Full wwPDB X-ray Structure Validation Report (i)

Sep 23, 2023 – 07:55 PM EDT

PDB ID	:	5SYT
Title	:	Crystal Structure of ZMPSTE24
Authors	:	Clark, K.; Jenkins, J.L.; Fedoriw, N.; Dumont, M.E.; Membrane Protein Structural Biology Consortium (MPSBC)
Deposited on	:	2016-08-11
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

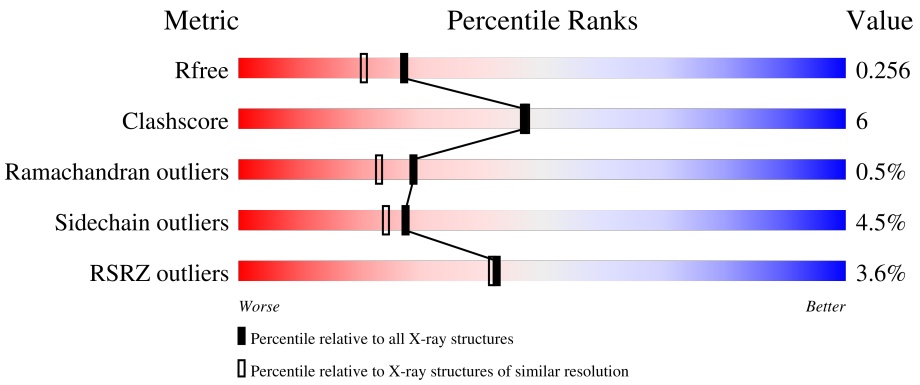
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	480	3% 79% 12% • 8%

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 7938 atoms, of which 3932 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.

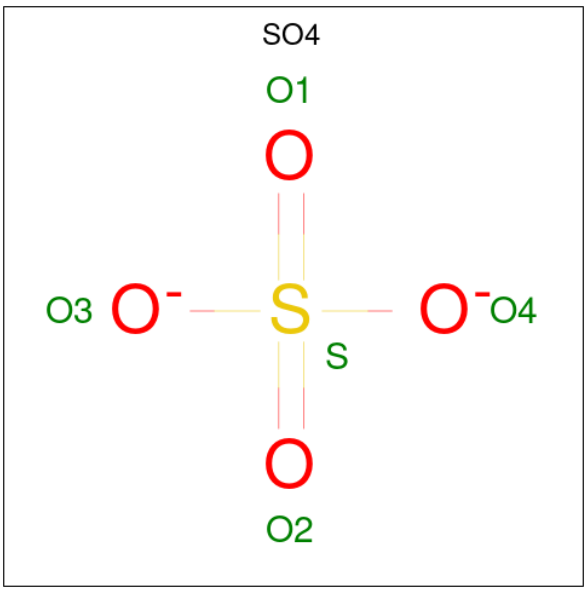
- Molecule 1 is a protein called CAAX prenyl protease 1 homolog.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	444	7123	2380	3554	556	621	12	0	1	0

There are 6 discrepancies between the modelled and reference sequences:

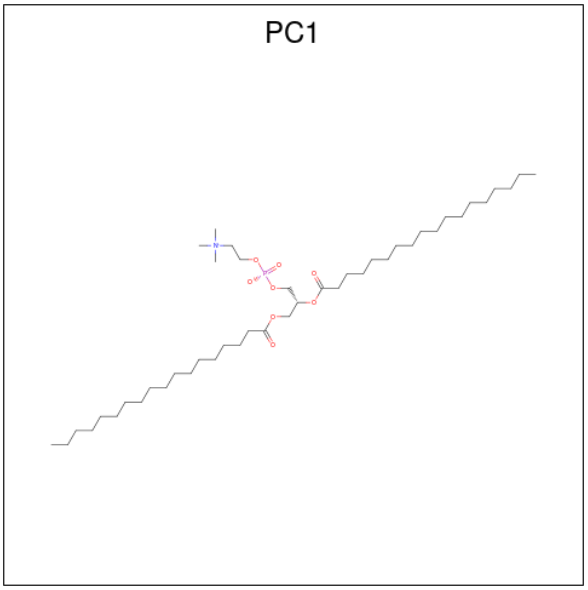
Chain	Residue	Modelled	Actual	Comment	Reference
A	475	SER	-	expression tag	UNP O75844
A	476	GLY	-	expression tag	UNP O75844
A	477	LEU	-	expression tag	UNP O75844
A	478	GLU	-	expression tag	UNP O75844
A	479	VAL	-	expression tag	UNP O75844
A	480	LEU	-	expression tag	UNP O75844

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



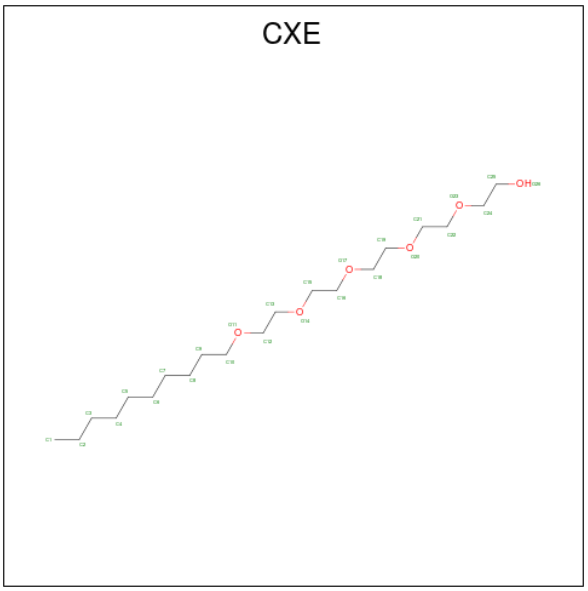
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
			Total	O	S		
2	A	1	5	4	1	0	0

- Molecule 3 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



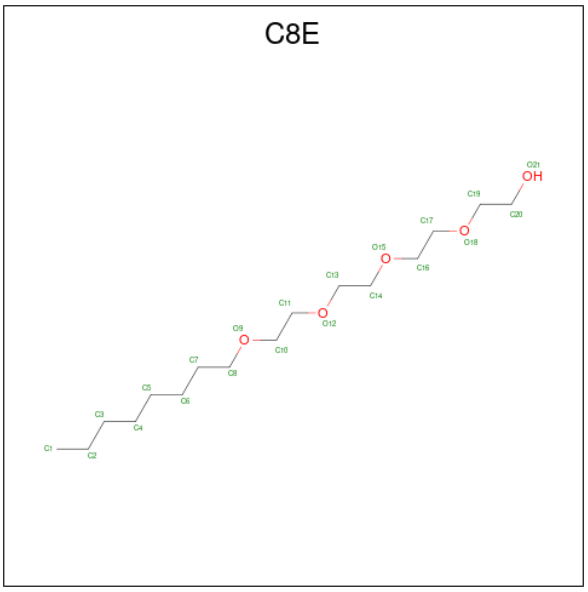
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
3	A	1	71	21	40	1	8	1	0	0

- Molecule 4 is PENTAETHYLENE GLYCOL MONODECYL ETHER (three-letter code: CXE) (formula: $C_{20}H_{42}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	A	1	61	18	37	6	0	0

- Molecule 5 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: $C_{16}H_{34}O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	A	1	55	16	34	5	0	0
			Total	C	H	O		
5	A	1	30	8	17	5	0	0

