WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Sep 11, 2023 – 03:23 PM EDT

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 wwPDB X-ray Structure Validation Summary 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 ⓘ

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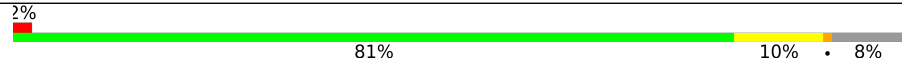*X-RAY DIFFRACTION*

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.
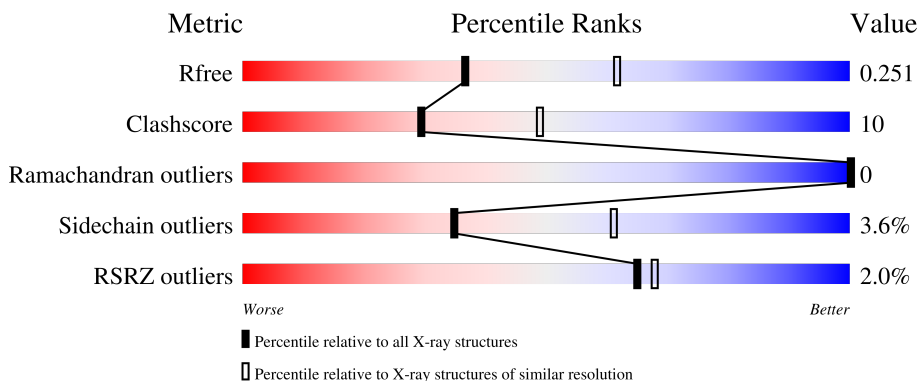
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 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	192	2% / 79% / 12% · 8%
1	B	192	2% / 81% / 10% · 8%

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 (i)

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: $C_{13}H_{17}N_3OS$).
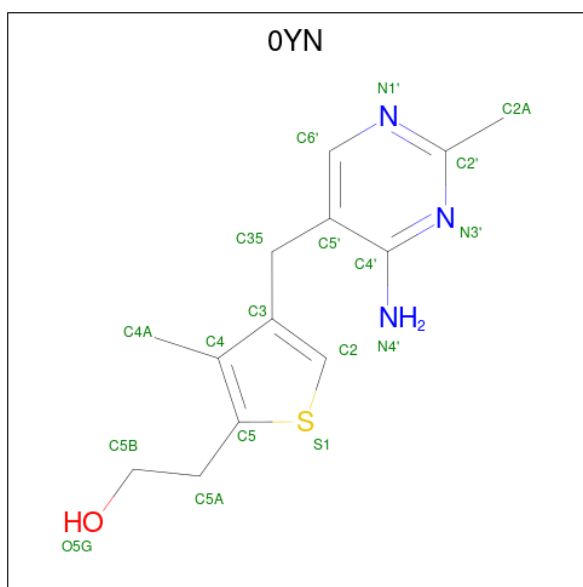
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			18	13	3	1	1		
2	B	1	Total	C	N	O	S	0	0
			18	13	3	1	1		

- Molecule 3 is nonyl beta-D-glucopyranoside (three-letter code: BNG) (formula: $C_{15}H_{30}O_6$).
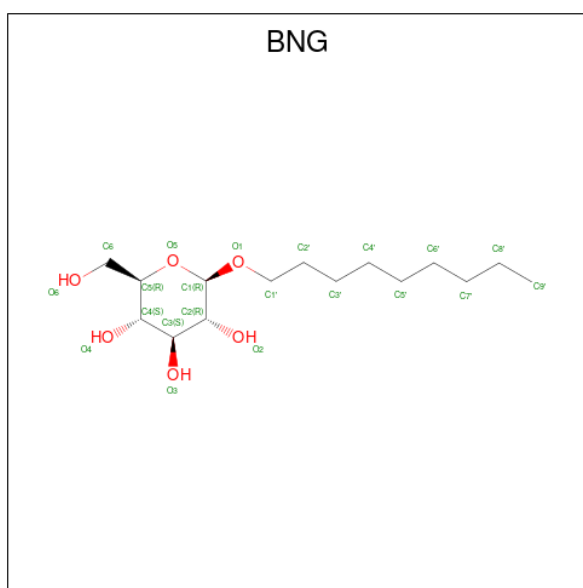
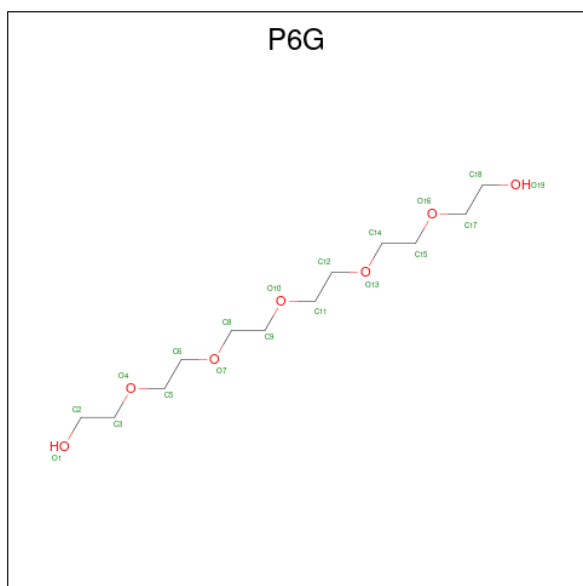| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	15	6		
3	B	1	Total	C	O	0	0
			21	15	6		

