wwPDB X-ray Structure Validation Summary Report (i)

Jun 16, 2024 – 09:59 AM EDT

PDB ID	:	5E9S
Title	:	Crystal structure of substrate-bound glutamate transporter homologue GltTk
Authors	:	Guskov, A.; Slotboom, D.J.
Deposited on	:	2015-10-15
Resolution	:	2.80 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:

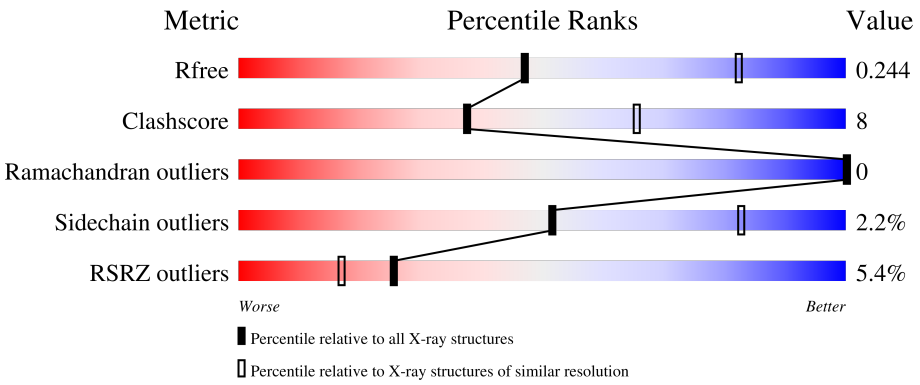
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	438	4% 76% 21%
1	B	438	6% 80% 17%
1	C	438	6% 78% 19%

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	DMU	A	505	-	-	-	X
5	1PE	B	506	-	-	-	X
5	1PE	B	507	-	-	-	X
6	PEG	B	511	-	-	-	X
6	PEG	B	516	-	-	-	X
6	PEG	B	519	-	-	-	X
6	PEG	B	522	-	-	-	X
6	PEG	C	509	-	-	-	X
6	PEG	C	513	-	-	-	X
6	PEG	C	514	-	-	-	X
8	P6G	C	520	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 10213 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 Proton/glutamate symporter, SDF family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	427	3196	2108	518	553	17	0	1	0
1	B	427	3188	2103	517	552	16	0	0	0
1	C	426	3186	2102	515	552	17	0	1	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	431	HIS	-	expression tag	UNP Q5JID0
A	432	HIS	-	expression tag	UNP Q5JID0
A	433	HIS	-	expression tag	UNP Q5JID0
A	434	HIS	-	expression tag	UNP Q5JID0
A	435	HIS	-	expression tag	UNP Q5JID0
A	436	HIS	-	expression tag	UNP Q5JID0
A	437	HIS	-	expression tag	UNP Q5JID0
A	438	HIS	-	expression tag	UNP Q5JID0
B	431	HIS	-	expression tag	UNP Q5JID0
B	432	HIS	-	expression tag	UNP Q5JID0
B	433	HIS	-	expression tag	UNP Q5JID0
B	434	HIS	-	expression tag	UNP Q5JID0
B	435	HIS	-	expression tag	UNP Q5JID0
B	436	HIS	-	expression tag	UNP Q5JID0
B	437	HIS	-	expression tag	UNP Q5JID0
B	438	HIS	-	expression tag	UNP Q5JID0
C	431	HIS	-	expression tag	UNP Q5JID0
C	432	HIS	-	expression tag	UNP Q5JID0
C	433	HIS	-	expression tag	UNP Q5JID0
C	434	HIS	-	expression tag	UNP Q5JID0
C	435	HIS	-	expression tag	UNP Q5JID0
C	436	HIS	-	expression tag	UNP Q5JID0
C	437	HIS	-	expression tag	UNP Q5JID0

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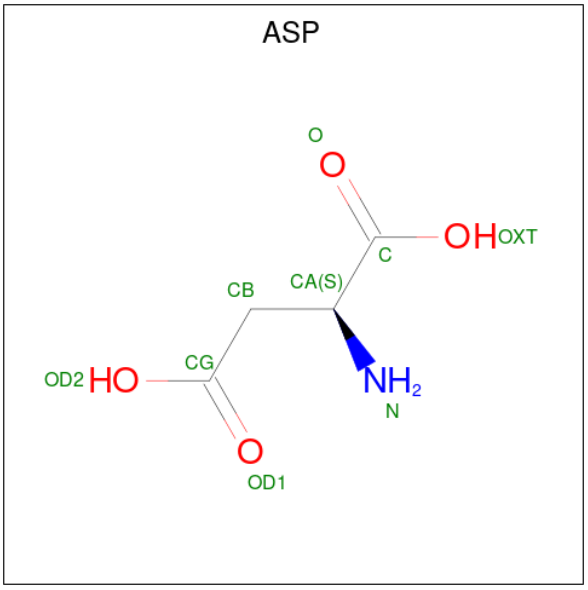
Chain	Residue	Modelled	Actual	Comment	Reference
C	438	HIS	-	expression tag	UNP Q5JID0

- Molecule 2 is ASPARTIC ACID (three-letter code: ASP) (formula: $C_4H_7NO_4$).

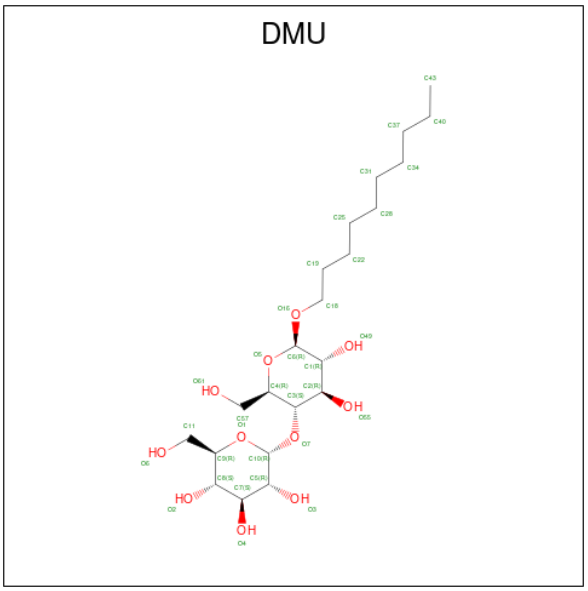


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	9	4	1	4	0	0
2	B	1	9	4	1	4	0	0
2	C	1	9	4	1	4	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

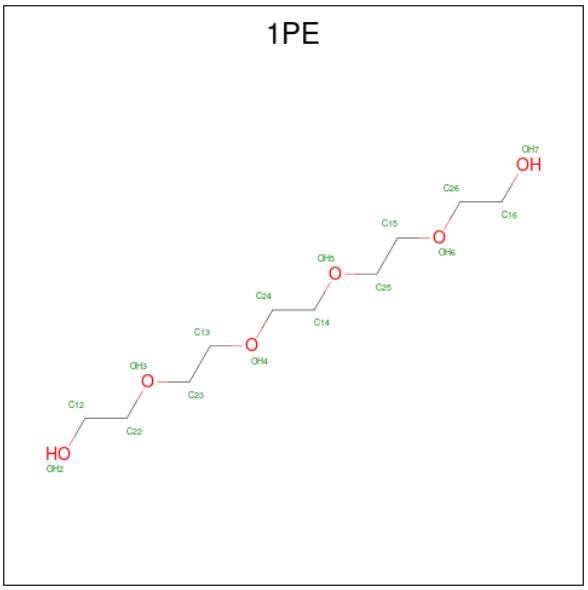
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
3	A	3	3	3	0	0
3	B	3	3	3	0	0
3	C	3	3	3	0	0

- Molecule 4 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	33	22	11	0	0
			Total	C	O		
4	B	1	33	22	11	0	0
			Total	C	O		
4	C	1	33	22	11	0	0

