



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 25, 2022 – 06:12 PM JST

PDB ID : 7W6G
Title : TKS-L190G mutant from Cannabis sativa in complex with lauroyl-CoA
Authors : Nakashima, Y.; Lee, Y.E.; Morita, H.
Deposited on : 2021-12-01
Resolution : 2.10 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 : 2.26
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) : 2.26

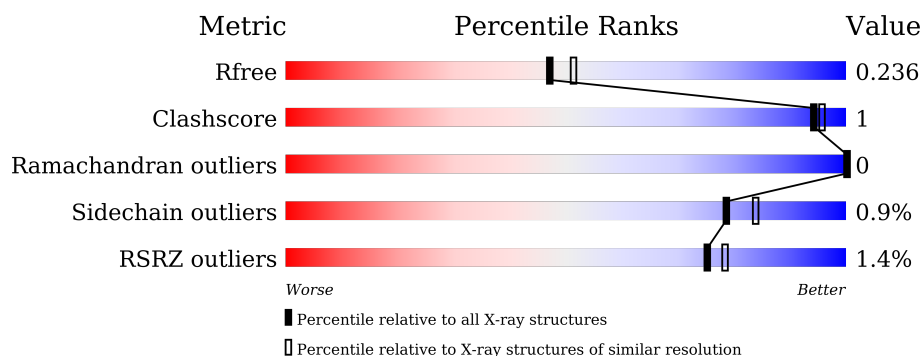
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 $\leq 5\%$. 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	385	<div> <div>%</div> <div> <div></div> <div>97%</div> <div>..</div> </div> </div>
1	B	385	<div> <div>3%</div> <div> <div></div> <div>94%</div> <div>5% .</div> </div> </div>
1	C	385	<div> <div>%</div> <div> <div></div> <div>94%</div> <div>5% .</div> </div> </div>
1	D	385	<div> <div>%</div> <div> <div></div> <div>96%</div> <div>..</div> </div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 25007 atoms, of which 12162 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.

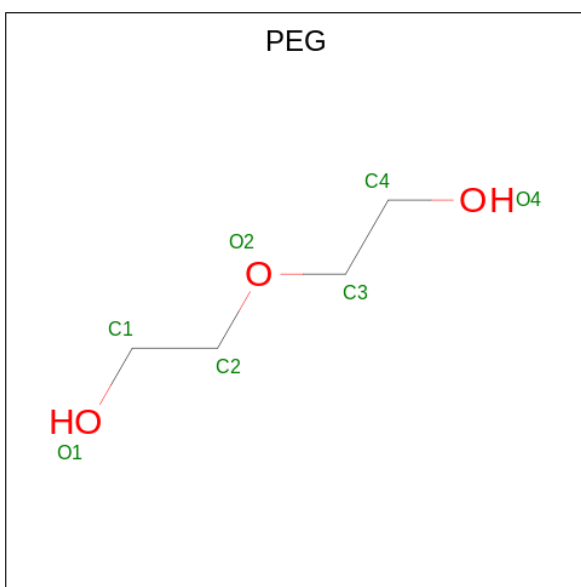
- Molecule 1 is a protein called 3,5,7-trioxododecanoyl-CoA synthase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	383	Total	C	H	N	O	S	0	13	0
			5973	1906	2973	512	558	24			
1	B	381	Total	C	H	N	O	S	0	10	0
			5895	1875	2935	511	551	23			
1	C	382	Total	C	H	N	O	S	0	15	0
			5981	1903	2979	509	566	24			
1	D	383	Total	C	H	N	O	S	0	15	0
			6039	1914	3013	520	570	22			

There are 4 discrepancies between the modelled and reference sequences:

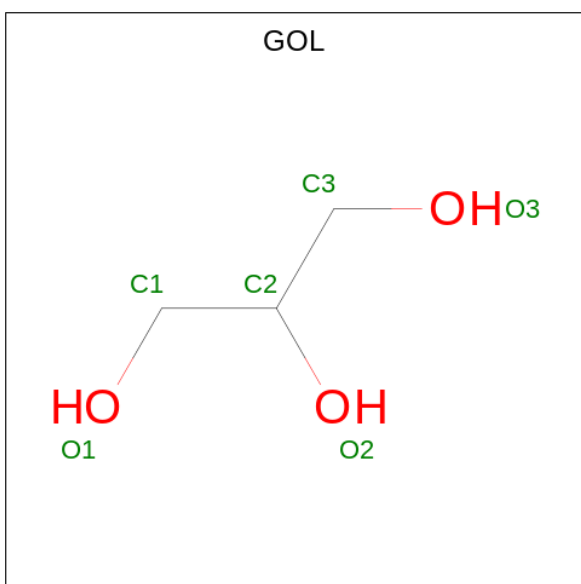
Chain	Residue	Modelled	Actual	Comment	Reference
A	190	GLY	LEU	engineered mutation	UNP B1Q2B6
B	190	GLY	LEU	engineered mutation	UNP B1Q2B6
C	190	GLY	LEU	engineered mutation	UNP B1Q2B6
D	190	GLY	LEU	engineered mutation	UNP B1Q2B6

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



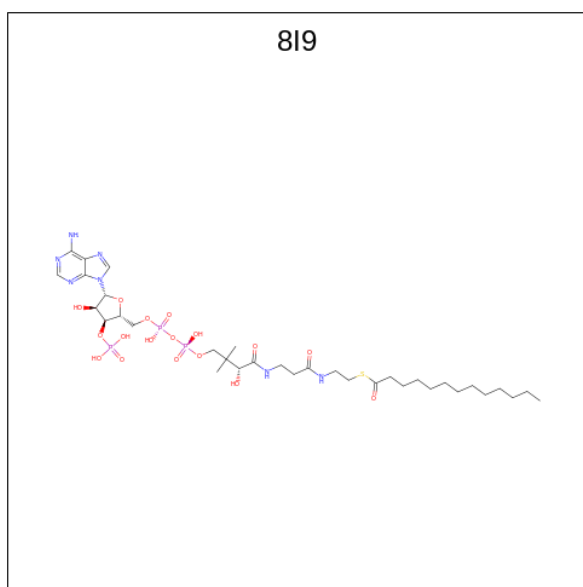
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			17	4	10	3		
2	A	1	Total	C	H	O	0	0
			17	4	10	3		
2	B	1	Total	C	H	O	0	0
			17	4	10	3		
2	C	1	Total	C	H	O	0	0
			17	4	10	3		
2	C	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