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

- 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 19	C 12	O 7	0	0
4	A	1	Total 19	C 12	O 7	0	0

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

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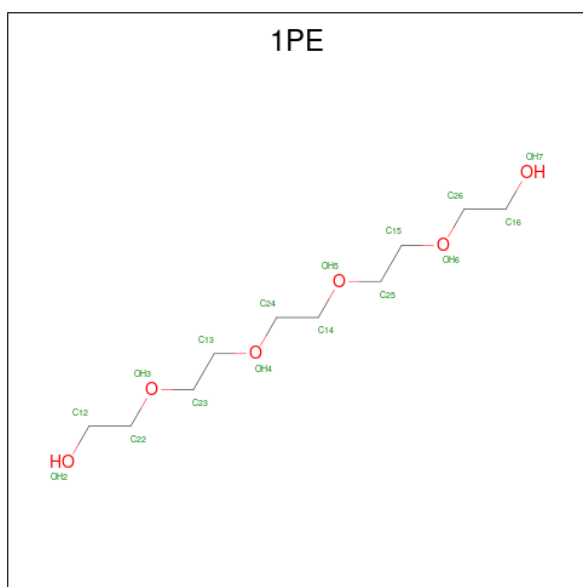
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 16	C 10	O 6	0	0
5	B	1	Total 16	C 10	O 6	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).

PEG

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

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

- Molecule 7 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: $C_{16}H_{34}O_8$).
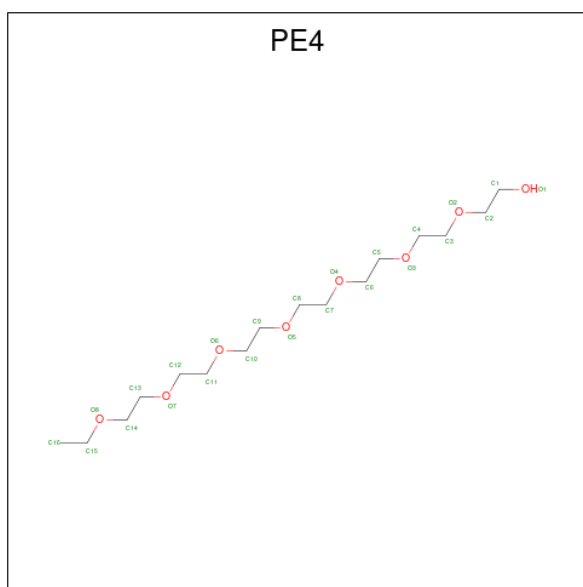
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 24	C 16	O 8	0	0