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



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

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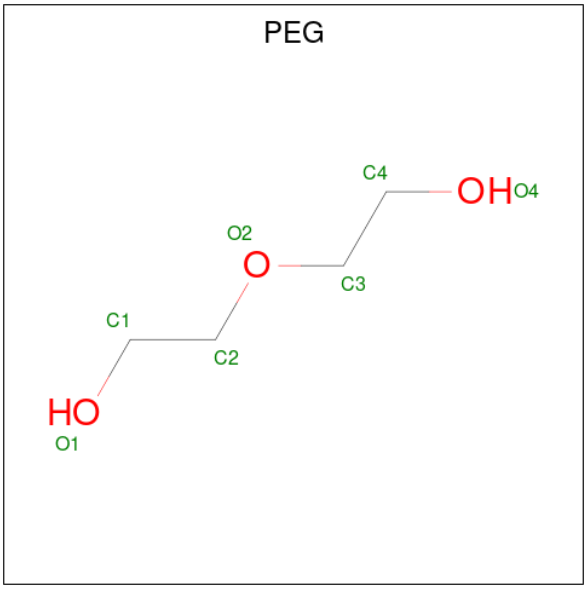
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	16	10	6	0	0
5	B	1	16	10	6	0	0
5	B	1	16	10	6	0	0
5	B	1	16	10	6	0	0
5	C	1	16	10	6	0	0
5	C	1	16	10	6	0	0

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



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

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

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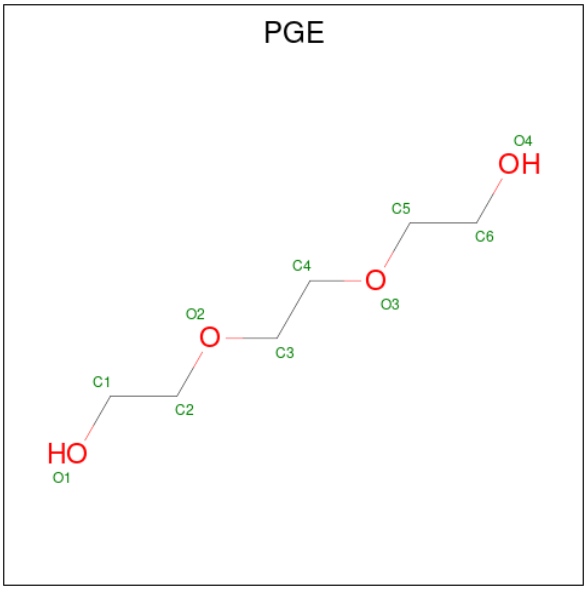
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 7 4 3	0	0
6	C	1	Total C O 7 4 3	0	0
6	C	1	Total C O 7 4 3	0	0
6	C	1	Total C O 7 4 3	0	0
6	C	1	Total C O 7 4 3	0	0
6	C	1	Total C O 7 4 3	0	0
6	C	1	Total C O 7 4 3	0	0

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



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

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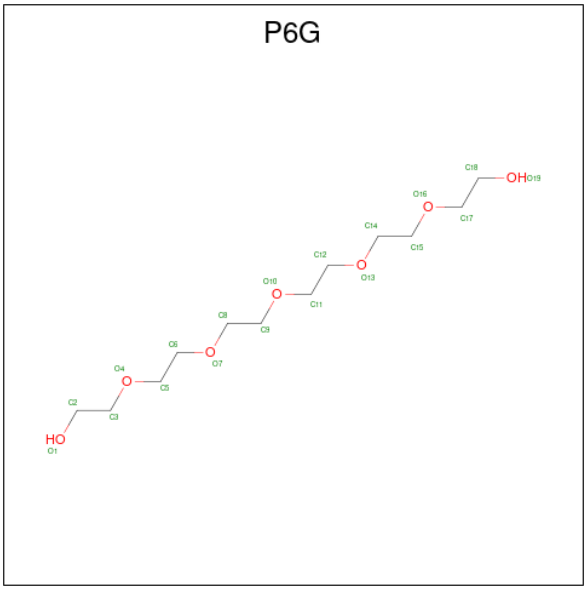
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	B	1	10	6	4	0	0
			Total	C	O		
7	C	1	10	6	4	0	0
			Total	C	O		
7	C	1	10	6	4	0	0

- Molecule 8 is HEXAETHYLENE GLYCOL (three-letter code: P6G) (formula: $C_{12}H_{26}O_7$).



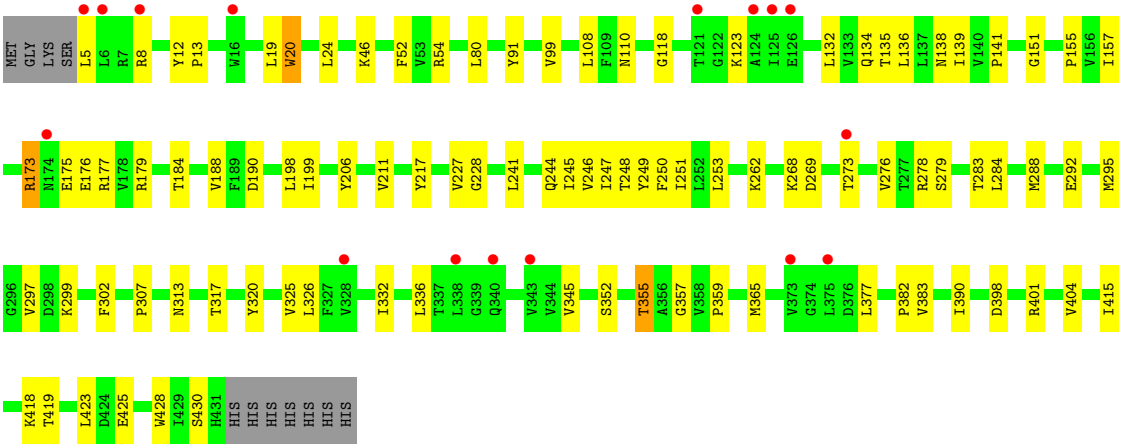
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	A	1	19	12	7	0	0
			Total	C	O		
8	B	1	19	12	7	0	0
			Total	C	O		
8	B	1	19	12	7	0	0
			Total	C	O		
8	C	1	19	12	7	0	0
			Total	C	O		
8	C	1	19	12	7	0	0

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.

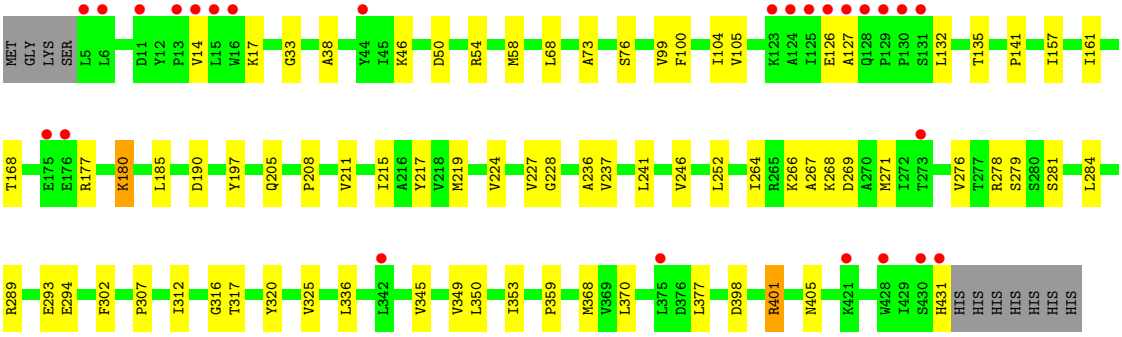
• Molecule 1: Proton/glutamate symporter, SDF family

Chain A:



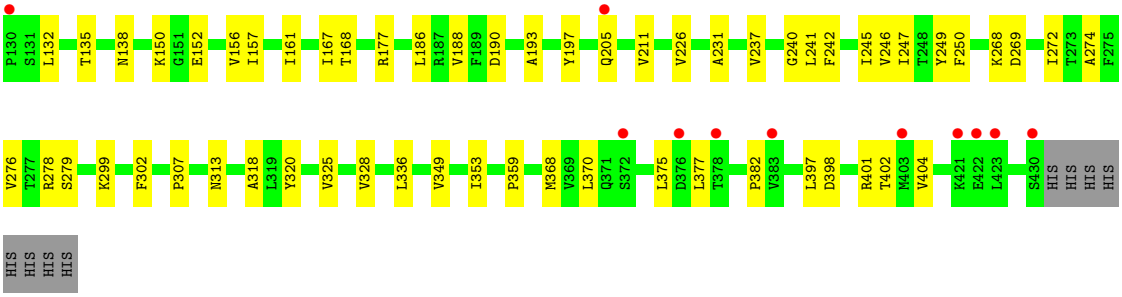
• Molecule 1: Proton/glutamate symporter, SDF family

Chain B:



• Molecule 1: Proton/glutamate symporter, SDF family

Chain C:


P130
S131
L132
T135
N138
K150
G151
E152
V156
I157
I161
I167
T168
R177
L186
R187
V188
F189
D190
A193
Y197
Q205
V211
V226
A231
V237
G240
L241
F242
I245
V246
I247
T248
Y249
F250
K268
D269
I272
T273
A274
F275
V276
T277
R278
S279
K299
F302
P307
N313
A318
L319
Y320
V325
V328
L336
V349
I353
P359
M368
V369
L370
Q371
S372
L375
D376
L377
T378
P382
Y383
L397
D398
R401
T402
M403
V404
K421
E422
L423
S430
HIS
HIS
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HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	117.52Å 117.52Å 310.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.36 – 2.80 48.36 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.4 (48.36-2.80) 97.4 (48.36-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.04 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.10_2155)	Depositor
R, R_{free}	0.213 , 0.242 0.215 , 0.244	Depositor DCC
R_{free} test set	2009 reflections (3.32%)	wwPDB-VP
Wilson B-factor (Å^2)	83.7	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 65.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,l	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	10213	wwPDB-VP
Average B, all atoms (Å^2)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: NA, PEG, DMU, P6G, PGE, 1PE

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	0.43	0/3256	0.64	0/4431
1	B	0.42	0/3248	0.61	0/4421
1	C	0.40	0/3245	0.63	0/4416
All	All	0.41	0/9749	0.63	0/13268

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	118	GLY	Peptide

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	3196	0	3402	64	0
1	B	3188	0	3394	45	0
1	C	3186	0	3395	53	0
2	A	9	0	3	2	0
2	B	9	0	3	3	0
2	C	9	0	3	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
4	A	33	0	42	0	0
4	B	33	0	42	1	0
4	C	33	0	42	2	0
5	A	32	0	44	2	0
5	B	48	0	66	4	0
5	C	32	0	44	0	0
6	A	70	0	100	1	0
6	B	98	0	140	3	0
6	C	63	0	90	5	0
7	A	40	0	56	2	0
7	B	10	0	14	0	0
7	C	20	0	28	0	0
8	A	19	0	26	0	0
8	B	38	0	52	2	0
8	C	38	0	52	1	0
All	All	10213	0	11038	163	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 8.

The worst 5 of 163 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)
5:B:508:1PE:H241	6:B:522:PEG:H22	1.63	0.81
1:A:357:GLY:H	7:A:520:PGE:H12	1.47	0.79
1:A:110:ASN:HB2	5:A:507:1PE:H251	1.65	0.78
1:A:177:ARG:NH1	1:B:190:ASP:OD2	2.20	0.74
1:C:241:LEU:HB3	1:C:404:VAL:HG21	1.72	0.70

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	426/438 (97%)	418 (98%)	8 (2%)	0	100	100
1	B	425/438 (97%)	415 (98%)	10 (2%)	0	100	100
1	C	425/438 (97%)	413 (97%)	12 (3%)	0	100	100
All	All	1276/1314 (97%)	1246 (98%)	30 (2%)	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	336/345 (97%)	331 (98%)	5 (2%)	65	89
1	B	335/345 (97%)	325 (97%)	10 (3%)	41	75
1	C	335/345 (97%)	329 (98%)	6 (2%)	59	86
All	All	1006/1035 (97%)	985 (98%)	21 (2%)	52	84

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	431	HIS
1	C	125	ILE
1	C	368[B]	MET
1	C	320	TYR
1	C	76	SER

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 67 ligands modelled in this entry, 9 are monoatomic - leaving 58 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	$\#\|Z\| > 2$
6	PEG	B	515	-	6,6,6	0.49	0	5,5,5	0.42	0
6	PEG	B	519	-	6,6,6	0.49	0	5,5,5	0.30	0
6	PEG	C	509	-	6,6,6	0.53	0	5,5,5	0.35	0
7	PGE	A	518	-	9,9,9	0.35	0	8,8,8	0.34	0
6	PEG	C	510	-	6,6,6	0.48	0	5,5,5	0.39	0
6	PEG	A	512	-	6,6,6	0.46	0	5,5,5	0.38	0
6	PEG	B	516	-	6,6,6	0.53	0	5,5,5	0.28	0
6	PEG	A	511	-	6,6,6	0.51	0	5,5,5	0.48	0
6	PEG	B	518	-	6,6,6	0.49	0	5,5,5	0.38	0
6	PEG	A	517	-	6,6,6	0.56	0	5,5,5	0.80	0
6	PEG	C	515	-	6,6,6	0.50	0	5,5,5	0.27	0
2	ASP	B	501	-	6,8,8	1.19	0	8,10,10	1.73	2 (25%)
2	ASP	A	501	-	6,8,8	1.18	1 (16%)	8,10,10	1.30	1 (12%)
6	PEG	C	513	-	6,6,6	0.50	0	5,5,5	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	PEG	A	509	-	6,6,6	0.49	0	5,5,5	0.29	0
6	PEG	B	521	-	6,6,6	0.49	0	5,5,5	0.30	0
6	PEG	B	514	-	6,6,6	0.49	0	5,5,5	0.31	0
6	PEG	B	510	-	6,6,6	0.52	0	5,5,5	0.28	0
5	1PE	B	508	-	15,15,15	0.54	0	14,14,14	0.24	0
6	PEG	B	520	-	6,6,6	0.53	0	5,5,5	0.41	0
6	PEG	A	508	-	6,6,6	0.47	0	5,5,5	0.31	0
6	PEG	A	513	-	6,6,6	0.50	0	5,5,5	0.36	0
4	DMU	B	505	-	34,34,34	1.61	8 (23%)	45,45,45	1.05	4 (8%)
5	1PE	A	506	-	15,15,15	0.54	0	14,14,14	0.36	0
7	PGE	A	519	-	9,9,9	0.38	0	8,8,8	0.32	0
6	PEG	C	516	-	6,6,6	0.45	0	5,5,5	0.30	0
6	PEG	A	516	-	6,6,6	0.53	0	5,5,5	0.30	0
8	P6G	C	519	-	18,18,18	0.60	0	17,17,17	0.55	0
6	PEG	C	512	-	6,6,6	0.51	0	5,5,5	0.35	0
6	PEG	A	515	-	6,6,6	0.51	0	5,5,5	0.26	0
4	DMU	C	505	-	34,34,34	1.60	9 (26%)	45,45,45	1.06	3 (6%)
5	1PE	C	507	-	15,15,15	0.54	0	14,14,14	0.22	0
7	PGE	B	523	-	9,9,9	0.43	0	8,8,8	0.27	0
6	PEG	A	514	-	6,6,6	0.51	0	5,5,5	0.25	0
7	PGE	A	521	-	9,9,9	0.36	0	8,8,8	0.40	0
5	1PE	B	507	-	15,15,15	0.55	0	14,14,14	0.33	0
6	PEG	A	510	-	6,6,6	0.49	0	5,5,5	0.32	0
6	PEG	B	509	-	6,6,6	0.52	0	5,5,5	0.31	0
7	PGE	C	517	-	9,9,9	0.34	0	8,8,8	0.26	0
4	DMU	A	505	-	34,34,34	1.68	9 (26%)	45,45,45	1.32	7 (15%)
5	1PE	A	507	-	15,15,15	0.54	0	14,14,14	0.42	0
6	PEG	B	511	-	6,6,6	0.48	0	5,5,5	0.30	0
6	PEG	C	508	-	6,6,6	0.50	0	5,5,5	0.43	0
6	PEG	B	517	-	6,6,6	0.50	0	5,5,5	0.24	0
8	P6G	C	520	-	18,18,18	0.54	0	17,17,17	0.50	0
5	1PE	C	506	-	15,15,15	0.52	0	14,14,14	0.58	0
6	PEG	C	511	-	6,6,6	0.52	0	5,5,5	0.38	0
7	PGE	A	520	-	9,9,9	0.45	0	8,8,8	0.35	0
8	P6G	B	524	-	18,18,18	0.54	0	17,17,17	0.47	0
5	1PE	B	506	-	15,15,15	0.56	0	14,14,14	0.49	0
6	PEG	B	522	-	6,6,6	0.51	0	5,5,5	0.28	0
7	PGE	C	518	-	9,9,9	0.31	0	8,8,8	0.58	0
8	P6G	A	522	-	18,18,18	0.59	0	17,17,17	0.48	0
8	P6G	B	525	-	18,18,18	0.56	0	17,17,17	0.49	0
6	PEG	B	513	-	6,6,6	0.51	0	5,5,5	0.38	0
2	ASP	C	501	-	6,8,8	1.12	0	8,10,10	1.37	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	PEG	B	512	-	6,6,6	0.54	0	5,5,5	0.32	0
6	PEG	C	514	-	6,6,6	0.51	0	5,5,5	0.38	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	B	515	-	-	2/4/4/4	-
6	PEG	B	519	-	-	2/4/4/4	-
6	PEG	C	509	-	-	1/4/4/4	-
7	PGE	A	518	-	-	6/7/7/7	-
6	PEG	C	510	-	-	3/4/4/4	-
6	PEG	A	512	-	-	3/4/4/4	-
6	PEG	B	516	-	-	4/4/4/4	-
6	PEG	A	511	-	-	3/4/4/4	-
6	PEG	B	518	-	-	1/4/4/4	-
6	PEG	A	517	-	-	2/4/4/4	-
6	PEG	C	515	-	-	4/4/4/4	-
2	ASP	B	501	-	-	4/8/8/8	-
2	ASP	A	501	-	-	2/8/8/8	-
6	PEG	C	513	-	-	0/4/4/4	-
6	PEG	A	509	-	-	2/4/4/4	-
6	PEG	B	521	-	-	2/4/4/4	-
6	PEG	B	514	-	-	2/4/4/4	-
6	PEG	B	510	-	-	2/4/4/4	-
5	1PE	B	508	-	-	6/13/13/13	-
6	PEG	B	520	-	-	2/4/4/4	-
6	PEG	A	508	-	-	2/4/4/4	-
6	PEG	A	513	-	-	1/4/4/4	-
4	DMU	B	505	-	-	10/19/59/59	0/2/2/2
5	1PE	A	506	-	-	7/13/13/13	-
7	PGE	A	519	-	-	4/7/7/7	-
6	PEG	C	516	-	-	1/4/4/4	-
6	PEG	A	516	-	-	3/4/4/4	-
8	P6G	C	519	-	-	9/16/16/16	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PEG	C	512	-	-	3/4/4/4	-
6	PEG	A	515	-	-	2/4/4/4	-
4	DMU	C	505	-	-	10/19/59/59	0/2/2/2
5	1PE	C	507	-	-	7/13/13/13	-
7	PGE	B	523	-	-	4/7/7/7	-
6	PEG	A	514	-	-	2/4/4/4	-
7	PGE	A	521	-	-	2/7/7/7	-
5	1PE	B	507	-	-	8/13/13/13	-
6	PEG	A	510	-	-	2/4/4/4	-
6	PEG	B	509	-	-	0/4/4/4	-
7	PGE	C	517	-	-	2/7/7/7	-
4	DMU	A	505	-	-	7/19/59/59	0/2/2/2
5	1PE	A	507	-	-	9/13/13/13	-
6	PEG	B	511	-	-	1/4/4/4	-
6	PEG	C	508	-	-	1/4/4/4	-
6	PEG	B	517	-	-	3/4/4/4	-
8	P6G	C	520	-	-	11/16/16/16	-
5	1PE	C	506	-	-	5/13/13/13	-
6	PEG	C	511	-	-	3/4/4/4	-
7	PGE	A	520	-	-	3/7/7/7	-
8	P6G	B	524	-	-	7/16/16/16	-
5	1PE	B	506	-	-	9/13/13/13	-
6	PEG	B	522	-	-	1/4/4/4	-
7	PGE	C	518	-	-	3/7/7/7	-
8	P6G	A	522	-	-	9/16/16/16	-
8	P6G	B	525	-	-	10/16/16/16	-
6	PEG	B	513	-	-	2/4/4/4	-
2	ASP	C	501	-	-	4/8/8/8	-
6	PEG	B	512	-	-	1/4/4/4	-
6	PEG	C	514	-	-	2/4/4/4	-