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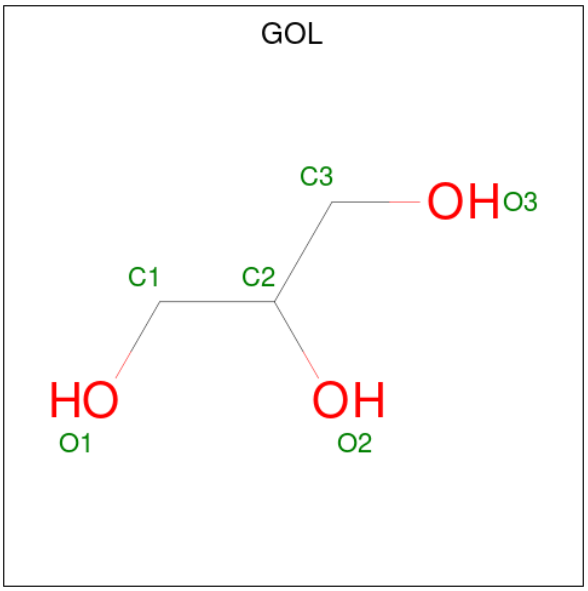
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	A	1	17	7	6	4	0	0
			Total	C	H	O		
5	A	1	55	16	34	5	0	0
			Total	C	H	O		
5	A	1	26	7	15	4	0	0
			Total	C	H	O		
5	A	1	30	8	17	5	0	0
			Total	C	H	O		
5	A	1	39	11	23	5	0	0
			Total	C	H	O		
5	A	1	50	15	31	4	0	0
			Total	C	H	O		
5	A	1	26	7	15	4	0	0
			Total	C	H	O		
5	A	1	29	8	17	4	0	0
			Total	C	H	O		
5	A	1	25	7	14	4	0	0
			Total	C	H	O		
5	A	1	55	16	34	5	0	0

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

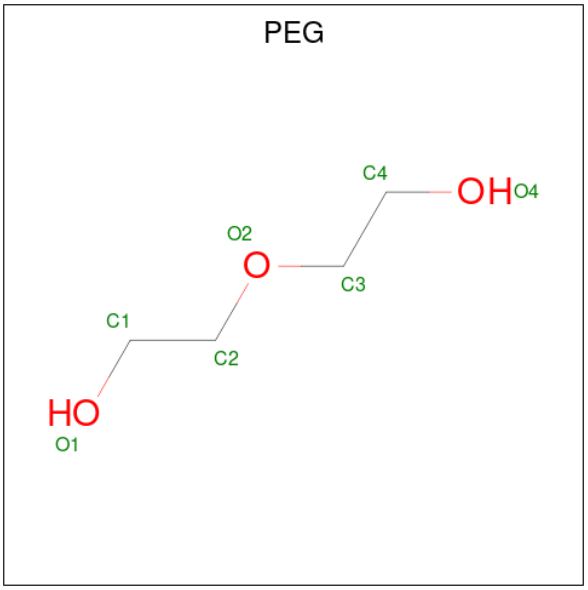
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
6	A	1	1	1	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



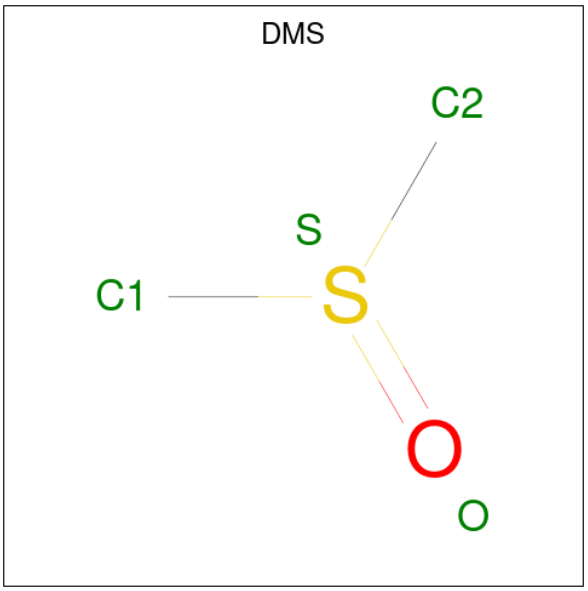
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
7	A	1	14	3	8	3	0	0
			Total	C	H	O		
7	A	1	14	3	8	3	0	0

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 9 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	S		
9	A	1	10	2	6	1	1	0	0
			Total	C	H	O	S		
9	A	1	10	2	6	1	1	0	0
			Total	C	H	O	S		
9	A	1	10	2	6	1	1	0	0

- Molecule 10 is water.

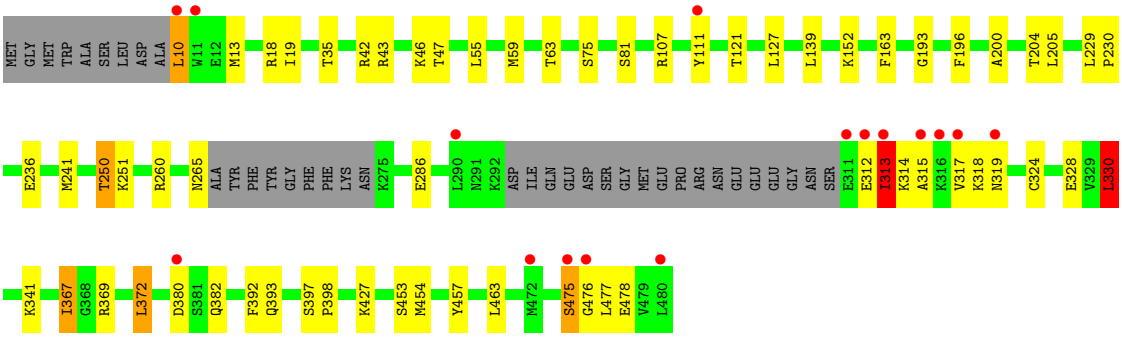
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	158	160	160	0	2

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: CAAX prenyl protease 1 homolog

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	149.46Å 84.56Å 76.89Å 90.00° 119.07° 90.00°	Depositor
Resolution (Å)	33.60 – 2.00 33.60 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (33.60-2.00) 93.7 (33.60-2.00)	Depositor EDS
R_{merge}	0.44	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.218 , 0.249 0.226 , 0.256	Depositor DCC
R_{free} test set	1997 reflections (3.54%)	wwPDB-VP
Wilson B-factor (Å^2)	19.7	Xtriage
Anisotropy	0.683	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 62.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.037 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7938	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.97% 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: ZN, DMS, SO4, PC1, GOL, CXE, C8E, PEG

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	0.58	0/3671	0.68	1/4983 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	330	LEU	CA-CB-CG	5.79	128.63	115.30

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	3569	3554	3549	46	1
2	A	10	0	0	0	0
3	A	31	40	36	4	1
4	A	24	37	35	2	0
5	A	180	257	252	6	0
6	A	1	0	0	0	0
7	A	12	16	16	4	0
8	A	7	10	10	0	0
9	A	12	18	18	0	0
10	A	160	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4006	3932	3916	48	1

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 6.