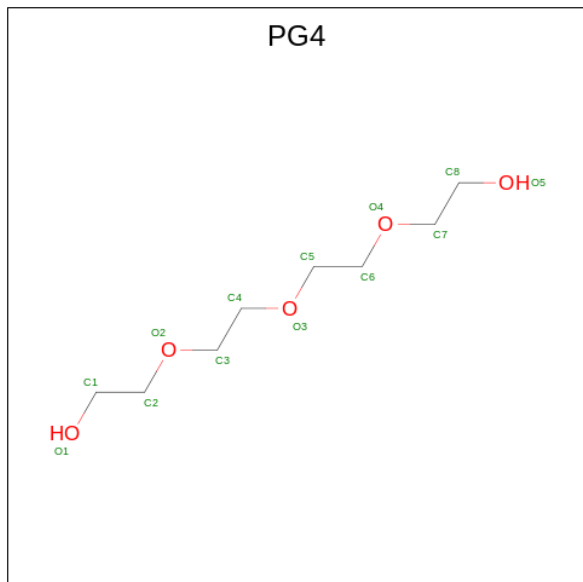
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			13	3	7	3		
3	C	1	Total	C	H	O	0	0
			13	3	7	3		
3	C	1	Total	C	H	O	0	0
			14	3	8	3		
3	C	1	Total	C	H	O	0	0
			14	3	8	3		
3	C	1	Total	C	H	O	0	0
			14	3	8	3		
3	D	1	Total	C	H	O	0	0
			13	3	7	3		
3	D	1	Total	C	H	O	0	0
			13	3	7	3		
3	D	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 4 is {S}-[2-[3-[[[(2 {R})-4-[[[(2 {R},3 {S},4 {R},5 {R})-5-(6-aminopurin-9-yl)-4-oxidanyl-3-phosphonoxy-oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl]oxy-3,3-dimethyl-2-oxidanyl-butanoyl]amino]propanoylamino]ethyl]tridecanethioate (three-letter code: 8I9) (formula: C₃₄H₆₀N₇O₁₇P₃S) (labeled as "Ligand of Interest" by depositor).



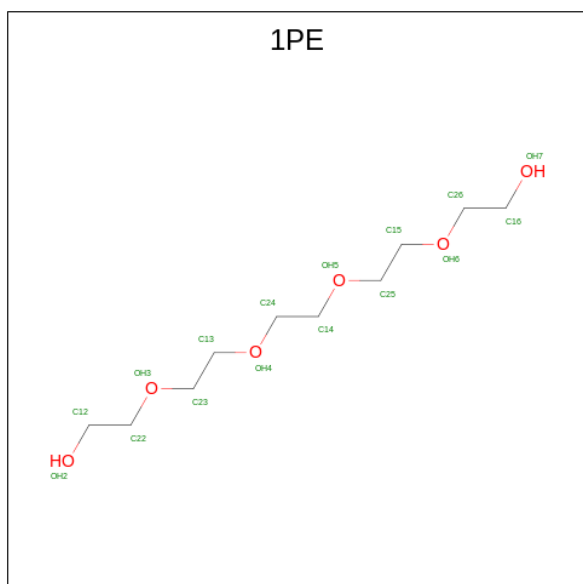
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	C	1	Total	C	H	N	O	P	S	0	0
			118	34	56	7	17	3	1		
4	D	1	Total	C	H	N	O	P	S	0	0
			118	34	56	7	17	3	1		

- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	H	O	0	0
			38	10	22	6		

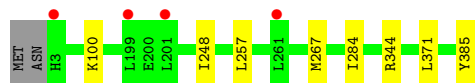
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	155	Total 155	O 155	0	0
7	B	160	Total 160	O 160	0	0
7	C	153	Total 153	O 153	0	0
7	D	153	Total 153	O 153	0	0

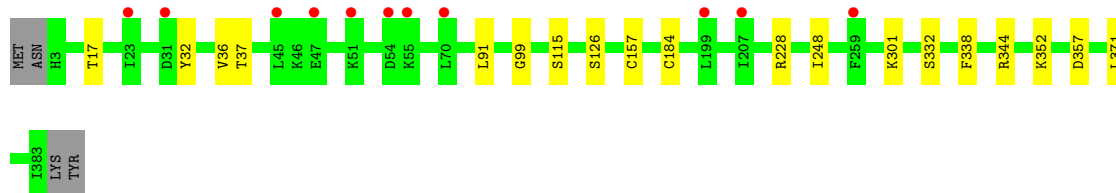
3 Residue-property plots [i](#)

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.

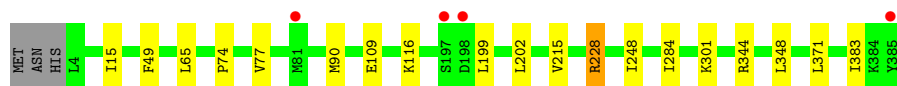
- Molecule 1: 3,5,7-trioxododecanoyl-CoA synthase



- Molecule 1: 3,5,7-trioxododecanoyl-CoA synthase



- Molecule 1: 3,5,7-trioxododecanoyl-CoA synthase



- Molecule 1: 3,5,7-trioxododecanoyl-CoA synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	58.02Å 66.93Å 95.09Å 93.45° 102.11° 100.20°	Depositor
Resolution (Å)	47.18 – 2.10 47.18 – 2.10	Depositor EDS
% Data completeness (in resolution range)	92.9 (47.18-2.10) 92.7 (47.18-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.194 , 0.236 0.194 , 0.236	Depositor DCC
R_{free} test set	3635 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25007	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 57.54 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3313e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE, PG4, GOL, CSD, PEG, 8I9

