	PG4	O3-C5-C6-O4
6	A	206	PEG	O1-C1-C2-O2
6	B	205	PEG	C1-C2-O2-C3
6	B	211	PEG	C1-C2-O2-C3
6	B	206	PEG	C1-C2-O2-C3
5	B	204	1PE	C12-C22-OH3-C23
7	A	212	PE4	C10-C9-O5-C8
6	B	208	PEG	C1-C2-O2-C3
5	B	204	1PE	C25-C15-OH6-C26
8	B	215	PG0	O1-C3-C4-O2
9	B	220	PG4	C6-C5-O3-C4
9	B	219	PG4	C3-C4-O3-C5
6	B	212	PEG	C4-C3-O2-C2
9	A	214	PG4	C4-C3-O2-C2
6	B	213	PEG	C1-C2-O2-C3
4	A	203	P6G	C9-C8-O7-C6

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Mol	Chain	Res	Type	Atoms
3	B	202	BNG	C6'-C7'-C8'-C9'
6	A	206	PEG	C4-C3-O2-C2
6	A	207	PEG	C1-C2-O2-C3
5	A	205	1PE	OH5-C14-C24-OH4
4	A	204	P6G	C6-C5-O4-C3
5	A	205	1PE	C25-C15-OH6-C26
9	A	216	PG4	O1-C1-C2-O2
6	B	214	PEG	O1-C1-C2-O2
4	A	203	P6G	C14-C15-O16-C17
6	A	206	PEG	C1-C2-O2-C3
3	A	202	BNG	C3'-C4'-C5'-C6'
8	A	213	PG0	C3-C4-O2-C5
6	B	207	PEG	C4-C3-O2-C2
3	B	203	BNG	C4'-C5'-C6'-C7'
6	A	208	PEG	C1-C2-O2-C3
4	A	204	P6G	O13-C14-C15-O16
7	A	212	PE4	O3-C5-C6-O4
8	A	213	PG0	C4-C3-O1-C2
5	A	205	1PE	C15-C25-OH5-C14
9	B	220	PG4	C1-C2-O2-C3
8	B	218	PG0	OTT-C1-C2-O1
3	B	202	BNG	O5-C1-O1-C1'
7	A	212	PE4	C9-C10-O6-C11
5	B	204	1PE	C23-C13-OH4-C24
9	A	214	PG4	C1-C2-O2-C3
4	A	203	P6G	C8-C9-O10-C11
6	A	210	PEG	C4-C3-O2-C2
7	A	212	PE4	C11-C12-O7-C13
7	A	212	PE4	O7-C13-C14-O8
6	A	210	PEG	C1-C2-O2-C3
8	B	216	PG0	C1-C2-O1-C3
3	B	203	BNG	C2'-C3'-C4'-C5'
4	A	204	P6G	C8-C9-O10-C11
6	B	211	PEG	C4-C3-O2-C2
6	B	206	PEG	C4-C3-O2-C2
4	A	204	P6G	C12-C11-O10-C9
6	A	208	PEG	C4-C3-O2-C2
9	B	220	PG4	C4-C3-O2-C2
4	A	204	P6G	O16-C17-C18-O19
3	B	202	BNG	C2'-C3'-C4'-C5'
9	A	215	PG4	C5-C6-O4-C7
5	B	204	1PE	OH4-C13-C23-OH3

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Mol	Chain	Res	Type	Atoms
7	A	212	PE4	O4-C7-C8-O5
6	A	209	PEG	O2-C3-C4-O4
4	A	203	P6G	C18-C17-O16-C15
9	B	219	PG4	C8-C7-O4-C6
6	B	210	PEG	O2-C3-C4-O4
9	A	216	PG4	C4-C3-O2-C2
6	B	212	PEG	O2-C3-C4-O4
5	B	204	1PE	OH5-C14-C24-OH4
9	A	215	PG4	O2-C3-C4-O3
9	B	219	PG4	O3-C5-C6-O4