All (48) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:SER:OG	1:A:476:GLY:N	2.13	0.81
1:A:265:ASN:ND2	10:A:602:HOH:O	2.20	0.73
1:A:314:LYS:HA	1:A:315:ALA:HB3	1.74	0.68
1:A:43:ARG:NH2	3:A:503:PC1:O12	2.29	0.65
1:A:397:SER:HB2	1:A:398:PRO:HD3	1.84	0.60
1:A:369:ARG:HB2	1:A:372:LEU:HD22	1.82	0.60
1:A:367:ILE:HD12	7:A:518:GOL:H11	1.88	0.54
1:A:13:MET:O	1:A:18:ARG:NH1	2.38	0.54
1:A:19:ILE:HD13	1:A:372:LEU:HD12	1.90	0.54
1:A:241:MET:HE2	1:A:427:LYS:HE3	1.90	0.53
1:A:393:GLN:OE1	4:A:504:CXE:H252	2.09	0.53
1:A:369:ARG:HD2	7:A:519:GOL:H32	1.89	0.53
1:A:454:MET:HE2	10:A:738:HOH:O	2.09	0.52
1:A:369:ARG:CD	7:A:519:GOL:H32	2.40	0.52
1:A:382:GLN:OE1	10:A:601:HOH:O	2.18	0.51
1:A:397:SER:CB	1:A:398:PRO:HD3	2.42	0.49
1:A:250:THR:HG22	1:A:251:LYS:N	2.26	0.49
1:A:312:GLU:O	1:A:313:ILE:HG23	2.13	0.49
1:A:152:LYS:HZ2	5:A:516:C8E:C17	2.25	0.49
1:A:46:LYS:HA	10:A:611:HOH:O	2.14	0.48
1:A:250:THR:HG22	1:A:251:LYS:H	1.77	0.48
1:A:229:LEU:HD12	1:A:230:PRO:HD2	1.95	0.48
1:A:250:THR:CG2	1:A:251:LYS:N	2.76	0.48
1:A:241:MET:HE3	1:A:330:LEU:HD12	1.96	0.47
1:A:286:GLU:H	1:A:286:GLU:CD	2.18	0.47
1:A:193:GLY:N	1:A:196:PHE:HB3	2.30	0.47
1:A:35:THR:HG22	3:A:503:PC1:H232	1.97	0.46
1:A:478:GLU:O	1:A:478:GLU:HG3	2.15	0.46
1:A:260:ARG:HH11	5:A:511:C8E:H72	1.81	0.46
1:A:43:ARG:NH2	3:A:503:PC1:H142	2.31	0.45
1:A:200:ALA:O	1:A:204:THR:HG23	2.17	0.45
5:A:510:C8E:H201	10:A:616:HOH:O	2.16	0.45
1:A:10:LEU:HD22	1:A:10:LEU:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:MET:HE3	1:A:63:THR:HG22	1.98	0.45
1:A:55:LEU:CD2	1:A:463:LEU:HD21	2.47	0.45
1:A:393:GLN:NE2	10:A:607:HOH:O	2.29	0.45
1:A:317:VAL:C	1:A:319:ASN:H	2.21	0.44
1:A:324:CYS:HB3	1:A:328:GLU:HB2	1.98	0.44
1:A:42:ARG:HD2	1:A:75:SER:OG	2.20	0.42
1:A:392:PHE:HE2	4:A:504:CXE:H191	1.85	0.42
1:A:453:SER:HB2	1:A:457:TYR:CD2	2.54	0.42
5:A:510:C8E:C20	10:A:616:HOH:O	2.68	0.41
1:A:43:ARG:NH2	3:A:503:PC1:H112	2.36	0.41
1:A:314:LYS:CA	1:A:315:ALA:HB3	2.48	0.41
1:A:163:PHE:CD2	5:A:511:C8E:H101	2.56	0.40
1:A:367:ILE:CD1	7:A:518:GOL:H11	2.49	0.40
1:A:205:LEU:HD23	1:A:205:LEU:C	2.42	0.40
1:A:397:SER:OG	5:A:510:C8E:H192	2.22	0.40

All (1) 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)
1:A:121:THR:OG1	3:A:503:PC1:O14[4_346]	1.97	0.23

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	439/480 (92%)	422 (96%)	15 (3%)	2 (0%)	29 23

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	313	ILE

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Mol	Chain	Res	Type
1	A	318	LYS

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	378/424 (89%)	361 (96%)	17 (4%)	27 24

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	47	THR
1	A	81	SER
1	A	107	ARG
1	A	111	TYR
1	A	127	LEU
1	A	139	LEU
1	A	236	GLU
1	A	250	THR
1	A	313	ILE
1	A	330	LEU
1	A	341	LYS
1	A	367	ILE
1	A	372	LEU
1	A	380	ASP
1	A	475	SER
1	A	477	LEU

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 23 ligands modelled in this entry, 1 is monoatomic - leaving 22 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
7	GOL	A	519	-	5,5,5	0.45	0	5,5,5	0.51	0
5	C8E	A	506	-	12,12,20	0.46	0	11,11,19	0.50	0
5	C8E	A	510	-	12,12,20	0.51	0	11,11,19	0.49	0
5	C8E	A	512	-	18,18,20	0.33	0	17,17,19	0.71	0
5	C8E	A	511	-	15,15,20	0.59	0	14,14,19	0.46	0
5	C8E	A	513	-	10,10,20	0.45	0	9,9,19	0.39	0
3	PC1	A	503	-	30,30,53	1.27	2 (6%)	36,38,61	1.54	5 (13%)
9	DMS	A	522	-	3,3,3	0.75	0	3,3,3	0.99	0
9	DMS	A	521	-	3,3,3	0.61	0	3,3,3	0.69	0
5	C8E	A	516	-	20,20,20	0.36	0	19,19,19	0.81	1 (5%)
5	C8E	A	509	-	10,10,20	0.37	0	9,9,19	0.47	0
5	C8E	A	505	-	20,20,20	0.46	0	19,19,19	0.44	0
7	GOL	A	518	-	5,5,5	0.38	0	5,5,5	0.87	0
5	C8E	A	515	-	10,10,20	0.47	0	9,9,19	0.31	0
8	PEG	A	520	-	6,6,6	0.56	0	5,5,5	0.82	0
2	SO4	A	502	-	4,4,4	0.20	0	6,6,6	0.38	0
2	SO4	A	501	-	4,4,4	0.20	0	6,6,6	0.41	0
5	C8E	A	507	-	10,10,20	0.41	0	9,9,19	0.33	0
5	C8E	A	508	-	20,20,20	0.44	0	19,19,19	0.49	0
5	C8E	A	514	-	11,11,20	0.48	0	10,10,19	0.58	0
4	CXE	A	504	-	23,23,25	0.51	0	22,22,24	0.52	0
9	DMS	A	523	-	3,3,3	0.67	0	3,3,3	1.03	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
5	C8E	A	516	-	-	9/18/18/18	-
5	C8E	A	509	-	-	4/8/8/18	-
5	C8E	A	505	-	-	12/18/18/18	-
5	C8E	A	508	-	-	9/18/18/18	-
5	C8E	A	515	-	-	1/8/8/18	-
5	C8E	A	514	-	-	8/9/9/18	-
7	GOL	A	518	-	-	3/4/4/4	-
7	GOL	A	519	-	-	4/4/4/4	-
5	C8E	A	506	-	-	4/10/10/18	-
8	PEG	A	520	-	-	2/4/4/4	-
4	CXE	A	504	-	-	11/21/21/23	-
5	C8E	A	510	-	-	6/10/10/18	-
5	C8E	A	512	-	-	8/16/16/18	-
5	C8E	A	511	-	-	4/13/13/18	-
5	C8E	A	513	-	-	3/8/8/18	-
3	PC1	A	503	-	-	11/34/34/57	-
5	C8E	A	507	-	-	5/8/8/18	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	PC1	O31-C31	3.42	1.43	1.33
3	A	503	PC1	O21-C21	3.19	1.43	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	503	PC1	O21-C21-C22	4.49	121.19	111.50
3	A	503	PC1	O31-C31-C32	3.79	121.31	111.38
3	A	503	PC1	C23-C22-C21	-3.39	101.28	113.62
5	A	516	C8E	O12-C11-C10	2.31	120.82	110.39
3	A	503	PC1	C15-N-C13	2.17	114.55	108.97
3	A	503	PC1	C15-N-C14	-2.07	103.66	108.97

There are no chirality outliers.