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	0.28	0/3064	0.47	0/4140
1	B	0.27	0/3016	0.46	0/4076
1	C	0.28	0/3078	0.48	0/4155
1	D	0.29	0/3094	0.47	0/4179
All	All	0.28	0/12252	0.47	0/16550

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3000	2973	2953	4	0
1	B	2960	2935	2919	9	0
1	C	3002	2979	2946	9	1
1	D	3026	3013	2984	9	1
2	A	14	20	20	2	0
2	B	7	10	10	0	0
2	C	14	20	20	0	0
3	A	6	7	8	0	0
3	C	24	31	32	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	18	22	24	0	0
4	C	62	56	0	0	0
4	D	62	56	0	3	0
5	C	13	18	18	0	0
6	C	16	22	22	0	0
7	A	155	0	0	0	0
7	B	160	0	0	0	1
7	C	153	0	0	0	0
7	D	153	0	0	1	1
All	All	12845	12162	11956	31	2

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 1.

All (31) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:270:SER:O	7:D:501:HOH:O	2.07	0.73
1:C:348:LEU:HD23	1:C:383:ILE:HD13	1.75	0.68
1:C:74:PRO:O	1:C:77:VAL:HG22	1.98	0.64
1:B:248:ILE:HD12	1:B:371:LEU:HG	1.91	0.53
1:B:228:ARG:O	1:B:228:ARG:HG3	2.12	0.49
1:D:74:PRO:O	1:D:77:VAL:HG22	2.13	0.49
1:B:36:VAL:HG23	1:B:37:THR:HG23	1.95	0.49
1:A:385:TYR:OXT	2:A:501:PEG:O4	2.20	0.48
1:A:257:LEU:HD21	2:A:502:PEG:H32	1.94	0.48
1:B:17:THR:HG23	1:B:338:PHE:CZ	2.48	0.48
1:D:55:LYS:HD3	4:D:401:8I9:O26	2.13	0.48
1:C:65:LEU:HD13	1:C:90[B]:MET:HE1	1.96	0.46
1:B:32:TYR:CZ	1:B:36:VAL:HG11	2.51	0.45
1:D:284:ILE:O	1:D:284:ILE:HG22	2.17	0.45
1:C:284:ILE:HG22	1:C:284:ILE:O	2.17	0.44
1:C:109:GLU:OE2	1:C:228:ARG:NH1	2.39	0.44
1:C:199:LEU:HD23	1:C:202:LEU:HD12	2.00	0.43
1:D:261:LEU:HD11	4:D:401:8I9:O57	2.18	0.43
1:D:55:LYS:CD	4:D:401:8I9:O26	2.66	0.43
1:D:107:ILE:HD13	1:D:114[A]:LYS:HZ2	1.82	0.43
1:B:157:CSD:SG	1:B:332:SER:HA	2.59	0.43
1:D:55:LYS:O	1:D:301:LYS:HD2	2.18	0.43
1:C:15:ILE:HG12	1:C:215:VAL:HG12	2.01	0.42
1:B:99:GLY:CA	1:B:184[B]:CYS:SG	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:LEU:HD13	1:B:126:SER:O	2.19	0.42
1:C:248:ILE:HD12	1:C:371:LEU:HG	2.00	0.42
1:D:319:VAL:HG13	1:D:320:ASP:N	2.35	0.41
1:A:284:ILE:HG22	1:A:284:ILE:O	2.19	0.41
1:A:248:ILE:HD12	1:A:371:LEU:HG	2.03	0.41
1:B:352:LYS:NZ	1:B:357:ASP:OD1	2.47	0.40
1:C:49:PHE:HB2	1:C:202:LEU:HD13	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:605:HOH:O	7:D:611:HOH:O[1_445]	2.01	0.19
1:C:116:LYS:NZ	1:D:243:ASN:OD1[1_454]	2.10	0.10

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	393/385 (102%)	384 (98%)	9 (2%)	0	100	100
1	B	388/385 (101%)	375 (97%)	13 (3%)	0	100	100
1	C	394/385 (102%)	387 (98%)	7 (2%)	0	100	100
1	D	395/385 (103%)	388 (98%)	7 (2%)	0	100	100
All	All	1570/1540 (102%)	1534 (98%)	36 (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	317/326 (97%)	313 (99%)	4 (1%)	69	75
1	B	315/326 (97%)	312 (99%)	3 (1%)	76	82
1	C	322/326 (99%)	319 (99%)	3 (1%)	78	84
1	D	327/326 (100%)	325 (99%)	2 (1%)	86	90
All	All	1281/1304 (98%)	1269 (99%)	12 (1%)	78	84

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	LYS
1	A	267[A]	MET
1	A	267[B]	MET
1	A	344	ARG
1	B	115	SER
1	B	301	LYS
1	B	344	ARG
1	C	228	ARG
1	C	301	LYS
1	C	344	ARG
1	D	228	ARG
1	D	344	ARG

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](#)

4 non-standard protein/DNA/RNA residues 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
1	CSD	B	157	1	3,7,8	1.04	0	1,8,10	1.31	0
1	CSD	A	157	1	3,7,8	0.97	0	1,8,10	0.38	0
1	CSD	C	157	1	3,7,8	1.01	0	1,8,10	1.70	0
1	CSD	D	157	1	3,7,8	1.05	0	1,8,10	1.20	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
1	CSD	B	157	1	-	1/2/6/8	-
1	CSD	A	157	1	-	1/2/6/8	-
1	CSD	C	157	1	-	2/2/6/8	-
1	CSD	D	157	1	-	1/2/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	157	CSD	CA-CB-SG-OD1
1	B	157	CSD	CA-CB-SG-OD1
1	C	157	CSD	N-CA-CB-SG
1	C	157	CSD	CA-CB-SG-OD1
1	D	157	CSD	CA-CB-SG-OD1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	157	CSD	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