- Molecule 8 is 2-(2-METHOXYETHOXY)ETHANOL (three-letter code: PG0) (formula: $C_5H_{12}O_3$).
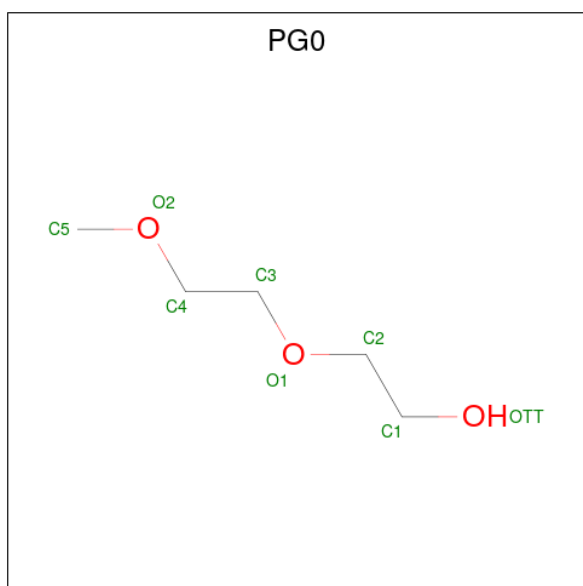
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total 8	C 5	O 3	0	0
8	B	1	Total 8	C 5	O 3	0	0

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

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

PG4
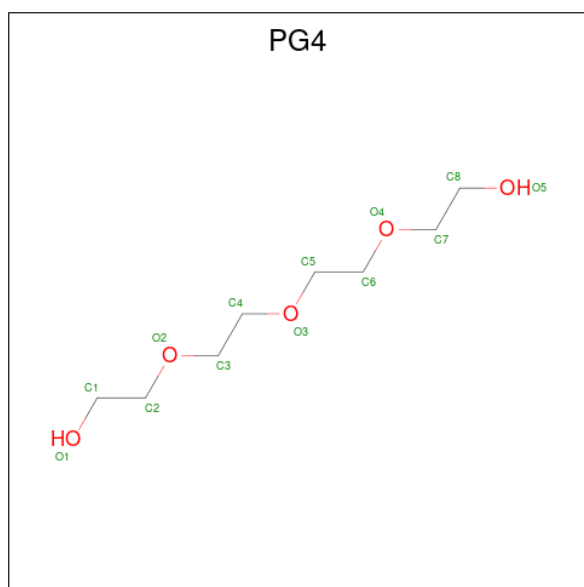
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total 13	C 8	O 5	0	0
9	A	1	Total 13	C 8	O 5	0	0
9	A	1	Total 13	C 8	O 5	0	0
9	B	1	Total 13	C 8	O 5	0	0
9	B	1	Total 13	C 8	O 5	0	0

- Molecule 10 is water.

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

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

3 Residue-property plots ⓘ

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
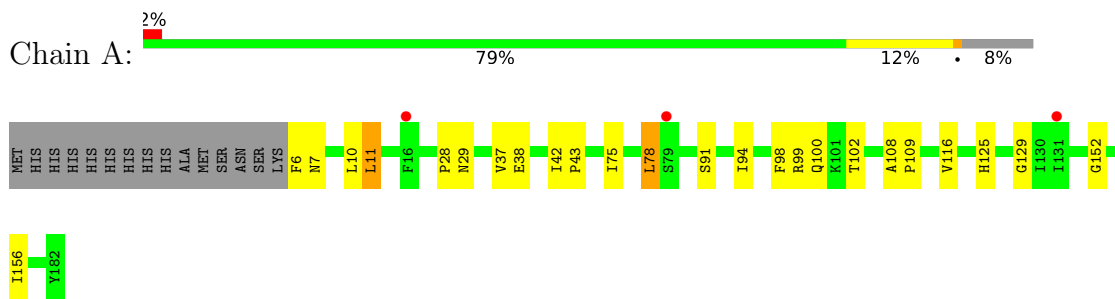
● Molecule 1: Thiamine transporter ThiT
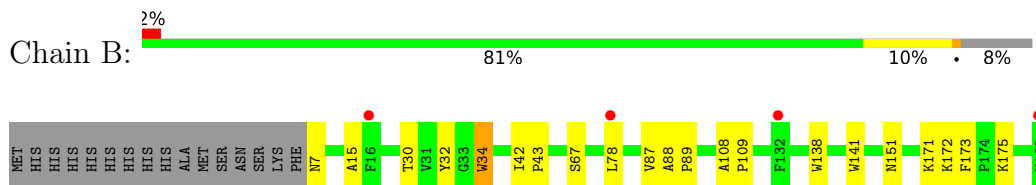
4 Data and refinement statistics ⓘ

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
$< I/\sigma(I) >$ [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]	$< |L| > = 0.49, < L^2 > = 0.32$	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.*

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[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: BNG, PG0, PEG, 1PE, PG4, 0YN, PE4, P6G

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.