All (104) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	PC1	O13-C11-C12-N
7	A	518	GOL	O1-C1-C2-C3
5	A	516	C8E	C10-C11-O12-C13
5	A	506	C8E	C13-C14-O15-C16
5	A	507	C8E	C16-C17-O18-C19
5	A	505	C8E	O12-C13-C14-O15
5	A	507	C8E	C17-C16-O15-C14
5	A	510	C8E	O15-C16-C17-O18
5	A	513	C8E	O12-C13-C14-O15
4	A	504	CXE	O11-C12-C13-O14
4	A	504	CXE	O14-C15-C16-O17
4	A	504	CXE	O17-C18-C19-O20
5	A	508	C8E	O9-C10-C11-O12
3	A	503	PC1	C22-C21-O21-C2
5	A	510	C8E	O9-C10-C11-O12
5	A	512	C8E	O9-C10-C11-O12
5	A	505	C8E	C6-C7-C8-O9
3	A	503	PC1	C21-C22-C23-C24
3	A	503	PC1	O22-C21-O21-C2
5	A	509	C8E	O18-C19-C20-O21
5	A	512	C8E	O12-C13-C14-O15
4	A	504	CXE	C5-C6-C7-C8
5	A	516	C8E	C3-C4-C5-C6
5	A	512	C8E	C3-C4-C5-C6
7	A	519	GOL	O1-C1-C2-C3
5	A	506	C8E	O9-C10-C11-O12
5	A	510	C8E	O18-C19-C20-O21
5	A	510	C8E	O12-C13-C14-O15
7	A	518	GOL	O1-C1-C2-O2
3	A	503	PC1	C23-C24-C25-C26
5	A	505	C8E	C2-C3-C4-C5
5	A	512	C8E	C4-C5-C6-C7
5	A	508	C8E	C4-C5-C6-C7
5	A	516	C8E	C6-C7-C8-O9
5	A	507	C8E	O18-C19-C20-O21
5	A	514	C8E	O18-C19-C20-O21
5	A	514	C8E	O15-C16-C17-O18
7	A	519	GOL	O1-C1-C2-O2
5	A	505	C8E	O15-C16-C17-O18
5	A	514	C8E	C20-C19-O18-C17
5	A	508	C8E	C2-C3-C4-C5
4	A	504	CXE	C22-C21-O20-C19

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Mol	Chain	Res	Type	Atoms
5	A	513	C8E	O15-C16-C17-O18
3	A	503	PC1	C1-O11-P-O13
5	A	512	C8E	C16-C17-O18-C19
7	A	518	GOL	O2-C2-C3-O3
3	A	503	PC1	O11-C1-C2-O21
4	A	504	CXE	C6-C7-C8-C9
3	A	503	PC1	O11-C1-C2-C3
5	A	512	C8E	C1-C2-C3-C4
5	A	511	C8E	C20-C19-O18-C17
5	A	505	C8E	C10-C11-O12-C13
3	A	503	PC1	C26-C27-C28-C29
5	A	508	C8E	C14-C13-O12-C11
5	A	505	C8E	C11-C10-O9-C8
5	A	514	C8E	C13-C14-O15-C16
7	A	519	GOL	O2-C2-C3-O3
5	A	508	C8E	O18-C19-C20-O21
5	A	516	C8E	O9-C10-C11-O12
5	A	505	C8E	C16-C17-O18-C19
5	A	511	C8E	C13-C14-O15-C16
5	A	510	C8E	C17-C16-O15-C14
5	A	511	C8E	C11-C10-O9-C8
5	A	513	C8E	O18-C19-C20-O21
5	A	516	C8E	C7-C8-O9-C10
5	A	514	C8E	C17-C16-O15-C14
5	A	509	C8E	O12-C13-C14-O15
5	A	516	C8E	C2-C3-C4-C5
5	A	508	C8E	C7-C8-O9-C10
5	A	510	C8E	C14-C13-O12-C11
4	A	504	CXE	C12-C13-O14-C15
4	A	504	CXE	C9-C10-O11-C12
5	A	514	C8E	C16-C17-O18-C19
4	A	504	CXE	C21-C22-O23-C24
8	A	520	PEG	O1-C1-C2-O2
5	A	512	C8E	C7-C8-O9-C10
5	A	505	C8E	C14-C13-O12-C11
8	A	520	PEG	C1-C2-O2-C3
5	A	505	C8E	C20-C19-O18-C17
5	A	505	C8E	C3-C4-C5-C6
5	A	508	C8E	C1-C2-C3-C4
3	A	503	PC1	C1-C2-C3-O31
7	A	519	GOL	C1-C2-C3-O3
4	A	504	CXE	C16-C15-O14-C13

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Mol	Chain	Res	Type	Atoms
5	A	516	C8E	C14-C13-O12-C11
4	A	504	CXE	O20-C21-C22-O23
5	A	511	C8E	O9-C10-C11-O12
5	A	506	C8E	O12-C13-C14-O15
5	A	512	C8E	C17-C16-O15-C14
5	A	516	C8E	O15-C16-C17-O18
5	A	507	C8E	O15-C16-C17-O18
5	A	505	C8E	O9-C10-C11-O12
5	A	515	C8E	O9-C10-C11-O12
3	A	503	PC1	O21-C2-C3-O31
5	A	508	C8E	C6-C7-C8-O9
5	A	508	C8E	C20-C19-O18-C17
5	A	509	C8E	C13-C14-O15-C16
5	A	505	C8E	C17-C16-O15-C14
5	A	507	C8E	O12-C13-C14-O15
5	A	506	C8E	O15-C16-C17-O18
5	A	516	C8E	O12-C13-C14-O15
5	A	509	C8E	C20-C19-O18-C17
5	A	514	C8E	O12-C13-C14-O15
5	A	514	C8E	C14-C13-O12-C11

There are no ring outliers.

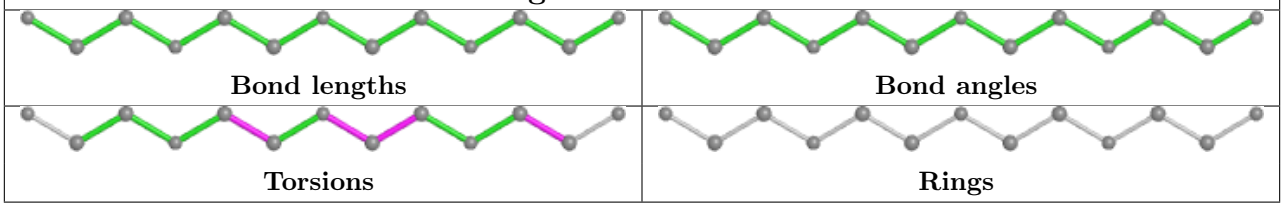
7 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	519	GOL	2	0
5	A	510	C8E	3	0
5	A	511	C8E	2	0
3	A	503	PC1	4	1
5	A	516	C8E	1	0
7	A	518	GOL	2	0
4	A	504	CXE	2	0