17 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
4	8I9	C	401	-	56,64,64	3.38	13 (23%)	67,90,90	1.50	8 (11%)
3	GOL	D	404	-	5,5,5	0.87	0	5,5,5	0.78	0
2	PEG	B	401	-	6,6,6	0.49	0	5,5,5	0.40	0
2	PEG	C	406	-	6,6,6	0.48	0	5,5,5	0.22	0
2	PEG	A	502	-	6,6,6	0.48	0	5,5,5	0.24	0
3	GOL	A	503	-	5,5,5	0.88	0	5,5,5	0.90	0
3	GOL	C	403	-	5,5,5	0.95	0	5,5,5	0.91	0
3	GOL	C	405	-	5,5,5	0.82	0	5,5,5	0.65	0
4	8I9	D	401	-	56,64,64	3.39	13 (23%)	67,90,90	1.53	12 (17%)
3	GOL	D	403	-	5,5,5	0.84	0	5,5,5	1.06	0
2	PEG	A	501	-	6,6,6	0.49	0	5,5,5	0.24	0
6	1PE	C	408	-	15,15,15	0.54	0	14,14,14	0.71	0
3	GOL	C	404	-	5,5,5	0.84	0	5,5,5	1.02	0
3	GOL	C	409	-	5,5,5	0.92	0	5,5,5	1.01	0
3	GOL	D	402	-	5,5,5	0.87	0	5,5,5	0.96	0
5	PG4	C	407	-	12,12,12	0.53	0	11,11,11	0.48	0
2	PEG	C	402	-	6,6,6	0.49	0	5,5,5	0.21	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
4	8I9	C	401	-	-	16/59/79/79	0/3/3/3
3	GOL	D	404	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	B	401	-	-	3/4/4/4	-
2	PEG	C	406	-	-	1/4/4/4	-
2	PEG	A	502	-	-	2/4/4/4	-
3	GOL	A	503	-	-	0/4/4/4	-
3	GOL	C	403	-	-	2/4/4/4	-
3	GOL	C	405	-	-	2/4/4/4	-
4	8I9	D	401	-	-	16/59/79/79	0/3/3/3
3	GOL	D	403	-	-	2/4/4/4	-
2	PEG	A	501	-	-	2/4/4/4	-
6	1PE	C	408	-	-	8/13/13/13	-
3	GOL	C	404	-	-	0/4/4/4	-
3	GOL	C	409	-	-	1/4/4/4	-
3	GOL	D	402	-	-	0/4/4/4	-
5	PG4	C	407	-	-	5/10/10/10	-
2	PEG	C	402	-	-	3/4/4/4	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	401	8I9	C12-C11	-14.70	1.31	1.53
4	C	401	8I9	C12-C11	-14.58	1.31	1.53
4	C	401	8I9	C14-C20	-10.13	1.25	1.52
4	D	401	8I9	C14-C20	-9.97	1.26	1.52
4	C	401	8I9	O62-C11	9.33	1.54	1.41
4	D	401	8I9	O62-C11	9.23	1.54	1.41
4	D	401	8I9	O62-C20	7.95	1.62	1.45
4	C	401	8I9	O62-C20	7.92	1.62	1.45
4	D	401	8I9	C12-C14	7.44	1.69	1.52
4	C	401	8I9	C12-C14	7.24	1.69	1.52
4	D	401	8I9	C34-N35	5.70	1.46	1.33
4	C	401	8I9	C34-N35	5.64	1.45	1.33
4	D	401	8I9	C38-N39	5.45	1.45	1.33
4	C	401	8I9	C38-N39	5.39	1.45	1.33
4	D	401	8I9	P16-O15	3.21	1.65	1.59
4	D	401	8I9	C02-N01	3.14	1.45	1.34
4	C	401	8I9	C02-N01	3.10	1.45	1.34
4	C	401	8I9	P16-O15	2.92	1.64	1.59
4	D	401	8I9	C43-S42	2.33	1.81	1.76
4	C	401	8I9	C43-S42	2.22	1.81	1.76
4	D	401	8I9	O58-C34	-2.16	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	401	8I9	O57-C38	-2.06	1.19	1.23
4	D	401	8I9	O57-C38	-2.06	1.19	1.23
4	D	401	8I9	C44-C43	2.05	1.52	1.50
4	C	401	8I9	C44-C43	2.05	1.52	1.50
4	C	401	8I9	O58-C34	-2.04	1.19	1.23

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	401	8I9	C44-C43-S42	5.82	120.23	113.46
4	C	401	8I9	C44-C43-S42	5.67	120.06	113.46
4	C	401	8I9	N05-C04-N03	-4.94	120.96	128.68
4	D	401	8I9	N05-C04-N03	-4.67	121.38	128.68
4	D	401	8I9	P25-O24-P23	-3.93	119.35	132.83
4	C	401	8I9	P25-O24-P23	-3.33	121.39	132.83
4	C	401	8I9	C36-C37-C38	3.33	117.90	112.36
4	D	401	8I9	C06-C07-N08	-3.33	105.93	109.40
4	D	401	8I9	O56-C43-C44	-3.19	120.22	123.99
4	C	401	8I9	O56-C43-C44	-3.01	120.44	123.99
4	C	401	8I9	C06-C07-N08	-3.01	106.27	109.40
4	D	401	8I9	C36-C37-C38	2.72	116.89	112.36
4	C	401	8I9	C41-S42-C43	2.55	109.80	101.87
4	D	401	8I9	C41-S42-C43	2.52	109.72	101.87
4	C	401	8I9	O56-C43-S42	-2.39	119.50	122.61
4	D	401	8I9	O56-C43-S42	-2.36	119.55	122.61
4	D	401	8I9	C12-C14-C20	2.32	107.34	103.22
4	D	401	8I9	C14-C12-C11	2.32	105.03	99.89
4	D	401	8I9	O27-C28-C29	-2.12	107.15	110.55
4	D	401	8I9	O57-C38-C37	-2.05	118.26	122.02

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	403	GOL	C1-C2-C3-O3
3	C	405	GOL	C1-C2-C3-O3
3	D	403	GOL	C1-C2-C3-O3
4	C	401	8I9	N35-C36-C37-C38
4	C	401	8I9	C40-C41-S42-C43
4	C	401	8I9	C43-C44-C45-C46
4	C	401	8I9	C21-O22-P23-O60
4	C	401	8I9	C21-O22-P23-O61