The worst 5 of 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

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

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	78	LEU
1	B	171	LYS
1	B	175	LYS
1	A	102	THR
1	B	7	ASN

Sometimes 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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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	A	208	-	6,6,6	0.59	0	5,5,5	0.40	0
6	PEG	B	210	-	6,6,6	0.62	0	5,5,5	0.40	0
8	PG0	A	213	-	7,7,7	0.25	0	6,6,6	0.17	0
6	PEG	A	209	-	6,6,6	0.58	0	5,5,5	0.28	0
3	BNG	B	203	-	21,21,21	0.88	0	26,26,26	0.99	1 (3%)
4	P6G	A	204	-	18,18,18	0.72	0	17,17,17	0.50	0
3	BNG	A	202	-	21,21,21	0.83	0	26,26,26	1.05	0
6	PEG	B	205	-	6,6,6	0.57	0	5,5,5	0.40	0
6	PEG	B	209	-	6,6,6	0.64	0	5,5,5	0.41	0
6	PEG	B	208	-	6,6,6	0.62	0	5,5,5	0.55	0
5	1PE	A	205	-	15,15,15	0.81	0	14,14,14	0.43	0
7	PE4	A	212	-	23,23,23	0.80	0	22,22,22	0.34	0
6	PEG	B	211	-	6,6,6	0.62	0	5,5,5	0.25	0
8	PG0	B	218	-	7,7,7	0.40	0	6,6,6	0.45	0
5	1PE	B	204	-	15,15,15	0.77	0	14,14,14	0.36	0
2	0YN	B	201	-	17,19,19	2.85	3 (17%)	21,26,26	2.20	9 (42%)
6	PEG	A	207	-	6,6,6	0.65	0	5,5,5	0.52	0
4	P6G	A	203	-	18,18,18	0.79	0	17,17,17	0.39	0
9	PG4	A	215	-	12,12,12	0.76	0	11,11,11	0.33	0
2	0YN	A	201	-	17,19,19	2.27	4 (23%)	21,26,26	2.71	11 (52%)
6	PEG	B	206	-	6,6,6	0.65	0	5,5,5	0.50	0
9	PG4	B	219	-	12,12,12	0.77	0	11,11,11	0.34	0
6	PEG	B	212	-	6,6,6	0.56	0	5,5,5	0.47	0
6	PEG	B	214	-	6,6,6	0.60	0	5,5,5	0.52	0
6	PEG	B	207	-	6,6,6	0.56	0	5,5,5	0.37	0
6	PEG	A	210	-	6,6,6	0.53	0	5,5,5	1.03	0
9	PG4	B	220	-	12,12,12	0.81	0	11,11,11	0.48	0
8	PG0	B	217	-	7,7,7	0.36	0	6,6,6	0.48	0
9	PG4	A	216	-	12,12,12	0.74	0	11,11,11	0.36	0
6	PEG	A	206	-	6,6,6	0.53	0	5,5,5	0.70	0
9	PG4	A	214	-	12,12,12	0.75	0	11,11,11	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
8	PG0	B	216	-	7,7,7	0.50	0	6,6,6	0.48	0
6	PEG	B	213	-	6,6,6	0.52	0	5,5,5	0.60	0
3	BNG	B	202	-	21,21,21	0.85	0	26,26,26	1.39	2 (7%)
8	PG0	B	215	-	7,7,7	0.33	0	6,6,6	0.25	0
6	PEG	A	211	-	6,6,6	0.59	0	5,5,5	0.36	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
6	PEG	A	208	-	-	4/4/4/4	-
6	PEG	B	210	-	-	1/4/4/4	-
8	PG0	A	213	-	-	3/5/5/5	-
6	PEG	A	209	-	-	2/4/4/4	-
3	BNG	B	203	-	-	4/12/32/32	0/1/1/1
4	P6G	A	204	-	-	8/16/16/16	-
3	BNG	A	202	-	-	8/12/32/32	0/1/1/1
6	PEG	B	205	-	-	2/4/4/4	-
6	PEG	B	209	-	-	0/4/4/4	-
6	PEG	B	208	-	-	1/4/4/4	-
5	1PE	A	205	-	-	5/13/13/13	-
7	PE4	A	212	-	-	11/21/21/21	-
6	PEG	B	211	-	-	3/4/4/4	-
8	PG0	B	218	-	-	3/5/5/5	-
5	1PE	B	204	-	-	7/13/13/13	-
2	0YN	B	201	-	-	3/6/7/7	0/2/2/2
6	PEG	A	207	-	-	3/4/4/4	-
4	P6G	A	203	-	-	10/16/16/16	-
9	PG4	A	215	-	-	4/10/10/10	-
2	0YN	A	201	-	-	2/6/7/7	0/2/2/2
6	PEG	B	206	-	-	2/4/4/4	-
9	PG4	B	219	-	-	4/10/10/10	-
6	PEG	B	212	-	-	3/4/4/4	-
6	PEG	B	214	-	-	3/4/4/4	-
6	PEG	B	207	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PEG	A	210	-	-	4/4/4/4	-
9	PG4	B	220	-	-	8/10/10/10	-
8	PG0	B	217	-	-	1/5/5/5	-
9	PG4	A	216	-	-	4/10/10/10	-
6	PEG	A	206	-	-	3/4/4/4	-
9	PG4	A	214	-	-	7/10/10/10	-
8	PG0	B	216	-	-	5/5/5/5	-
6	PEG	B	213	-	-	1/4/4/4	-
3	BNG	B	202	-	-	5/12/32/32	0/1/1/1
8	PG0	B	215	-	-	1/5/5/5	-
6	PEG	A	211	-	-	1/4/4/4	-