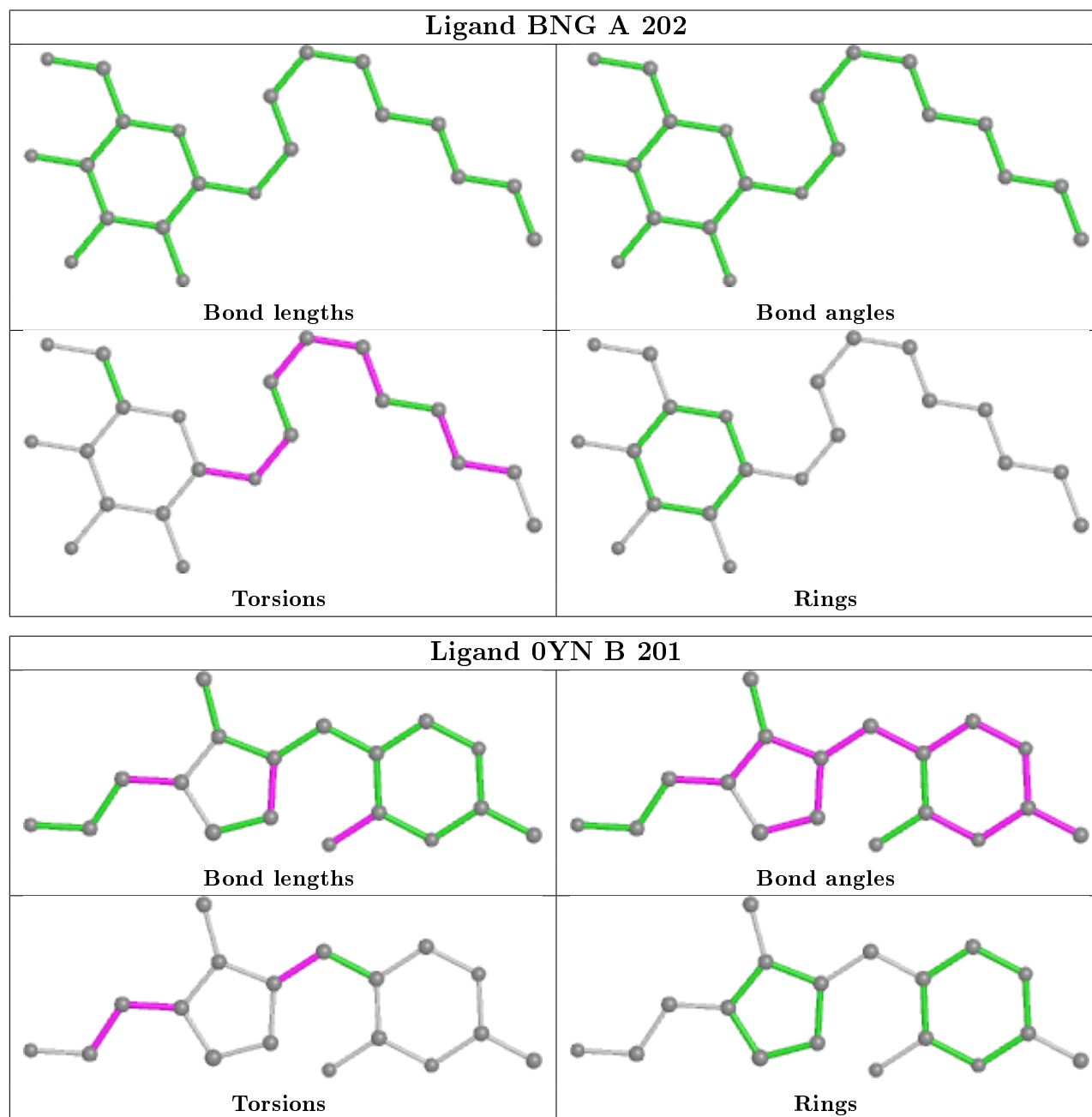
There are no ring outliers.