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Mol	Chain	Res	Type	Atoms
4	C	401	8I9	C28-O27-P25-O24
4	D	401	8I9	C40-C41-S42-C43
4	D	401	8I9	C43-C44-C45-C46
4	D	401	8I9	C21-O22-P23-O60
4	D	401	8I9	C21-O22-P23-O61
6	C	408	1PE	OH5-C14-C24-OH4
3	C	405	GOL	O2-C2-C3-O3
4	D	401	8I9	C48-C49-C50-C51
6	C	408	1PE	OH6-C15-C25-OH5
2	A	501	PEG	O1-C1-C2-O2
2	A	502	PEG	O1-C1-C2-O2
4	D	401	8I9	C47-C48-C49-C50
3	D	404	GOL	C1-C2-C3-O3
6	C	408	1PE	OH4-C13-C23-OH3
4	D	401	8I9	N39-C40-C41-S42
3	C	403	GOL	O2-C2-C3-O3
3	D	403	GOL	O2-C2-C3-O3
4	D	401	8I9	C50-C51-C52-C53
4	C	401	8I9	C47-C48-C49-C50
2	C	402	PEG	O2-C3-C4-O4
4	C	401	8I9	C48-C49-C50-C51
4	C	401	8I9	C49-C50-C51-C52
5	C	407	PG4	O3-C5-C6-O4
2	C	402	PEG	O1-C1-C2-O2
4	D	401	8I9	C49-C50-C51-C52
4	D	401	8I9	O56-C43-S42-C41
6	C	408	1PE	C13-C23-OH3-C22
6	C	408	1PE	C12-C22-OH3-C23
4	C	401	8I9	C50-C51-C52-C53
2	B	401	PEG	C1-C2-O2-C3
2	B	401	PEG	O2-C3-C4-O4
4	C	401	8I9	P23-O24-P25-O26
4	C	401	8I9	C28-O27-P25-O26
4	C	401	8I9	N39-C40-C41-S42
4	D	401	8I9	O27-C28-C29-C32
6	C	408	1PE	C23-C13-OH4-C24
5	C	407	PG4	C8-C7-O4-C6
4	D	401	8I9	O27-C28-C29-C30
6	C	408	1PE	C25-C15-OH6-C26
5	C	407	PG4	O1-C1-C2-O2
2	C	406	PEG	O2-C3-C4-O4
4	D	401	8I9	P23-O24-P25-O26

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Mol	Chain	Res	Type	Atoms
2	A	501	PEG	C4-C3-O2-C2
2	A	502	PEG	C1-C2-O2-C3
4	D	401	8I9	O27-C28-C29-C31
2	B	401	PEG	C4-C3-O2-C2
5	C	407	PG4	C6-C5-O3-C4
4	D	401	8I9	C44-C43-S42-C41
5	C	407	PG4	C5-C6-O4-C7
3	C	409	GOL	O1-C1-C2-O2
4	C	401	8I9	C21-O22-P23-O24
4	D	401	8I9	C21-O22-P23-O24
4	C	401	8I9	C52-C53-C54-C55
2	C	402	PEG	C4-C3-O2-C2
6	C	408	1PE	OH7-C16-C26-OH6
4	C	401	8I9	C28-O27-P25-O59

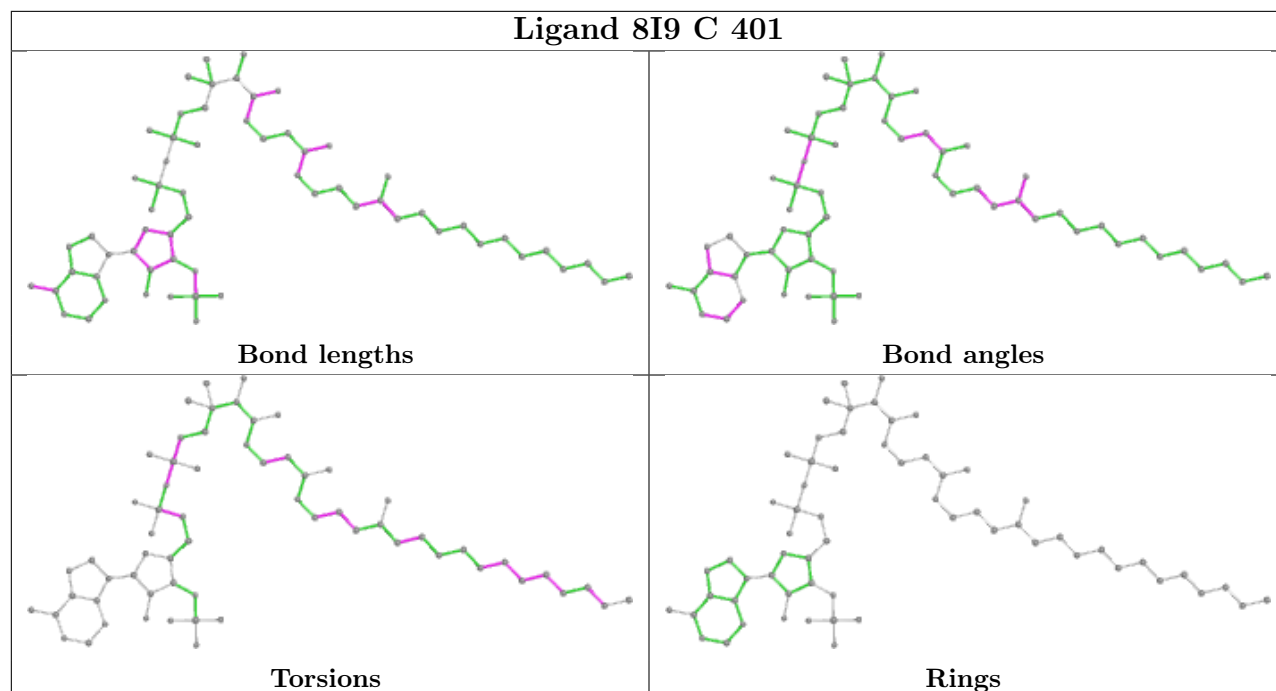
There are no ring outliers.