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	505	DMU	O1-C9	4.74	1.55	1.44
4	B	505	DMU	O1-C9	4.67	1.55	1.44
4	C	505	DMU	O1-C9	4.64	1.55	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	505	DMU	C11-C9	-3.33	1.40	1.51
4	B	505	DMU	C11-C9	-3.15	1.41	1.51

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	505	DMU	O5-C4-C3	3.79	117.73	109.75
4	A	505	DMU	C18-O16-C6	3.28	119.29	113.84
2	B	501	ASP	OXT-C-CA	3.16	124.16	113.38
4	C	505	DMU	O5-C4-C3	3.14	116.37	109.75
2	B	501	ASP	OXT-C-O	-3.08	117.10	124.09

There are no chirality outliers.

5 of 223 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	505	DMU	O5-C6-O16-C18
4	B	505	DMU	O5-C6-O16-C18
4	C	505	DMU	O5-C6-O16-C18
4	A	505	DMU	C2-C3-O7-C10
4	B	505	DMU	O6-C11-C9-O1

There are no ring outliers.

21 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	509	PEG	1	0
6	C	510	PEG	2	0
6	A	511	PEG	1	0
6	C	515	PEG	1	0
2	B	501	ASP	3	0
2	A	501	ASP	2	0
5	B	508	1PE	2	0
4	B	505	DMU	1	0
6	C	512	PEG	1	0
4	C	505	DMU	2	0
7	A	521	PGE	1	0
5	B	507	1PE	1	0
6	B	509	PEG	1	0
5	A	507	1PE	2	0
6	C	508	PEG	1	0

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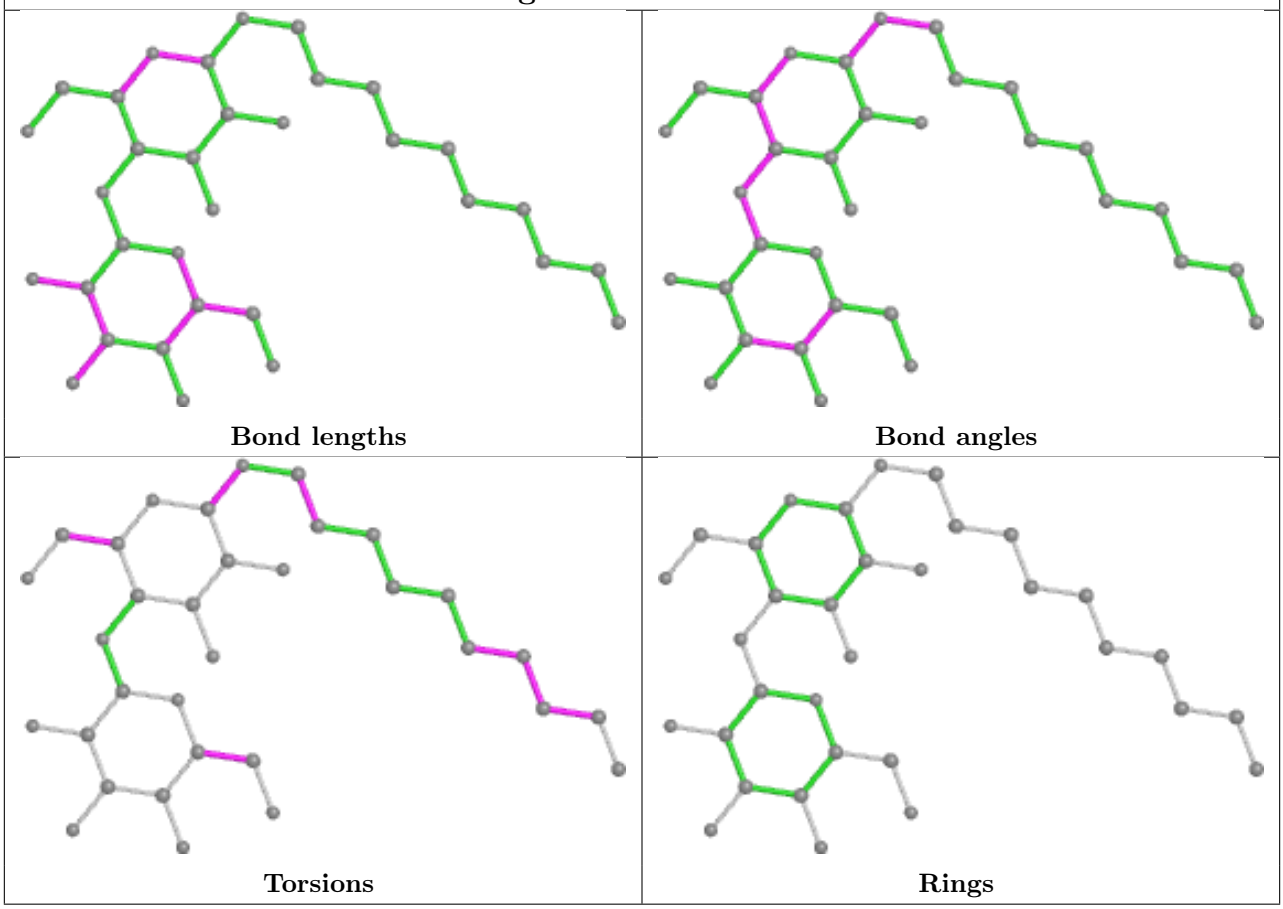
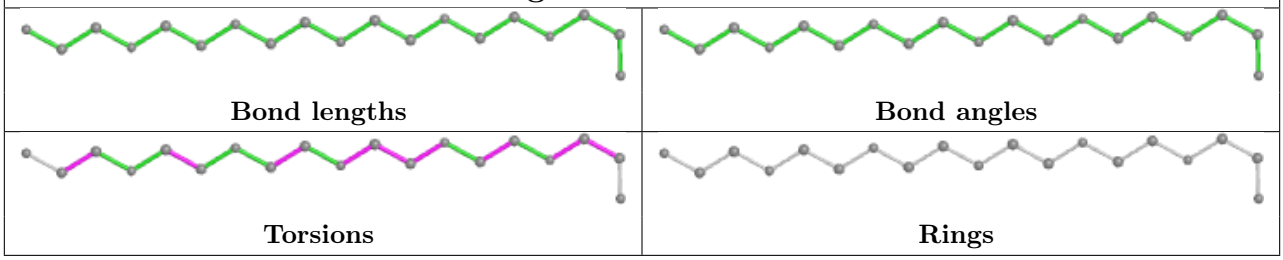
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	520	P6G	1	0
7	A	520	PGE	1	0
8	B	524	P6G	1	0
5	B	506	1PE	1	0
6	B	522	PEG	2	0
8	B	525	P6G	1	0