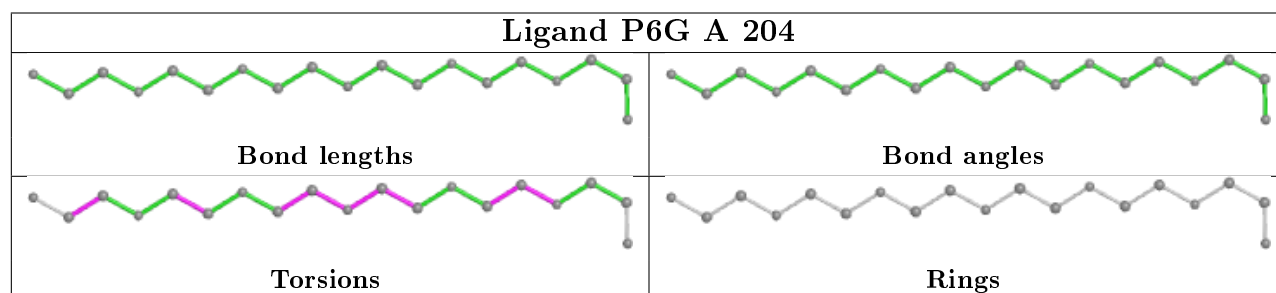
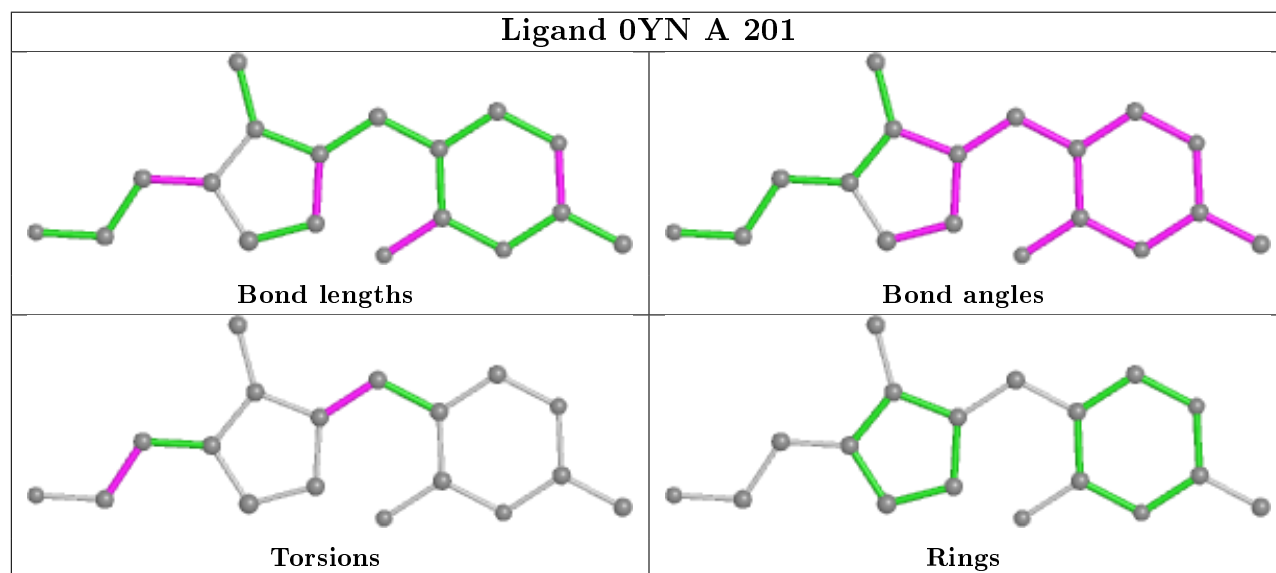
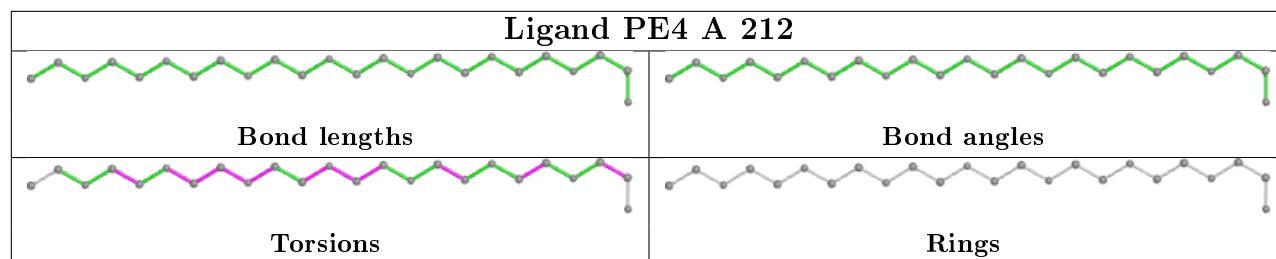
22 monomers are involved in 52 short contacts:

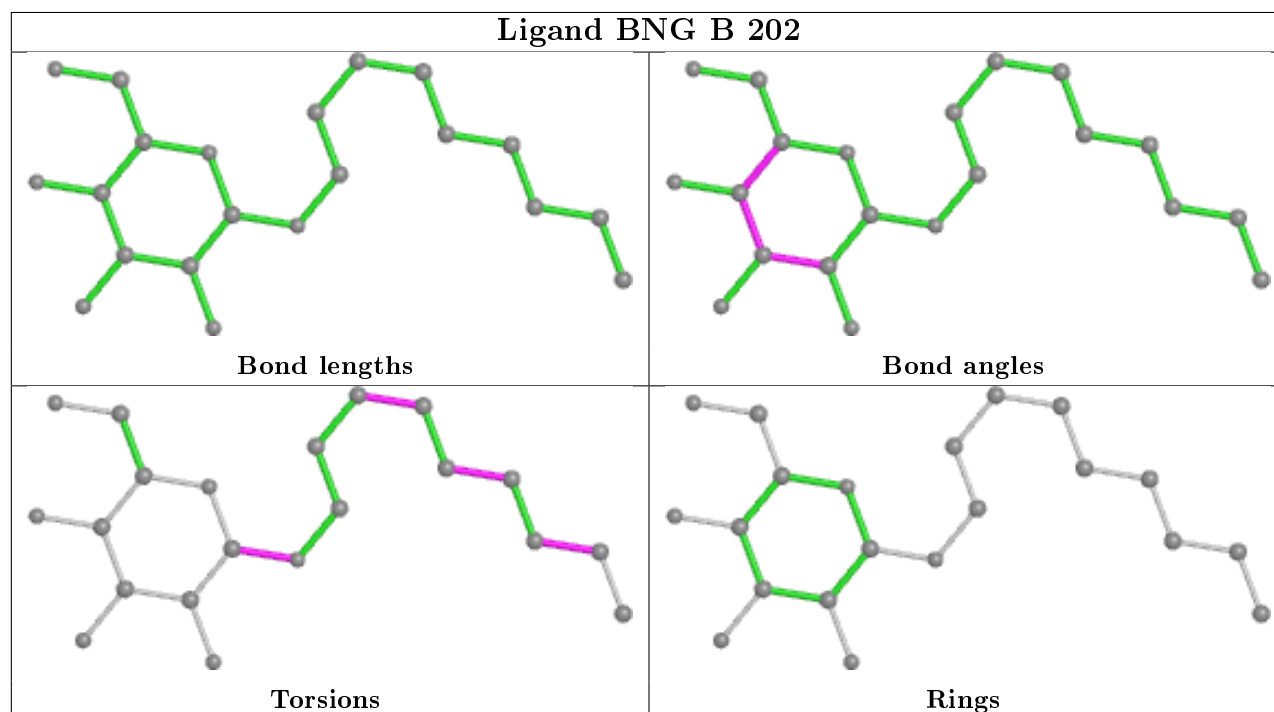
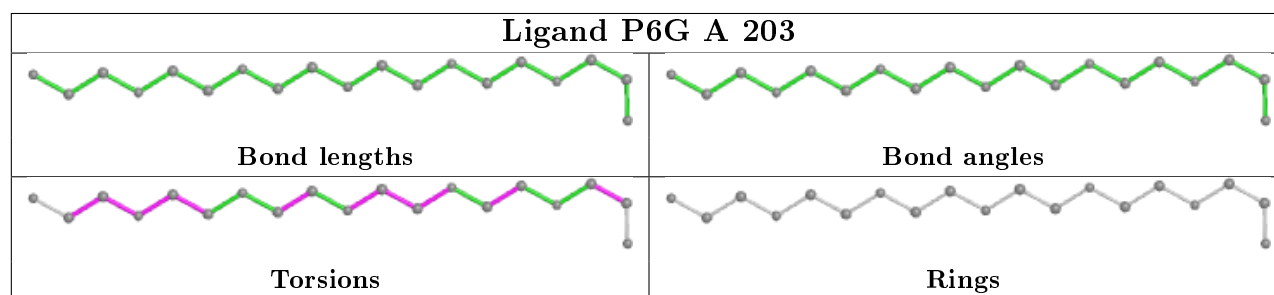
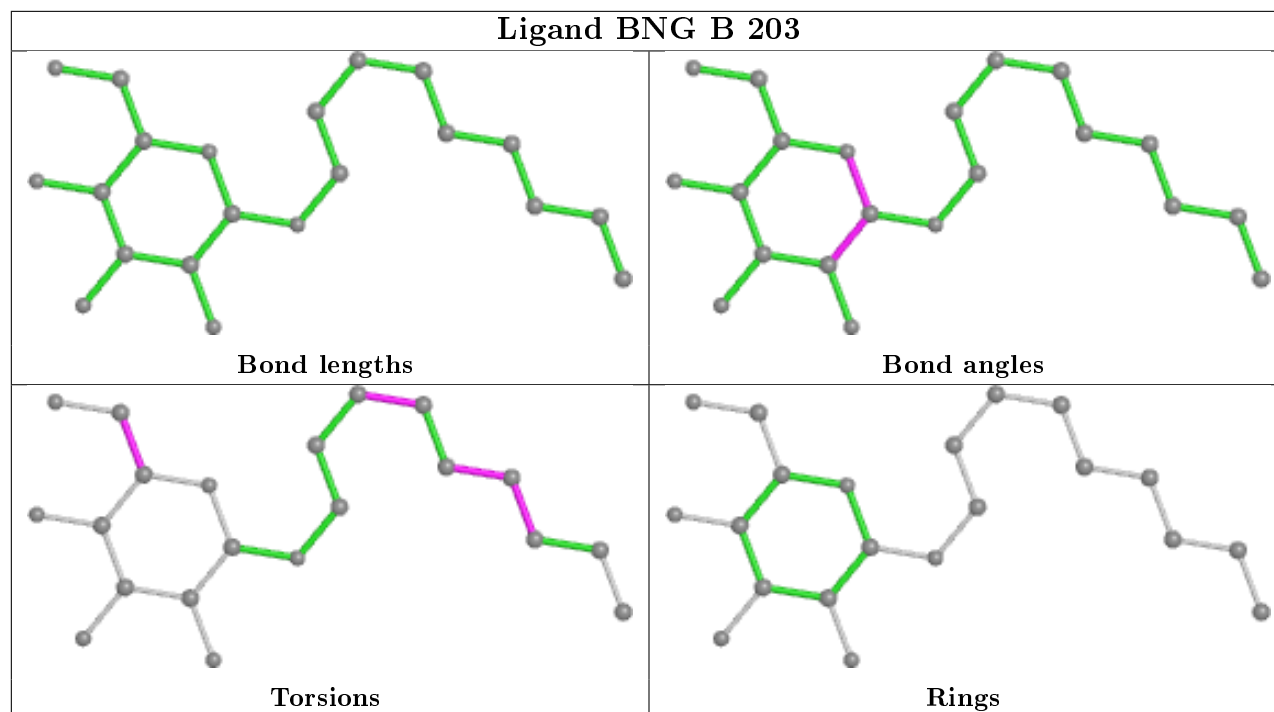
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	207	PEG	2	0
3	A	202	BNG	2	0
2	A	201	0YN	1	0
6	A	207	PEG	1	0
9	A	216	PG4	4	0
4	A	204	P6G	11	0
3	B	203	BNG	4	0
6	B	214	PEG	2	0
5	B	204	1PE	4	0
8	B	215	PG0	1	0
9	A	215	PG4	1	0
6	B	213	PEG	2	0
9	A	214	PG4	5	0
9	B	219	PG4	1	0
8	B	216	PG0	2	0
6	B	209	PEG	4	0
8	A	213	PG0	2	0
9	B	220	PG4	3	0
4	A	203	P6G	7	0
6	A	211	PEG	3	0
5	A	205	1PE	2	0
3	B	202	BNG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers

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 [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	177/192 (92%)	-0.22	3 (1%) 70 72	36, 53, 80, 152	0
1	B	176/192 (91%)	-0.21	4 (2%) 60 63	36, 55, 83, 123	0
All	All	353/384 (91%)	-0.21	7 (1%) 65 68	36, 54, 82, 152	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	132	PHE	2.6
1	B	16	PHE	2.5
1	A	16	PHE	2.5
1	B	182	TYR	2.4
1	B	78	LEU	2.4
1	A	79	SER	2.2
1	A	131	ILE	2.2

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](#)

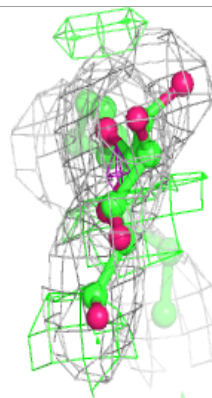
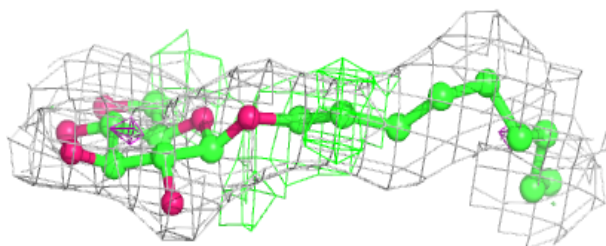
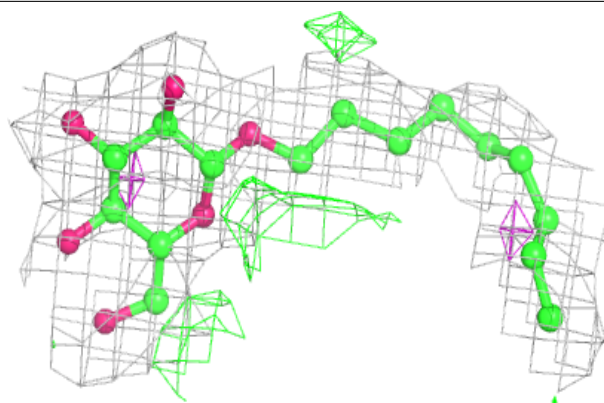
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	1PE	A	205	16/16	0.69	0.20	85,115,120,122	0
3	BNG	B	203	21/21	0.71	0.20	55,67,73,80	21
6	PEG	A	209	7/7	0.72	0.19	94,95,99,99	0
6	PEG	A	207	7/7	0.72	0.30	76,83,95,102	0
6	PEG	B	210	7/7	0.73	0.32	82,88,90,98	0
8	PG0	B	217	8/8	0.76	0.23	79,102,104,107	0
9	PG4	A	214	13/13	0.78	0.32	76,88,100,101	0
8	PG0	B	218	8/8	0.78	0.25	73,88,94,95	0
6	PEG	B	213	7/7	0.79	0.19	71,82,103,106	0
6	PEG	A	211	7/7	0.84	0.21	70,96,108,115	0
6	PEG	A	210	7/7	0.85	0.39	73,84,97,103	0
9	PG4	A	215	13/13	0.85	0.27	76,83,90,94	0
9	PG4	B	219	13/13	0.86	0.14	66,86,111,113	0
6	PEG	A	208	7/7	0.86	0.35	81,86,96,97	0
4	P6G	A	203	19/19	0.87	0.19	63,89,111,111	0
6	PEG	B	211	7/7	0.88	0.42	85,93,97,97	0
8	PG0	A	213	8/8	0.88	0.14	83,88,100,104	0
6	PEG	B	208	7/7	0.88	0.14	82,84,92,92	0
5	1PE	B	204	16/16	0.88	0.14	70,81,95,99	0
6	PEG	A	206	7/7	0.88	0.24	54,62,85,86	0
6	PEG	B	205	7/7	0.89	0.12	78,80,87,91	0
9	PG4	A	216	13/13	0.89	0.20	69,92,102,108	0
8	PG0	B	215	8/8	0.89	0.51	62,81,84,92	0
6	PEG	B	214	7/7	0.89	0.10	82,83,95,96	0
4	P6G	A	204	19/19	0.90	0.18	57,81,101,104	0
6	PEG	B	207	7/7	0.90	0.15	59,74,81,88	0
6	PEG	B	209	7/7	0.90	0.27	80,92,103,112	0
8	PG0	B	216	8/8	0.90	0.18	55,66,89,93	0
7	PE4	A	212	24/24	0.92	0.12	50,72,89,97	24
3	BNG	A	202	21/21	0.92	0.12	58,81,91,101	0
9	PG4	B	220	13/13	0.93	0.18	64,74,93,98	0
6	PEG	B	212	7/7	0.93	0.16	79,87,93,97	0
2	OYN	B	201	18/18	0.95	0.15	39,52,72,77	0
6	PEG	B	206	7/7	0.95	0.17	70,76,78,83	0
2	OYN	A	201	18/18	0.96	0.14	33,47,58,60	0
3	BNG	B	202	21/21	0.96	0.18	49,69,81,97	0

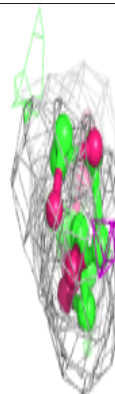
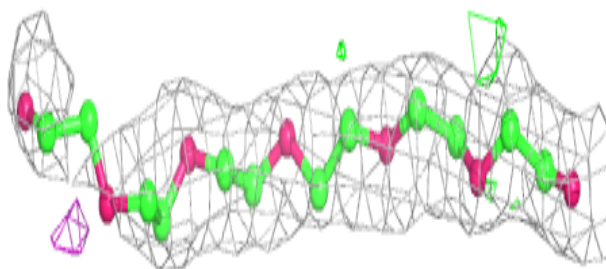
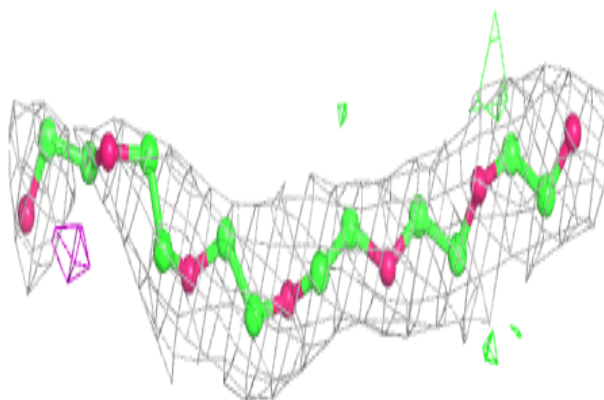
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BNG 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)