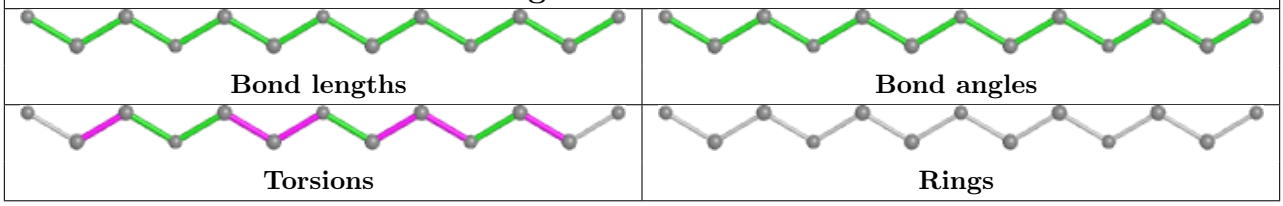
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

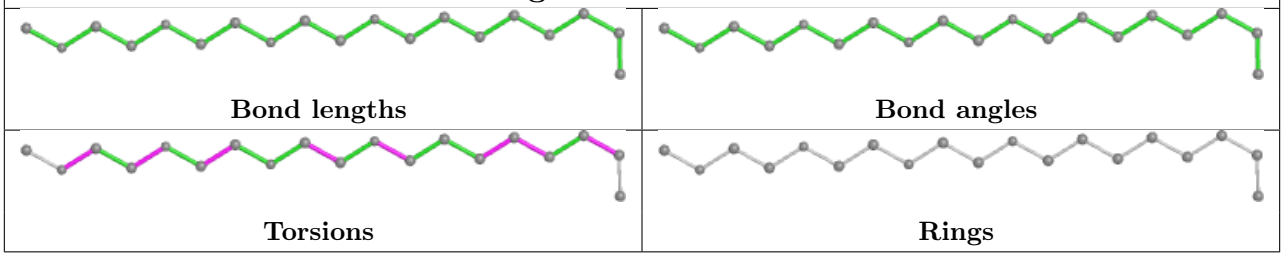
Ligand C8E A 506



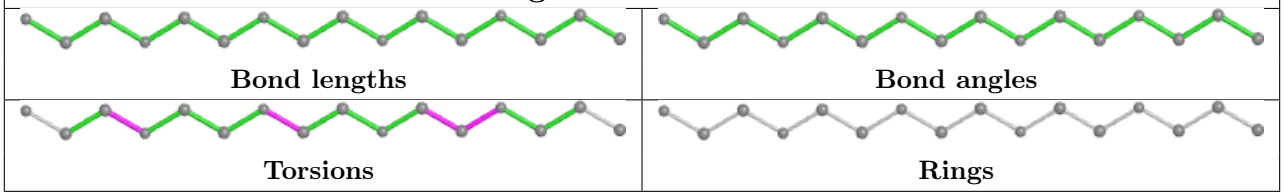
Ligand C8E A 510



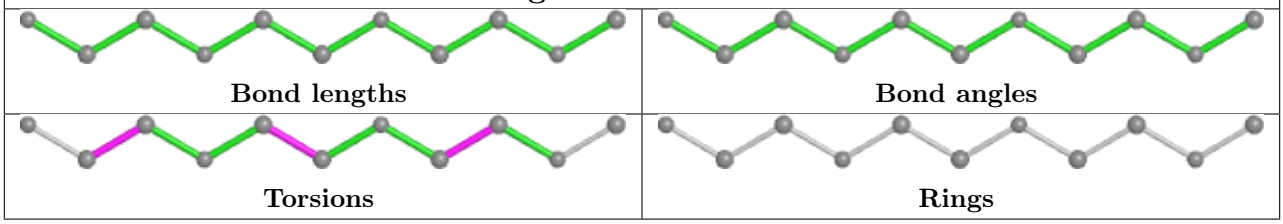
Ligand C8E A 512



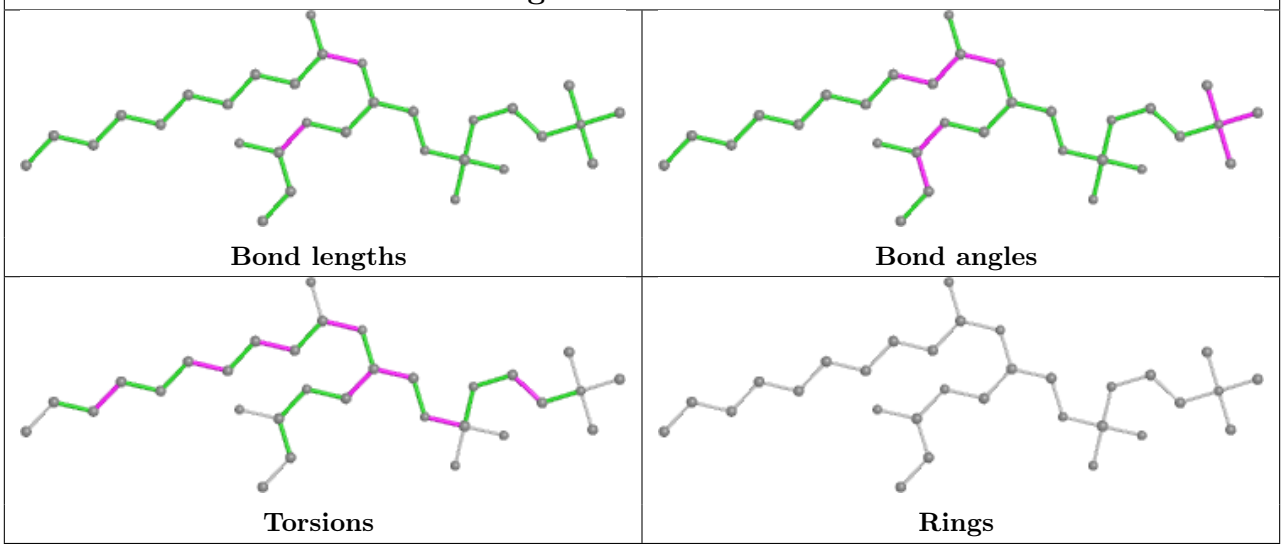
Ligand C8E A 511



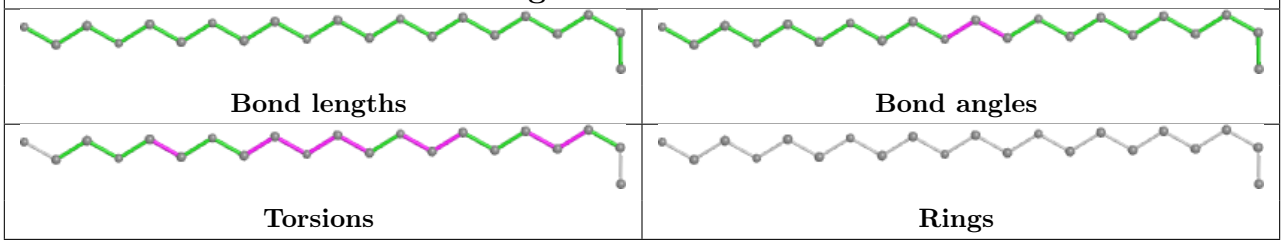
Ligand C8E A 513



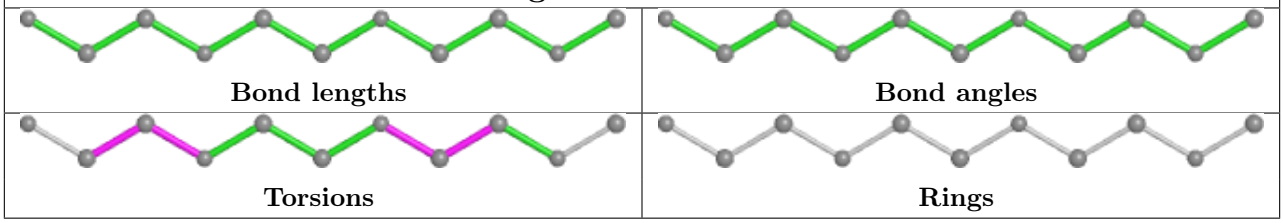
Ligand PC1 A 503



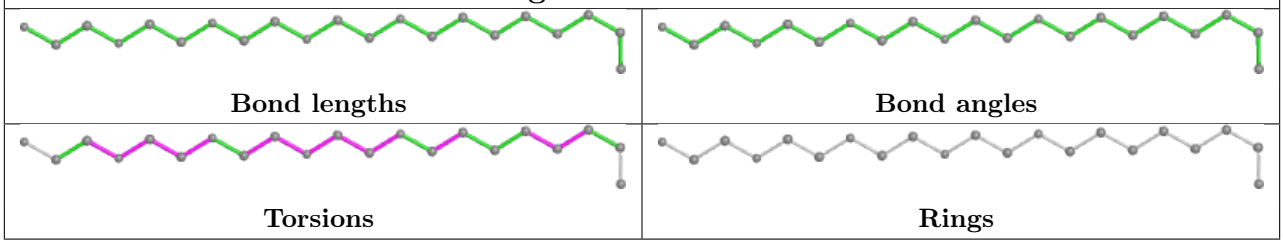
Ligand C8E A 516



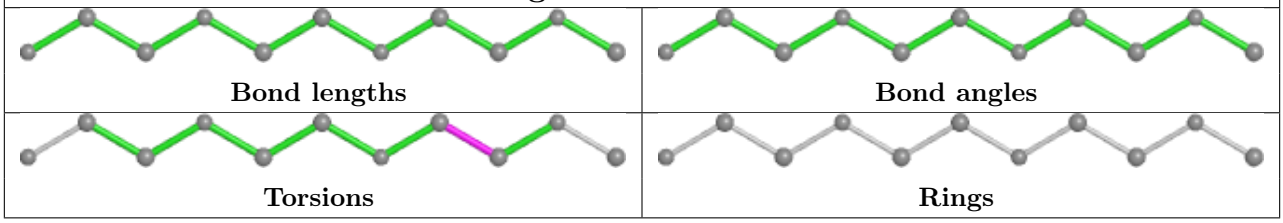