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 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.

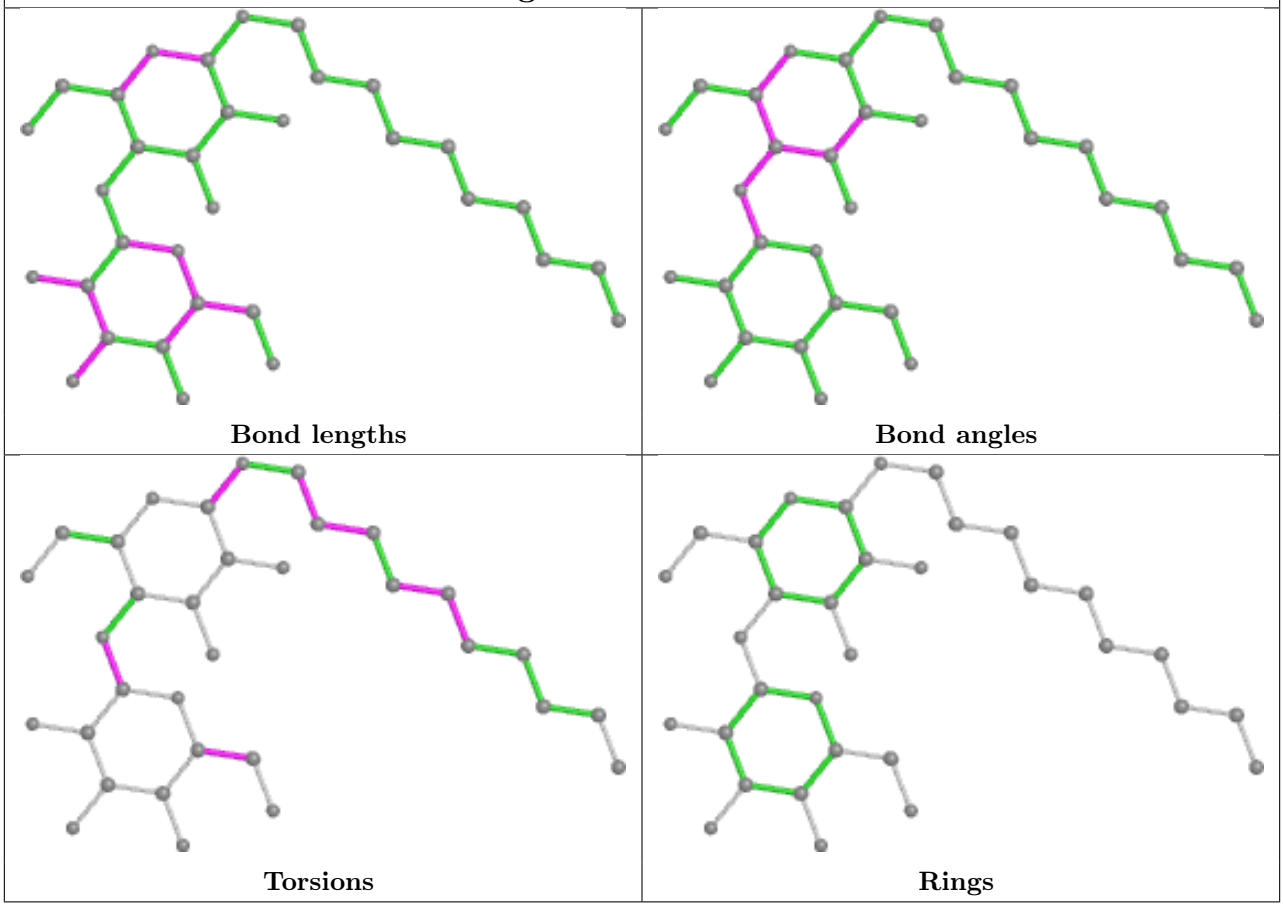
Ligand DMU B 505



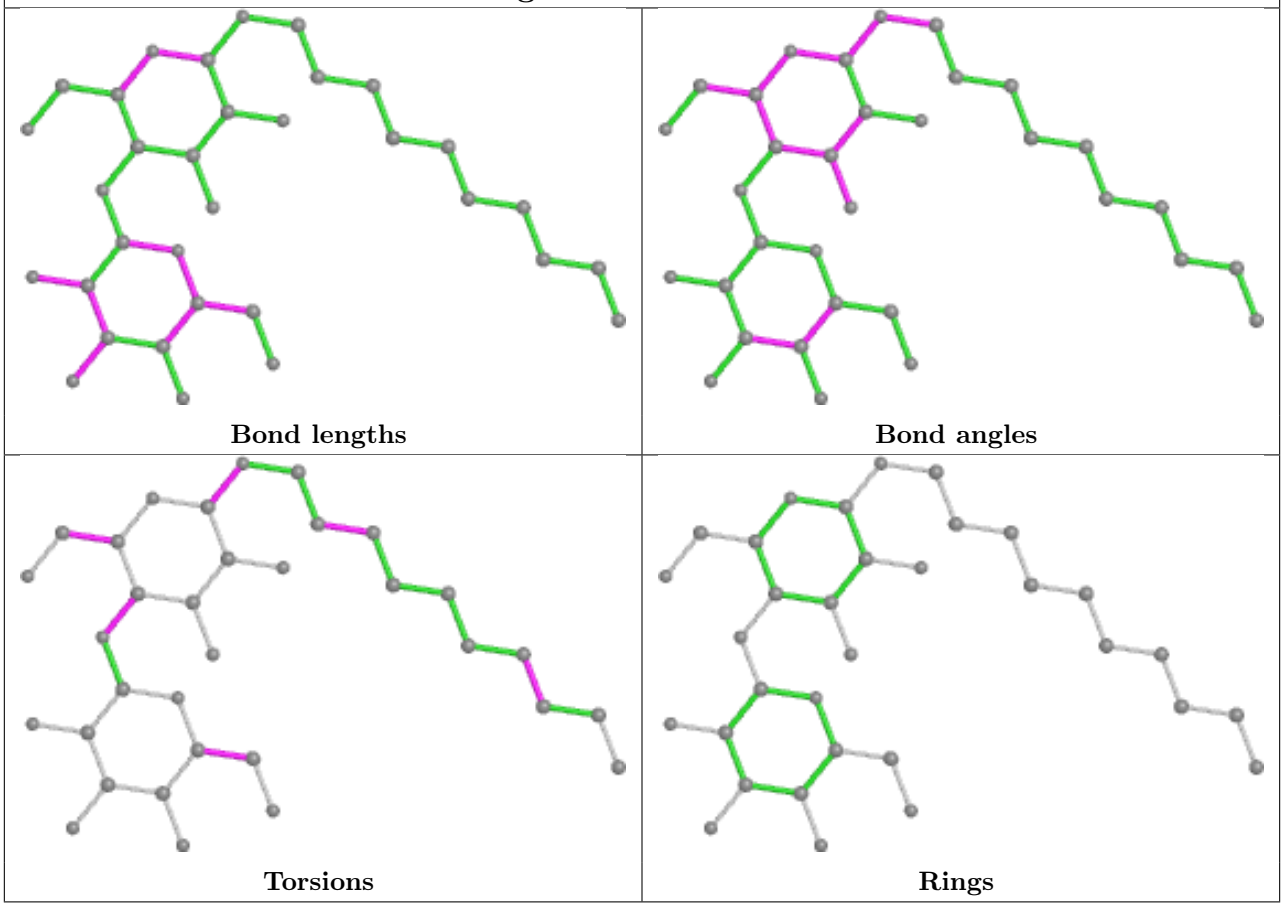
Ligand P6G C 519



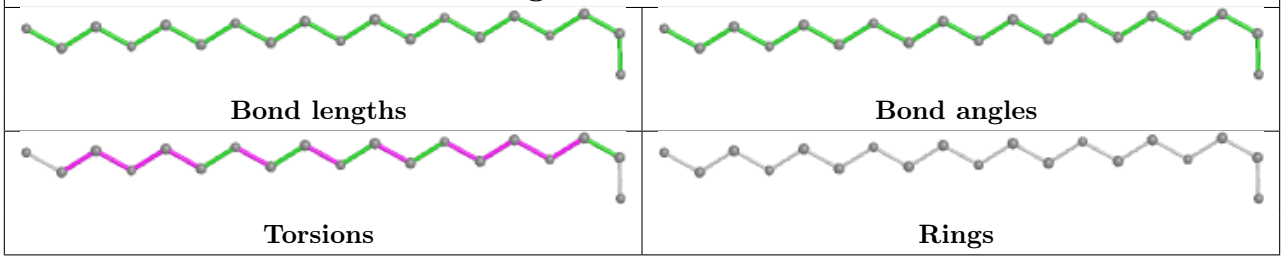
Ligand DMU C 505



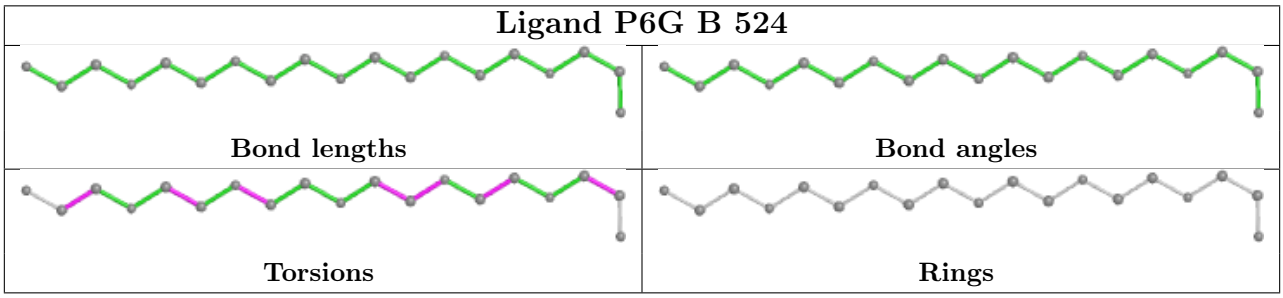
Ligand DMU A 505

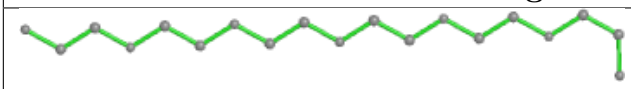
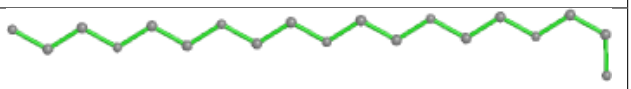
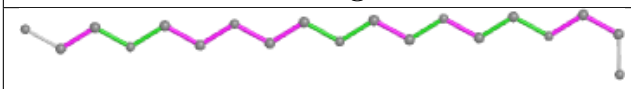
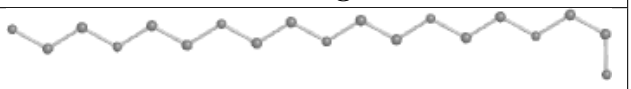


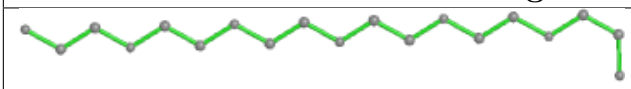
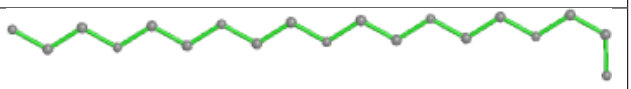
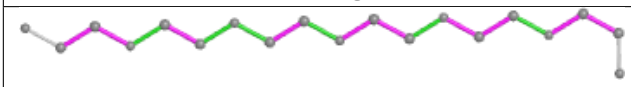
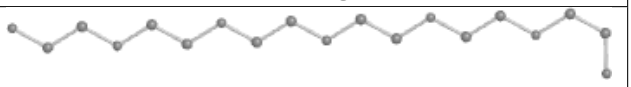
Ligand P6G C 520



Ligand P6G B 524



Ligand P6G A 522	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand P6G B 525	
 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	427/438 (97%)	-0.18	16 (3%)	41	31	55, 84, 153, 243	0
1	B	427/438 (97%)	0.06	26 (6%)	21	13	58, 90, 159, 234	0
1	C	426/438 (97%)	-0.08	27 (6%)	20	12	56, 94, 146, 212	0
All	All	1280/1314 (97%)	-0.07	69 (5%)	25	17	55, 89, 154, 243	0

The worst 5 of 69 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	430	SER	8.6
1	B	127	ALA	8.4
1	B	126	GLU	7.6
1	B	124	ALA	6.8
1	B	11	ASP	5.9

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
6	PEG	B	520	7/7	0.54	0.30	120,125,133,138	0
6	PEG	C	514	7/7	0.62	0.84	122,124,129,130	0
5	1PE	B	507	16/16	0.63	0.60	80,121,137,138	0
6	PEG	A	514	7/7	0.64	0.34	119,128,132,132	0
5	1PE	B	508	16/16	0.66	0.36	121,139,151,151	0
6	PEG	C	513	7/7	0.67	0.46	113,118,124,125	0
8	P6G	C	519	19/19	0.67	0.30	83,109,120,122	0