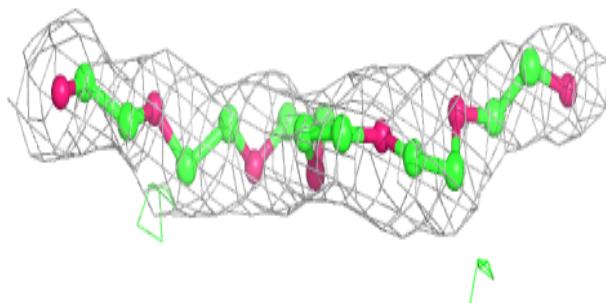
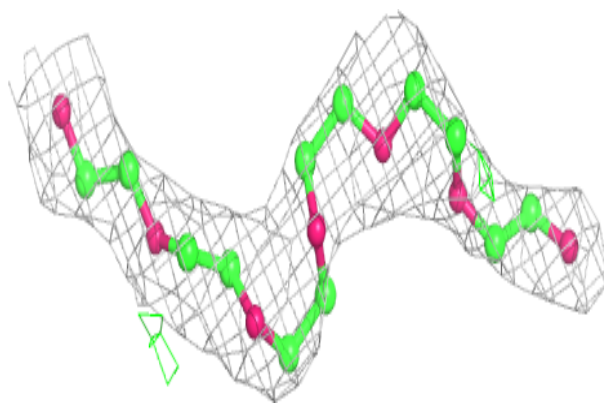
**Electron density around P6G A 203:**

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

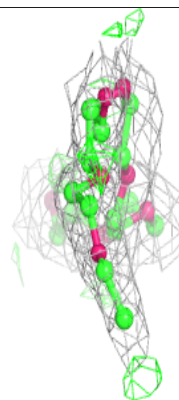
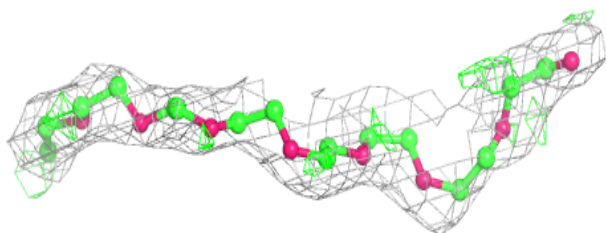
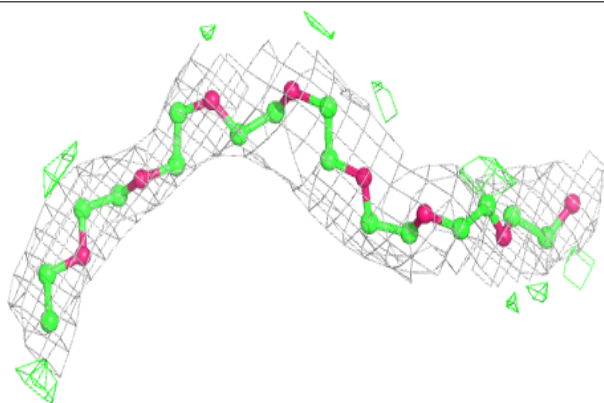


Electron density around P6G A 204:

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

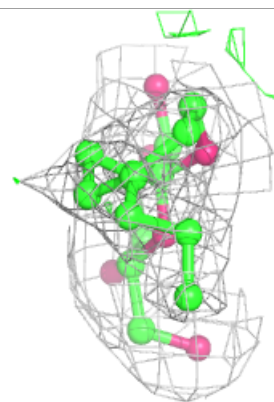
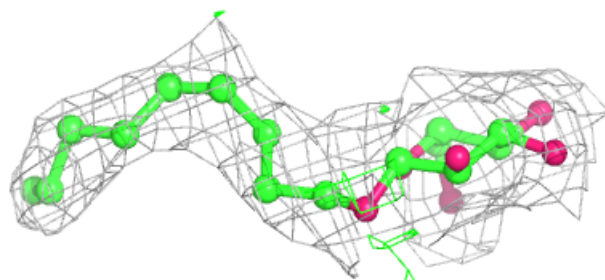
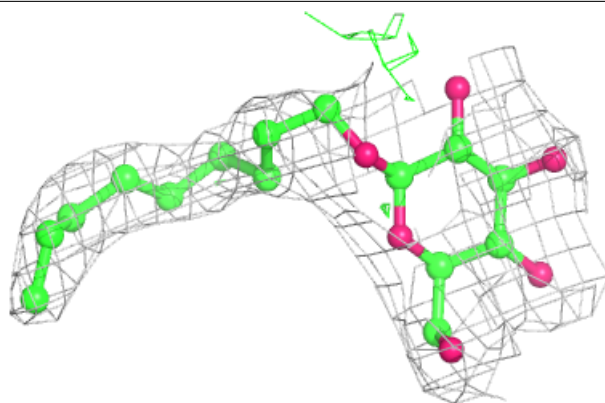
**Electron density around PE4 A 212:**