The worst 5 of 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

The worst 5 of 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

There are no chirality outliers.

5 of 139 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	0YN	C5-C5A-C5B-O5G
2	B	201	0YN	C4-C5-C5A-C5B
2	B	201	0YN	C5-C5A-C5B-O5G
3	A	202	BNG	C2-C1-O1-C1'
3	A	202	BNG	O5-C1-O1-C1'

There are no ring outliers.

22 monomers are involved in 52 short contacts:

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

Bond lengths

Bond angles

Torsions

Rings

Ligand P6G A 204

Bond lengths

Bond angles

Torsions

Rings

Ligand BNG A 202

Bond lengths

Bond angles

Torsions

Rings

Ligand PE4 A 212

Bond lengths

Bond angles

Torsions

Rings

Ligand 0YN B 201

Bond lengths

Bond angles

Torsions

Rings

Ligand P6G A 203

Bond lengths

Bond angles

Torsions

Rings

Ligand 0YN A 201

Bond lengths

Bond angles

Torsions

Rings

Ligand BNG B 202

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	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

The worst 5 of 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

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^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	207	7/7	0.72	0.30	76,83,95,102	0
6	PEG	A	209	7/7	0.72	0.19	94,95,99,99	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
8	PG0	B	218	8/8	0.78	0.25	73,88,94,95	0
9	PG4	A	214	13/13	0.78	0.32	76,88,100,101	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
6	PEG	A	208	7/7	0.86	0.35	81,86,96,97	0
9	PG4	B	219	13/13	0.86	0.14	66,86,111,113	0
4	P6G	A	203	19/19	0.87	0.19	63,89,111,111	0
6	PEG	B	208	7/7	0.88	0.14	82,84,92,92	0
6	PEG	A	206	7/7	0.88	0.24	54,62,85,86	0
6	PEG	B	211	7/7	0.88	0.42	85,93,97,97	0
5	1PE	B	204	16/16	0.88	0.14	70,81,95,99	0
8	PG0	A	213	8/8	0.88	0.14	83,88,100,104	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
9	PG4	A	216	13/13	0.89	0.20	69,92,102,108	0