6	PEG	B	515	7/7	0.68	0.14	109,110,118,120	0
6	PEG	A	511	7/7	0.68	0.21	111,116,121,121	0
6	PEG	B	521	7/7	0.68	0.24	124,124,128,129	0
6	PEG	B	519	7/7	0.69	0.58	132,133,142,142	0
8	P6G	B	525	19/19	0.69	0.25	95,125,130,131	0
5	1PE	C	507	16/16	0.69	0.15	127,143,149,151	0
7	PGE	B	523	10/10	0.70	0.23	108,130,138,139	0
5	1PE	B	506	16/16	0.72	0.47	94,113,121,125	0
6	PEG	B	522	7/7	0.73	0.56	120,125,133,134	0
6	PEG	B	517	7/7	0.73	0.22	110,113,118,119	0
4	DMU	A	505	33/33	0.73	0.58	108,156,169,172	0
7	PGE	C	518	10/10	0.74	0.36	124,133,135,137	0
8	P6G	A	522	19/19	0.74	0.26	99,124,135,137	0
5	1PE	A	507	16/16	0.76	0.30	111,124,133,133	0
6	PEG	B	511	7/7	0.76	0.55	109,122,129,132	0
6	PEG	A	513	7/7	0.76	0.26	125,130,134,137	0
8	P6G	C	520	19/19	0.76	0.41	111,120,138,139	0
6	PEG	C	515	7/7	0.77	0.16	121,121,123,123	0
6	PEG	C	509	7/7	0.78	0.57	92,105,108,108	0
6	PEG	B	512	7/7	0.78	0.32	100,106,116,117	0
6	PEG	B	516	7/7	0.79	0.42	105,118,124,124	0
7	PGE	A	520	10/10	0.79	0.25	97,102,114,117	0
6	PEG	C	511	7/7	0.80	0.29	115,118,120,120	0
8	P6G	B	524	19/19	0.81	0.22	78,96,112,114	0
5	1PE	A	506	16/16	0.81	0.30	107,117,124,125	0
6	PEG	C	512	7/7	0.81	0.14	106,115,124,124	0
6	PEG	A	515	7/7	0.81	0.18	128,133,136,138	0
6	PEG	A	510	7/7	0.82	0.36	105,106,110,113	0
6	PEG	A	517	7/7	0.83	0.18	112,123,133,133	0
6	PEG	C	516	7/7	0.83	0.39	130,134,140,144	0
3	NA	B	504	1/1	0.84	0.10	112,112,112,112	0
6	PEG	A	512	7/7	0.84	0.31	96,112,119,119	0
7	PGE	A	521	10/10	0.84	0.23	125,136,140,141	0
6	PEG	B	513	7/7	0.84	0.30	98,105,121,123	0
5	1PE	C	506	16/16	0.84	0.41	91,137,155,156	0
6	PEG	A	509	7/7	0.85	0.41	87,88,95,95	0