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

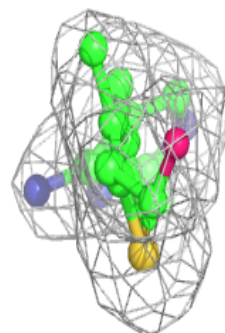
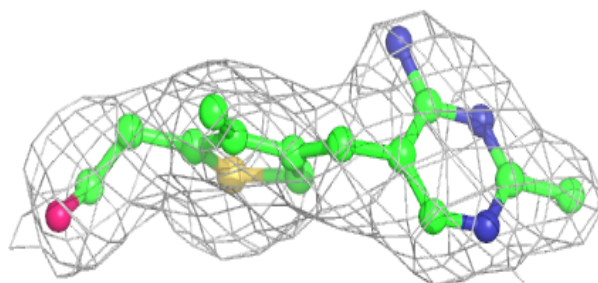
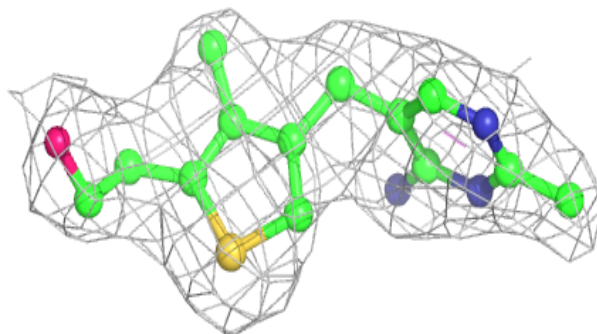


Electron density around BNG A 202:

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

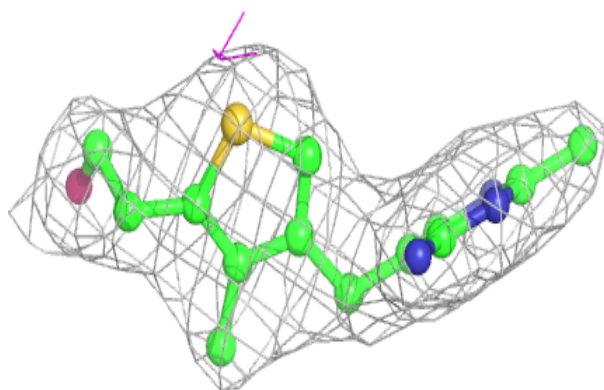
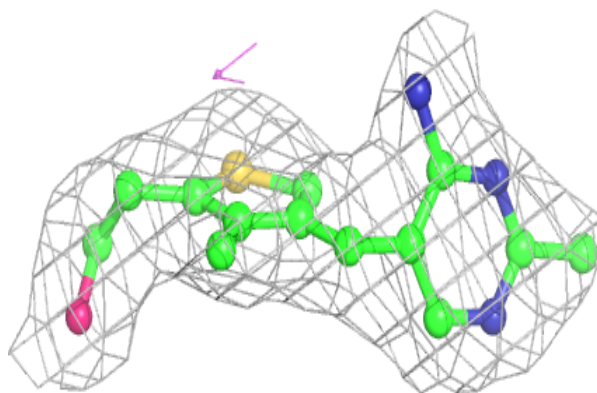
**Electron density around 0YN B 201:**

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

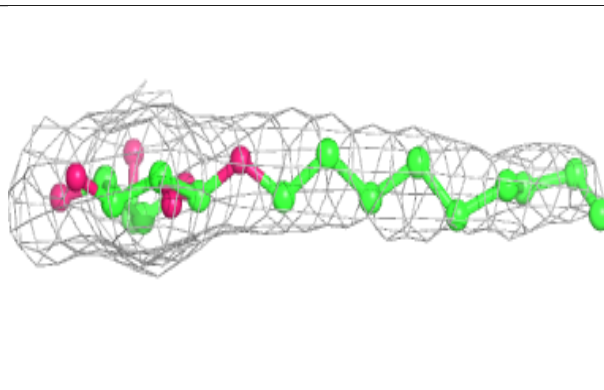
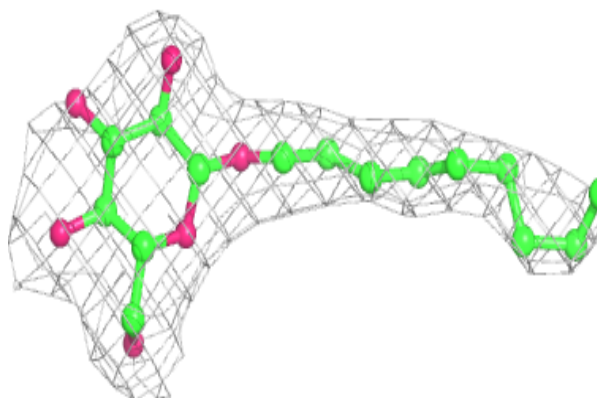


Electron density around 0YN A 201:

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

**Electron density around 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)



6.5 Other polymers

There are no such residues in this entry.