3 monomers are involved in 5 short contacts:

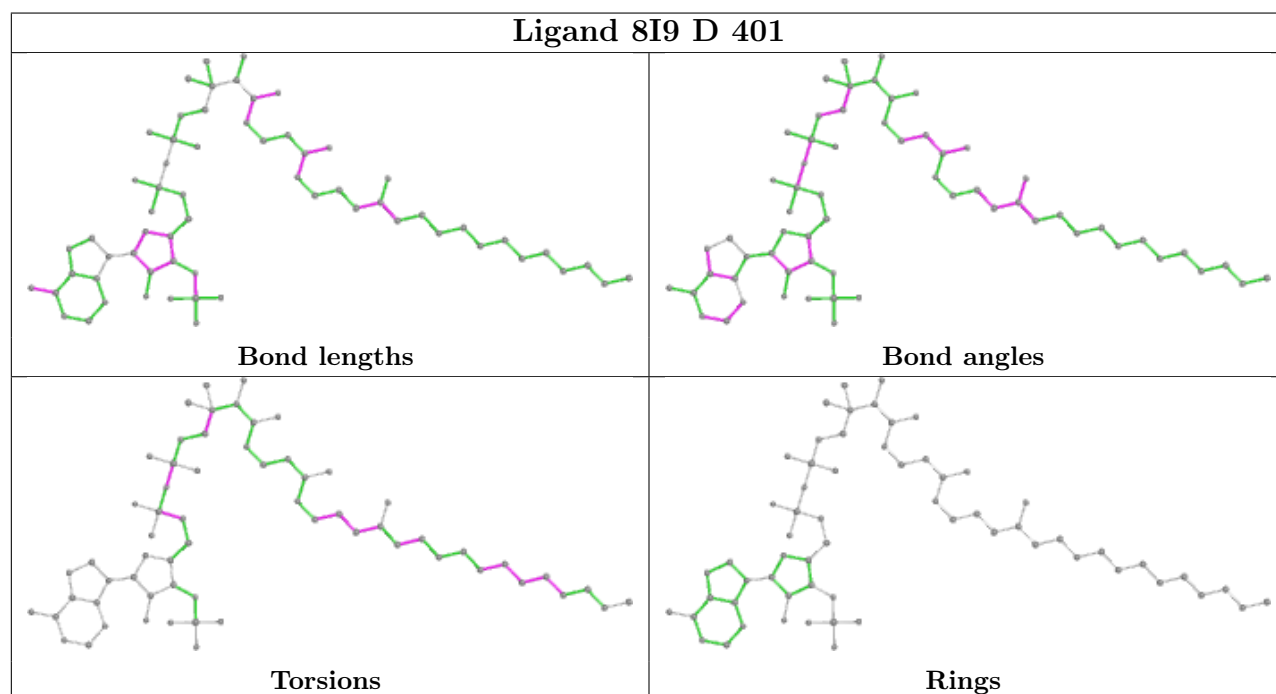
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	PEG	1	0
4	D	401	8I9	3	0
2	A	501	PEG	1	0

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.