6	PEG	B	205	7/7	0.89	0.12	78,80,87,91	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
6	PEG	B	207	7/7	0.90	0.15	59,74,81,88	0
4	P6G	A	204	19/19	0.90	0.18	57,81,101,104	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
6	PEG	B	212	7/7	0.93	0.16	79,87,93,97	0
9	PG4	B	220	13/13	0.93	0.18	64,74,93,98	0
6	PEG	B	206	7/7	0.95	0.17	70,76,78,83	0
2	0YN	B	201	18/18	0.95	0.15	39,52,72,77	0
2	0YN	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:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
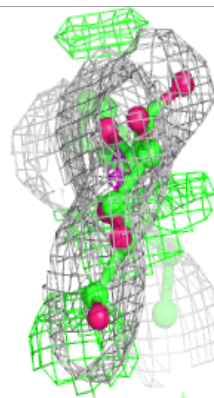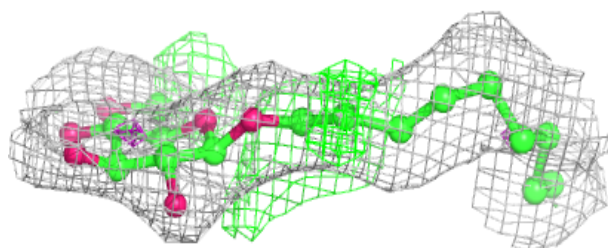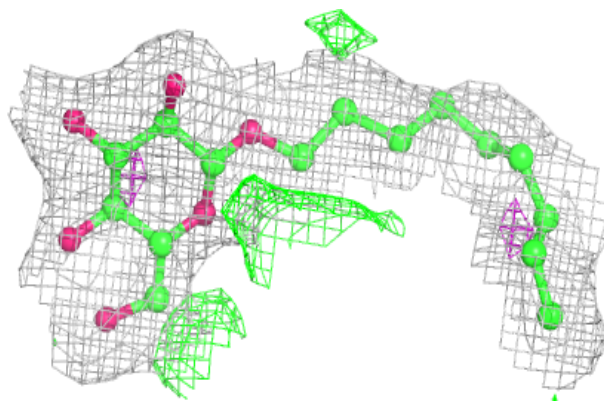
Electron density around P6G A 203:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
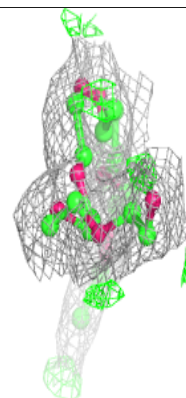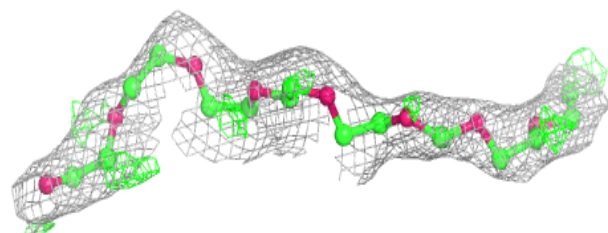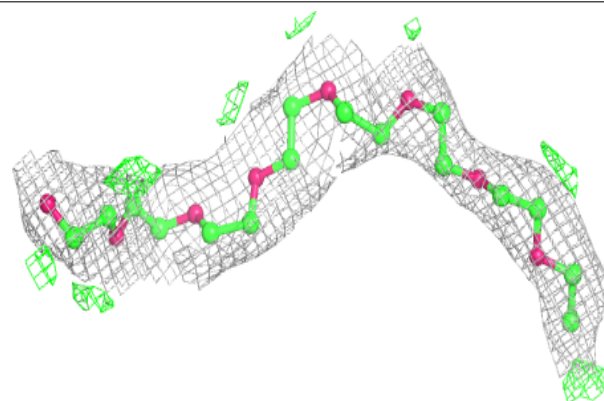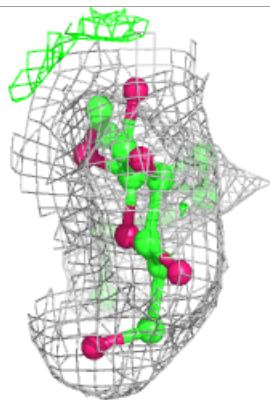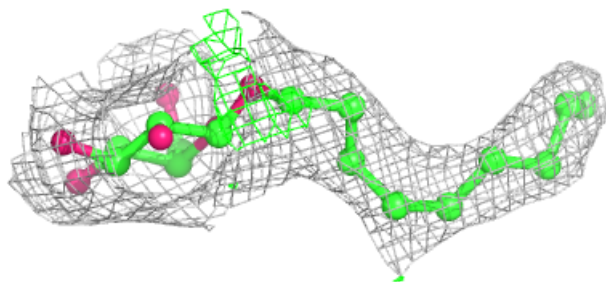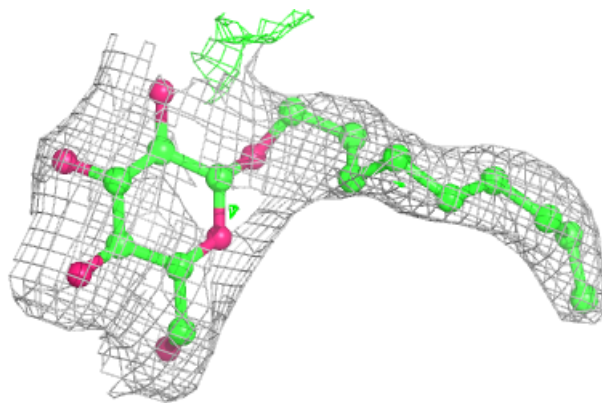$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