Ligand C8E A 509

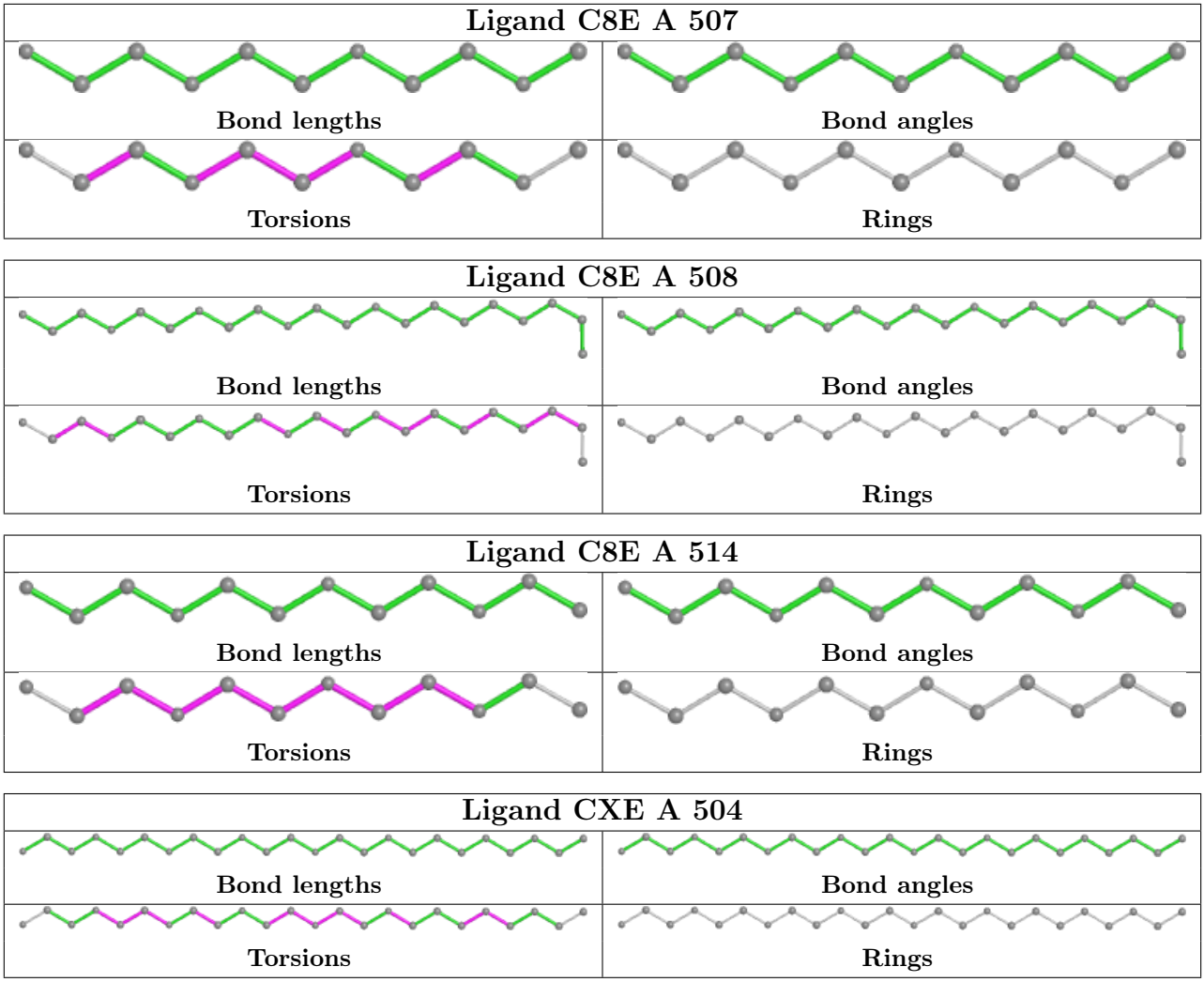


Ligand C8E A 505



Ligand C8E A 515





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	444/480 (92%)	0.05	16 (3%) 42 42	19, 32, 68, 96	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	11	TRP	4.9
1	A	317	VAL	4.4
1	A	319	ASN	4.4
1	A	475	SER	4.0
1	A	480	LEU	3.9
1	A	315	ALA	3.9
1	A	313	ILE	3.4
1	A	476	GLY	3.3
1	A	380	ASP	3.0
1	A	472	MET	2.9
1	A	312	GLU	2.6
1	A	10	LEU	2.4
1	A	316	LYS	2.4
1	A	111	TYR	2.4
1	A	311	GLU	2.1
1	A	290	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