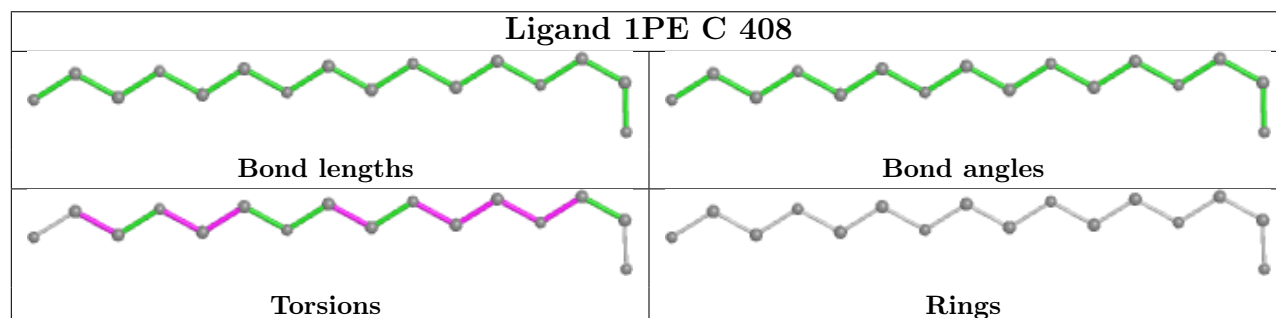
Ligand 8I9 C 401

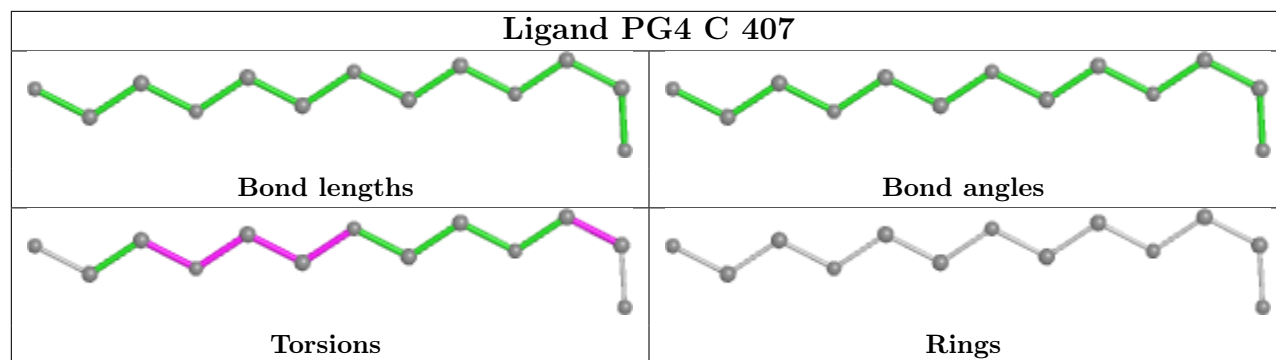


Ligand 8I9 D 401



Ligand 1PE C 408





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

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	382/385 (99%)	-0.28	4 (1%) 82 85	15, 30, 52, 86	0
1	B	380/385 (98%)	-0.10	11 (2%) 51 57	15, 30, 62, 89	0
1	C	381/385 (98%)	-0.25	4 (1%) 82 85	15, 28, 48, 93	0
1	D	382/385 (99%)	-0.30	2 (0%) 91 92	13, 28, 53, 76	0
All	All	1525/1540 (99%)	-0.23	21 (1%) 75 78	13, 29, 54, 93	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	197	SER	4.3
1	B	199	LEU	3.6
1	B	70	LEU	3.3
1	B	47	GLU	3.3
1	B	23	ILE	3.0
1	B	45	LEU	2.9
1	A	199[A]	LEU	2.8
1	B	51	LYS	2.5
1	B	54	ASP	2.4
1	C	198	ASP	2.4
1	B	55	LYS	2.4
1	A	3	HIS	2.4
1	C	385	TYR	2.4
1	A	261[A]	LEU	2.3
1	B	207	ILE	2.3
1	B	31	ASP	2.2
1	C	81[A]	MET	2.2
1	D	197	SER	2.2
1	B	259	PHE	2.1
1	D	40	GLU	2.1
1	A	201	LEU	2.0

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

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
1	CSD	C	157	8/9	0.92	0.19	25,32,40,47	0
1	CSD	A	157	8/9	0.94	0.12	25,36,44,53	0
1	CSD	B	157	8/9	0.96	0.12	25,32,40,46	0
1	CSD	D	157	8/9	0.96	0.13	24,29,35,41	0

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.

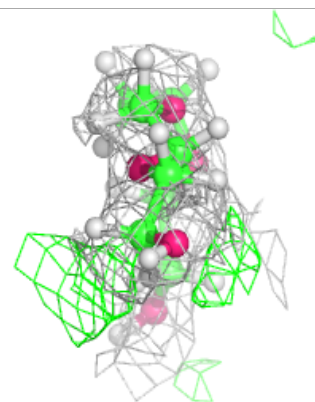
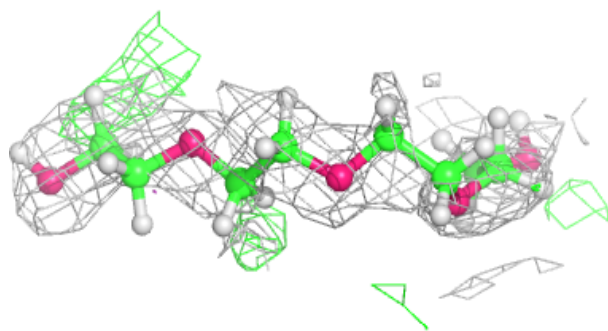
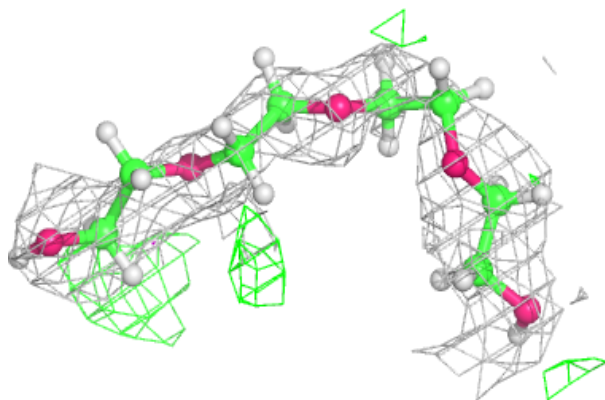
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PEG	B	401	7/7	0.49	0.29	62,75,87,87	0
5	PG4	C	407	13/13	0.52	0.21	71,86,95,95	0
2	PEG	C	406	7/7	0.61	0.23	63,75,80,80	0
2	PEG	A	502	7/7	0.71	0.20	65,78,85,85	0
2	PEG	C	402	7/7	0.71	0.23	65,78,88,89	0
2	PEG	A	501	7/7	0.72	0.14	52,63,75,76	0
3	GOL	D	404	6/6	0.73	0.26	77,92,94,94	0
6	1PE	C	408	16/16	0.76	0.16	40,62,75,76	0
3	GOL	C	409	6/6	0.79	0.21	66,80,85,86	0
3	GOL	A	503	6/6	0.80	0.18	52,59,70,71	0
4	8I9	D	401	62/62	0.88	0.14	34,57,71,77	0
3	GOL	C	405	6/6	0.89	0.23	70,85,86,86	0
4	8I9	C	401	62/62	0.90	0.13	29,44,69,70	0
3	GOL	D	403	6/6	0.91	0.17	31,38,46,46	0
3	GOL	C	403	6/6	0.93	0.14	40,52,61,64	0
3	GOL	D	402	6/6	0.94	0.10	29,35,39,42	0
3	GOL	C	404	6/6	0.97	0.09	20,25,31,33	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.

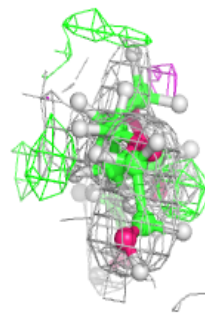
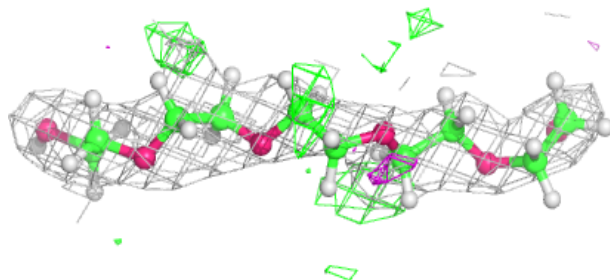
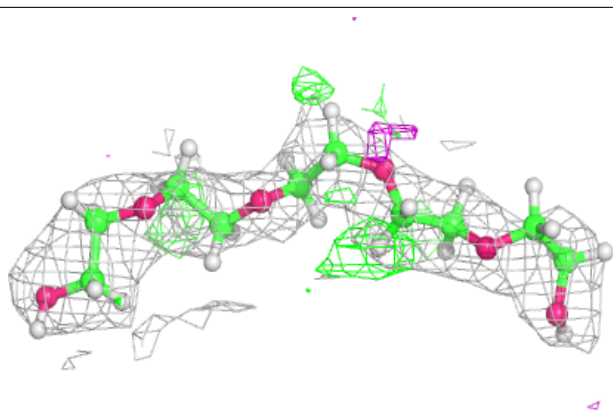
Electron density around PG4 C 407:

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

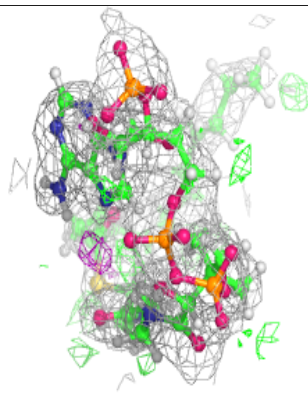
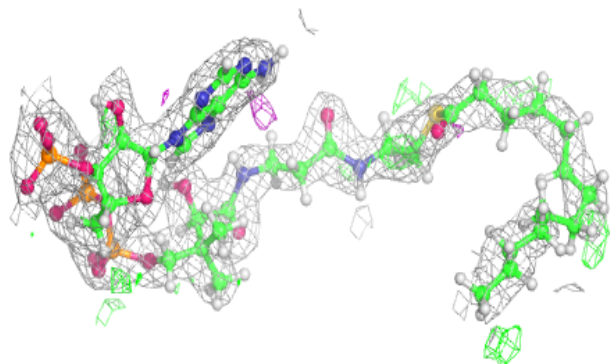
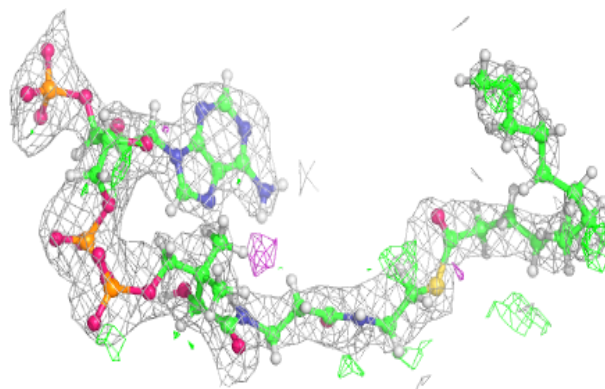


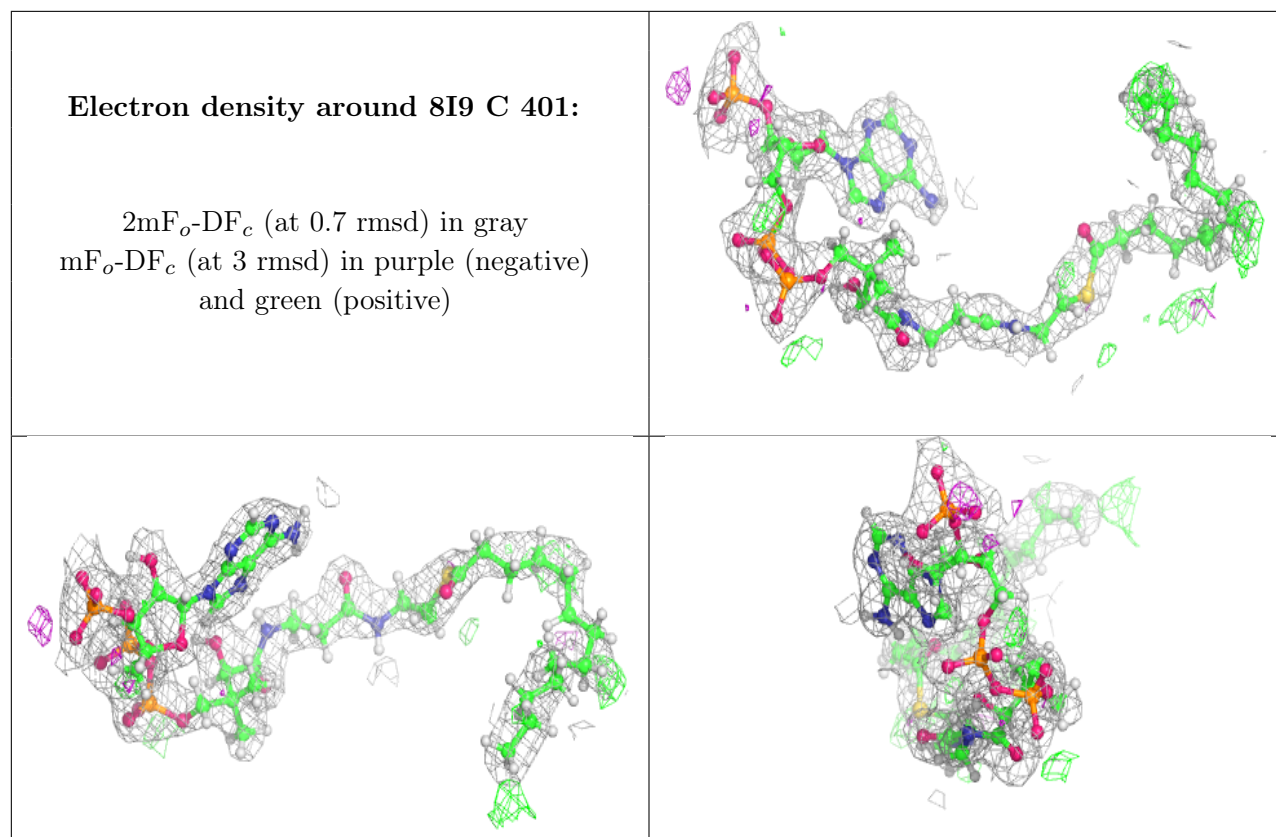
Electron density around 1PE C 408:

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

**Electron density around 8I9 D 401:**

$2mF_o-DF_c$ (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.