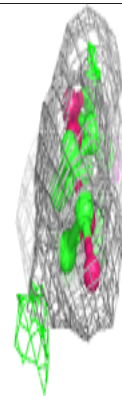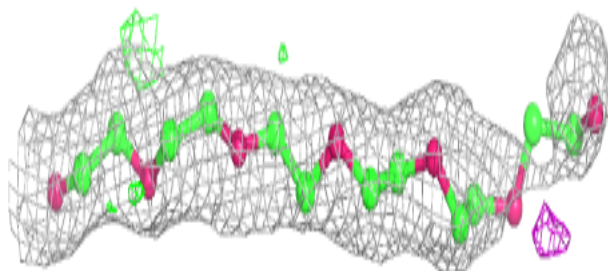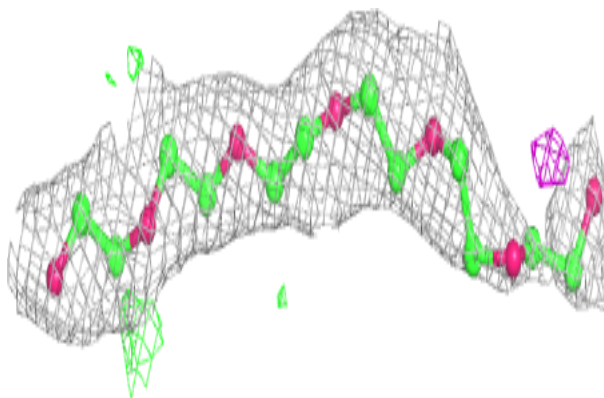
Electron density around P6G A 204:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
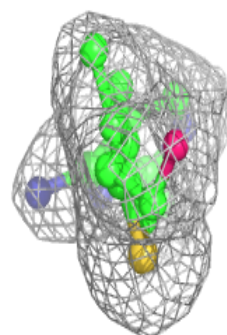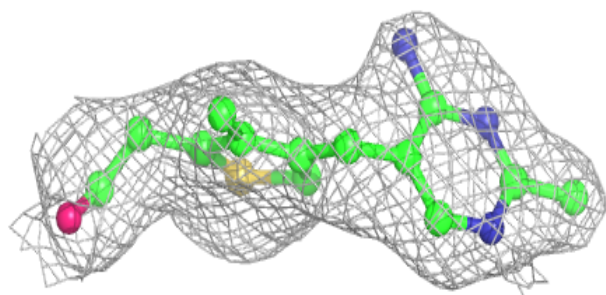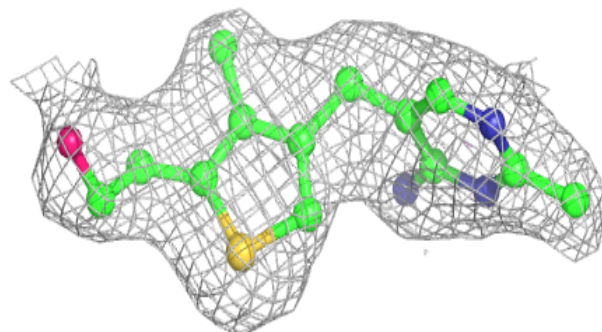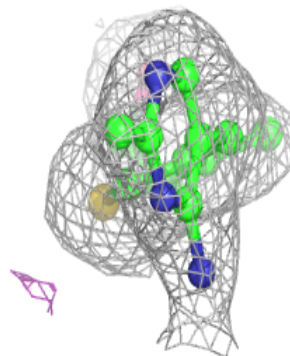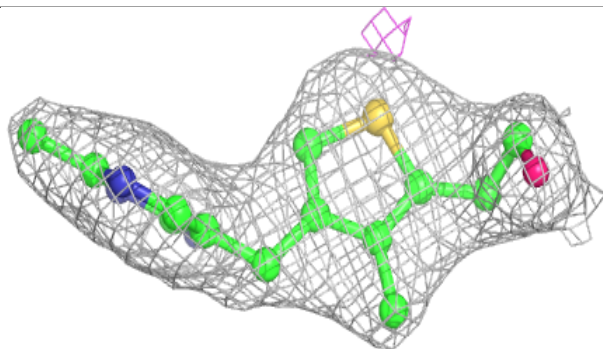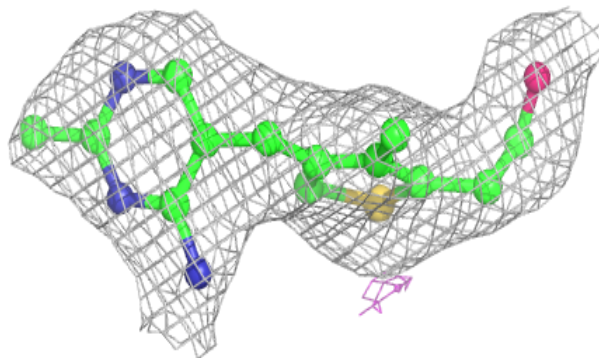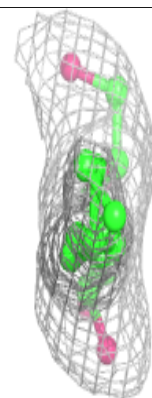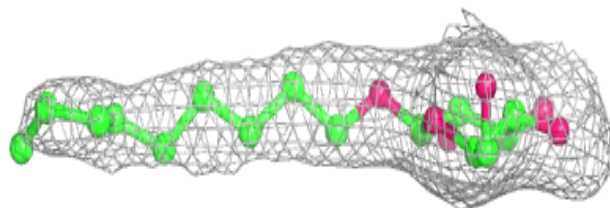mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
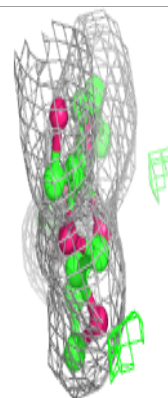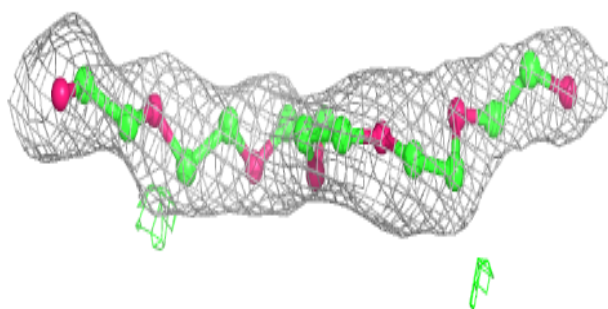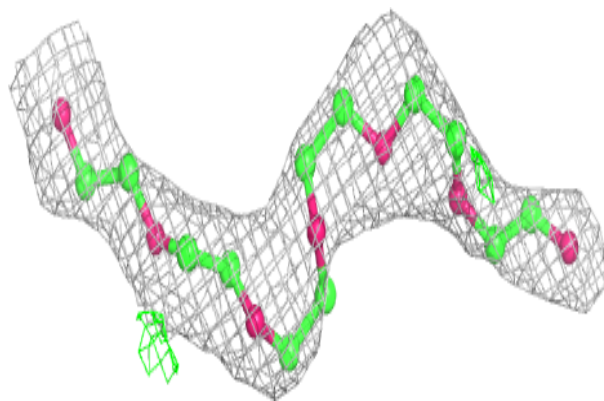
Electron density around PE4 A 212:

$2mF_o$-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)
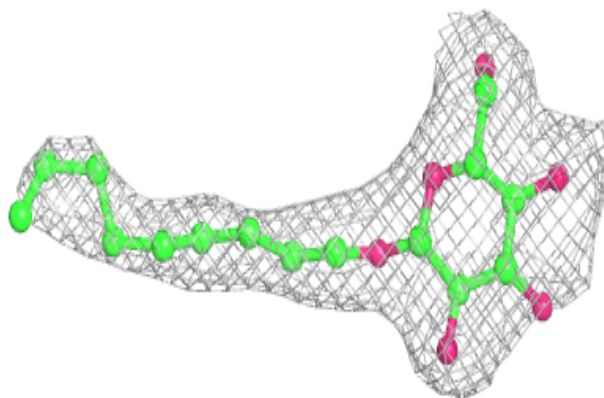and green (positive)

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.