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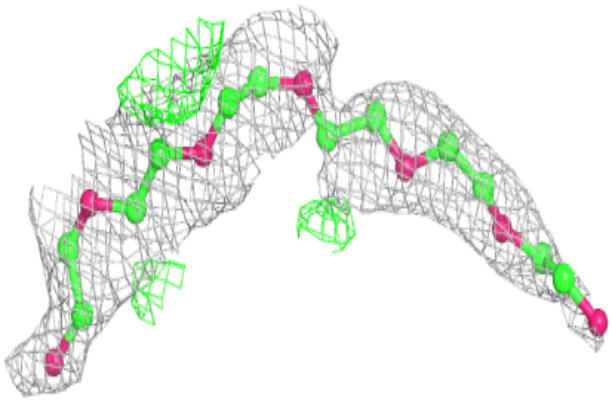
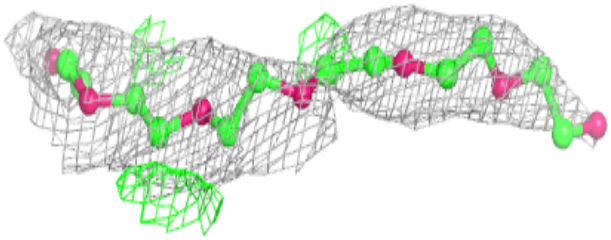
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	DMU	B	505	33/33	0.85	0.32	93,142,154,161	0
7	PGE	A	519	10/10	0.86	0.21	81,87,108,113	0
7	PGE	C	517	10/10	0.86	0.28	124,132,137,137	0
3	NA	C	504	1/1	0.87	0.14	85,85,85,85	0
6	PEG	C	508	7/7	0.88	0.52	93,96,97,97	0
4	DMU	C	505	33/33	0.88	0.64	81,140,149,151	0
6	PEG	C	510	7/7	0.88	0.61	102,109,111,115	0
6	PEG	B	518	7/7	0.88	0.44	103,114,121,125	0
6	PEG	B	514	7/7	0.88	0.13	104,110,117,118	0
3	NA	C	503	1/1	0.89	0.09	66,66,66,66	0
6	PEG	B	509	7/7	0.89	0.31	98,101,106,108	0
7	PGE	A	518	10/10	0.90	0.15	78,94,102,104	0
6	PEG	A	516	7/7	0.91	0.83	105,108,133,140	0
6	PEG	B	510	7/7	0.92	0.30	95,98,100,102	0
6	PEG	A	508	7/7	0.93	0.37	87,89,92,93	0
3	NA	B	502	1/1	0.93	0.08	68,68,68,68	0
3	NA	A	504	1/1	0.93	0.11	86,86,86,86	0
3	NA	A	503	1/1	0.94	0.12	65,65,65,65	0
2	ASP	A	501	9/9	0.95	0.21	63,70,79,87	0
3	NA	B	503	1/1	0.95	0.17	61,61,61,61	0
2	ASP	B	501	9/9	0.96	0.19	63,73,87,104	0
3	NA	A	502	1/1	0.97	0.24	63,63,63,63	0
2	ASP	C	501	9/9	0.98	0.18	71,76,81,86	0
3	NA	C	502	1/1	0.99	0.28	75,75,75,75	0

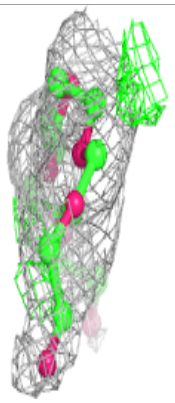
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around P6G C 519:

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

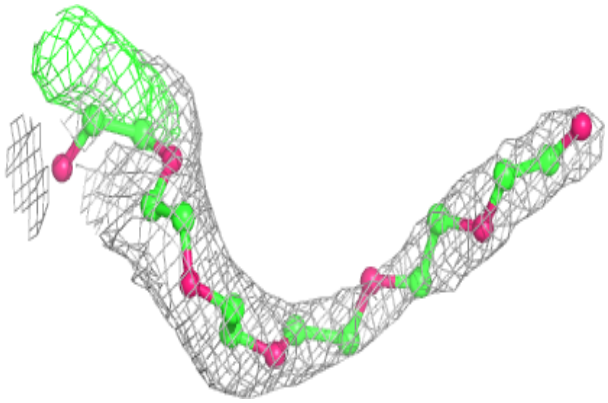


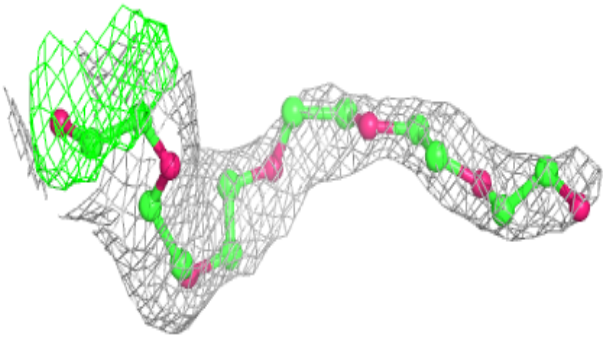


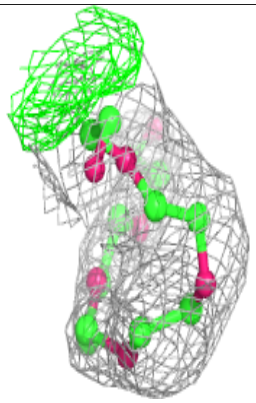


Electron density around P6G B 525:

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

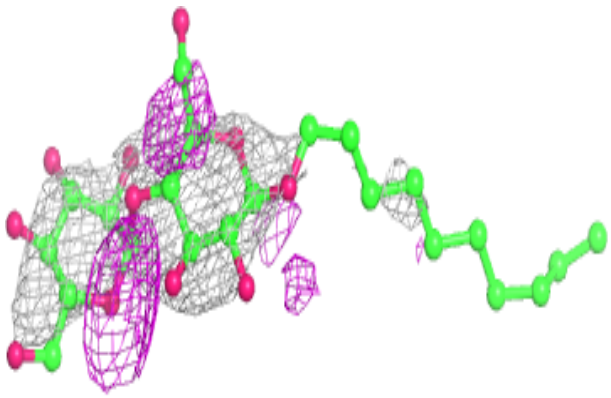


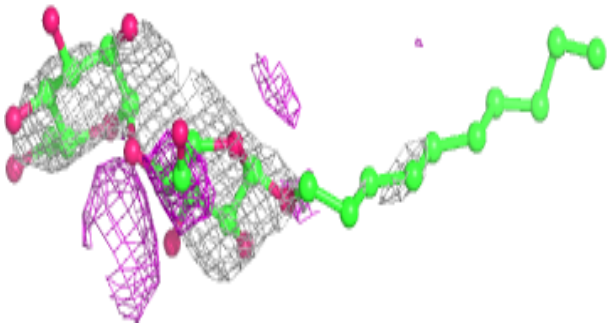


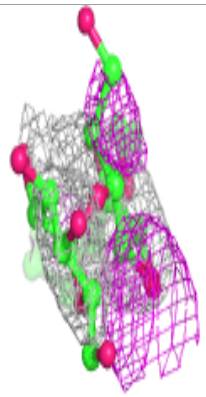


Electron density around DMU A 505:

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

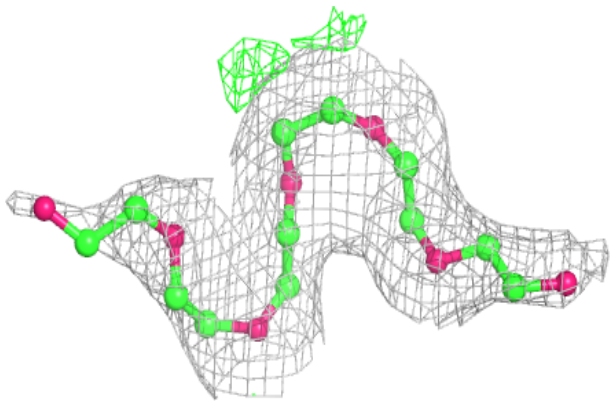


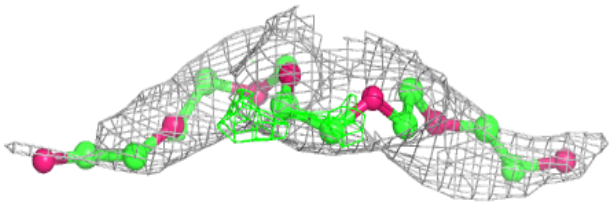


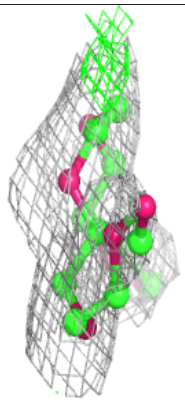


Electron density around P6G A 522:

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

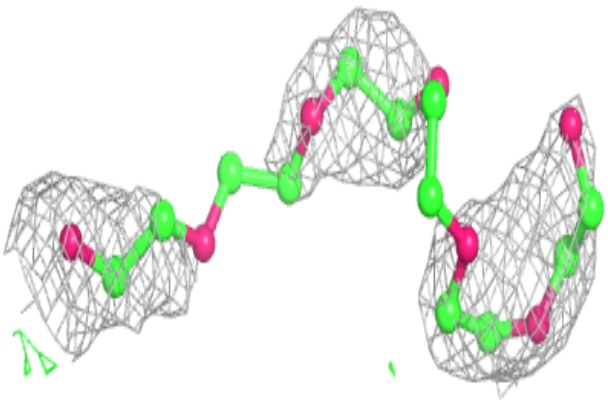


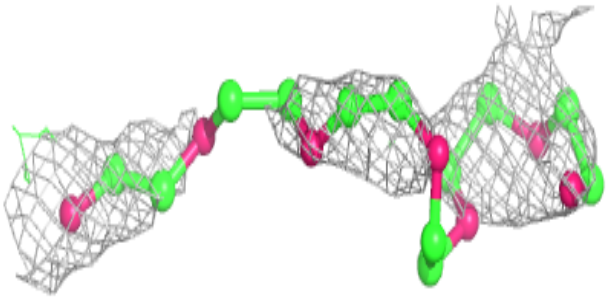


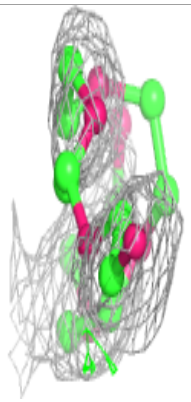


Electron density around P6G C 520:

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

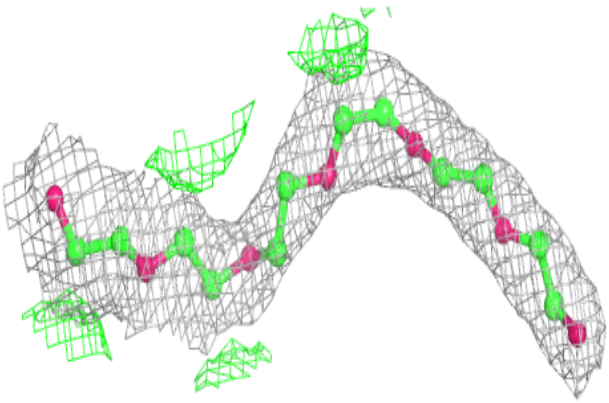


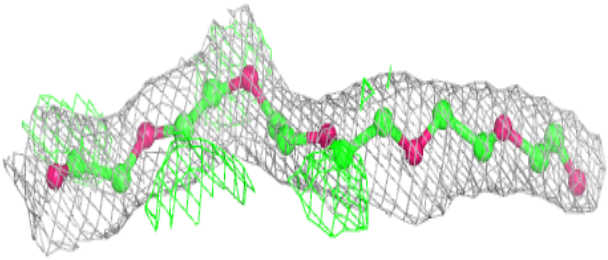


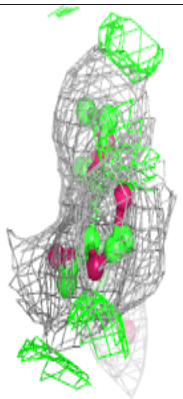


Electron density around P6G B 524:

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

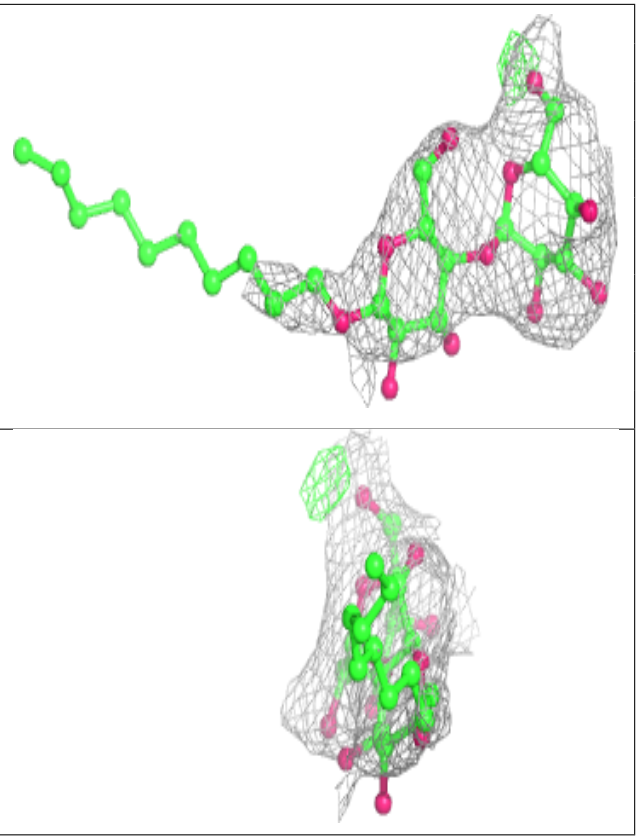






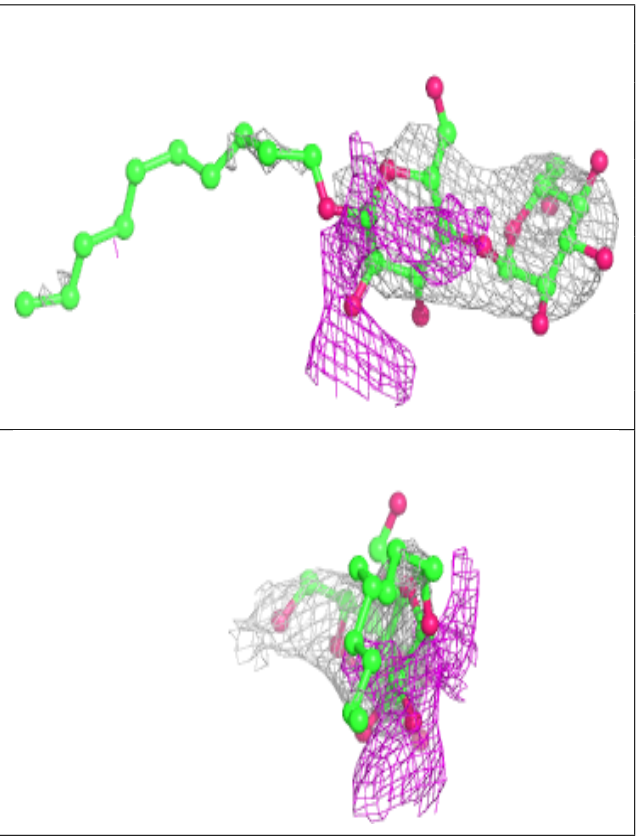
Electron density around DMU B 505:

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



Electron density around DMU C 505:

$2mF_o$-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.