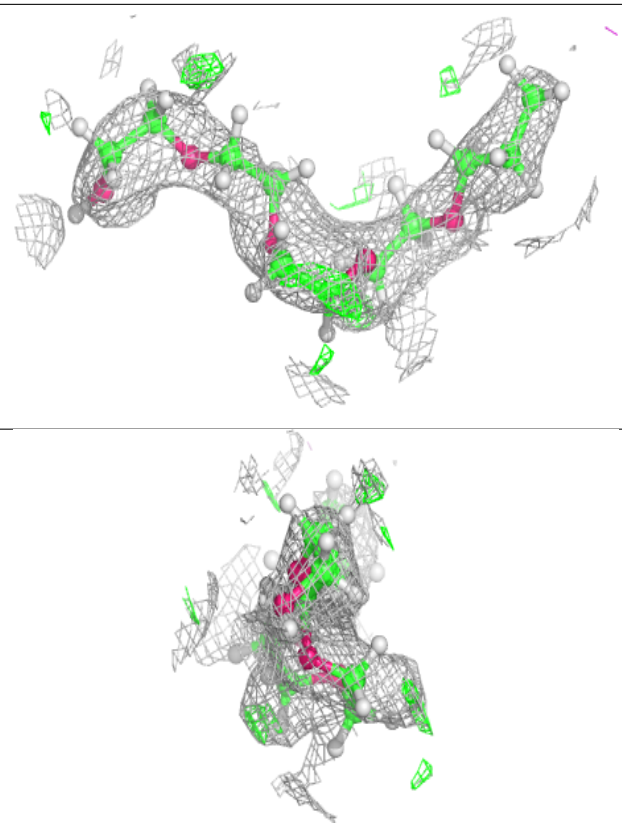
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

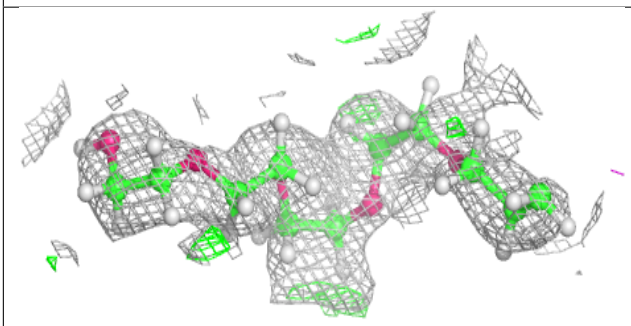
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	C8E	A	511	16/21	0.77	0.33	28,55,69,79	0
5	C8E	A	514	12/21	0.77	0.22	44,69,83,85	0
7	GOL	A	519	6/6	0.77	0.24	68,90,105,117	0
5	C8E	A	506	13/21	0.80	0.16	41,57,66,69	0
3	PC1	A	503	31/54	0.81	0.18	30,55,74,78	0
5	C8E	A	505	21/21	0.82	0.15	32,56,84,84	0
9	DMS	A	522	4/4	0.82	0.20	32,40,53,82	0
4	CXE	A	504	24/26	0.83	0.15	33,54,70,85	0
8	PEG	A	520	7/7	0.83	0.17	46,55,65,67	0
5	C8E	A	508	21/21	0.83	0.18	42,56,70,72	0
5	C8E	A	509	11/21	0.86	0.14	36,54,71,74	0
5	C8E	A	510	13/21	0.87	0.14	34,44,54,56	0
5	C8E	A	516	21/21	0.87	0.12	30,41,55,63	0
7	GOL	A	518	6/6	0.87	0.14	35,42,48,50	0
5	C8E	A	513	11/21	0.89	0.21	43,58,76,79	0
5	C8E	A	507	11/21	0.89	0.17	41,49,53,62	0
5	C8E	A	515	11/21	0.89	0.12	41,53,74,80	0
5	C8E	A	512	19/21	0.89	0.12	31,44,67,68	0
9	DMS	A	523	4/4	0.89	0.14	47,61,96,96	0
2	SO4	A	502	5/5	0.92	0.24	47,58,71,83	0
2	SO4	A	501	5/5	0.92	0.30	62,73,88,92	0
9	DMS	A	521	4/4	0.93	0.25	46,56,92,92	0
6	ZN	A	517	1/1	0.99	0.11	30,30,30,30	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 C8E A 511:

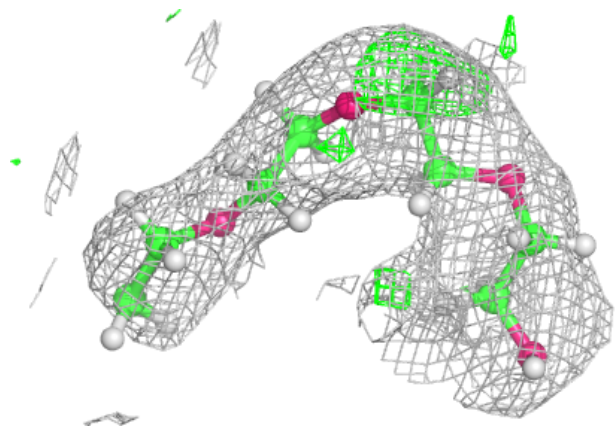
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

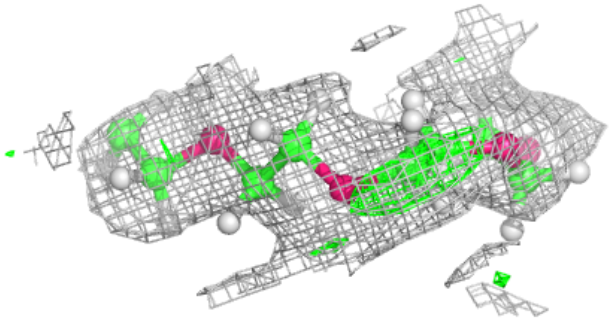


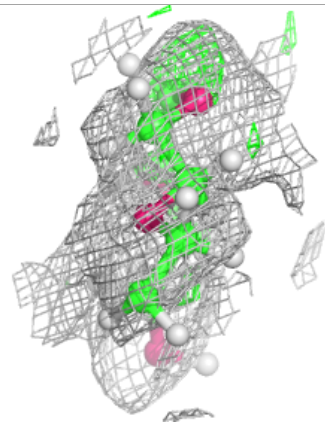


Electron density around C8E A 514:

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

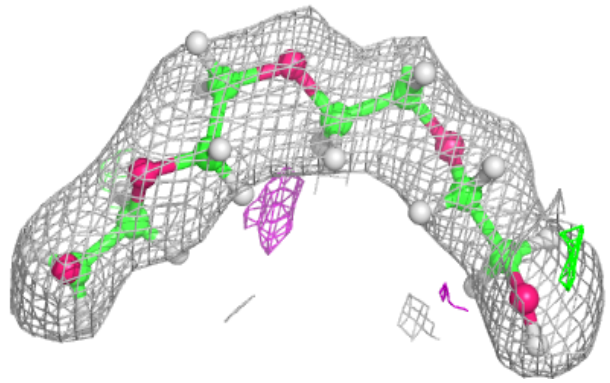


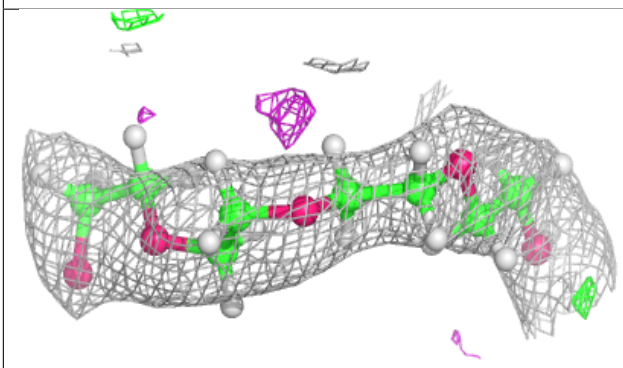


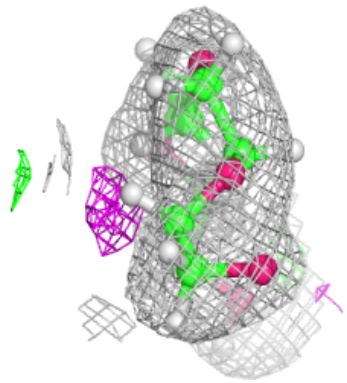


Electron density around C8E A 506:

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

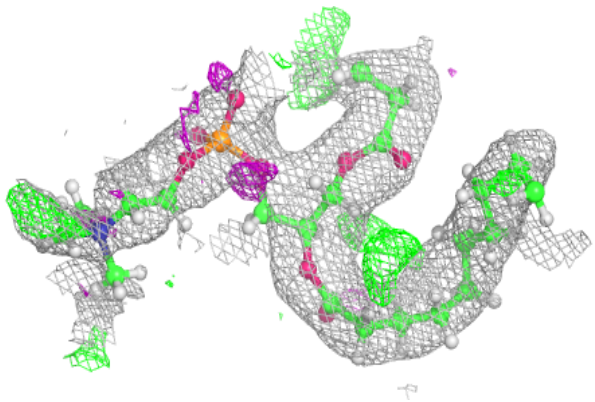


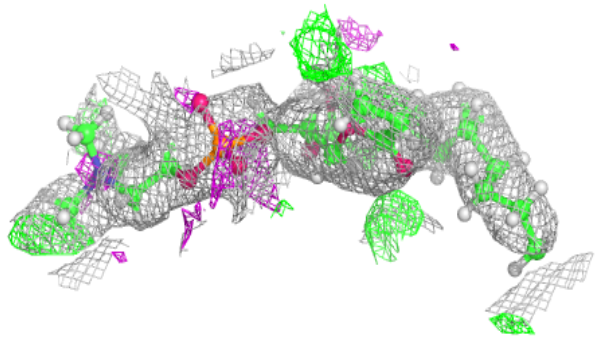




Electron density around PC1 A 503:

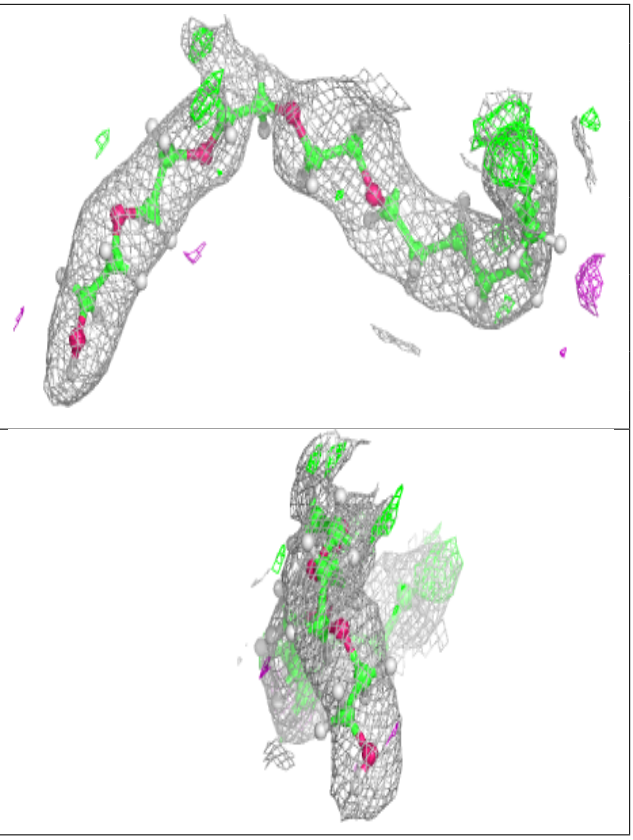
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





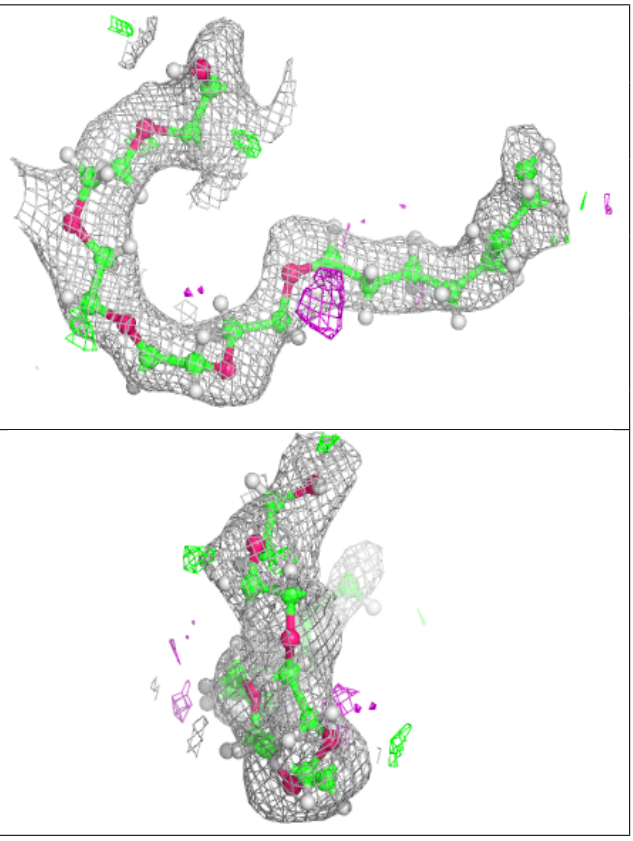
Electron density around C8E A 505:

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



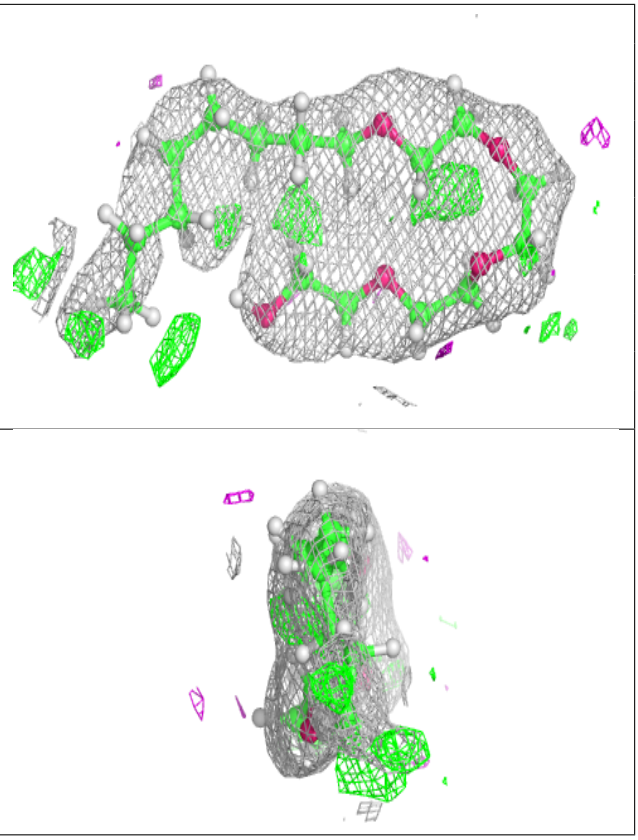
Electron density around CXE A 504:

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



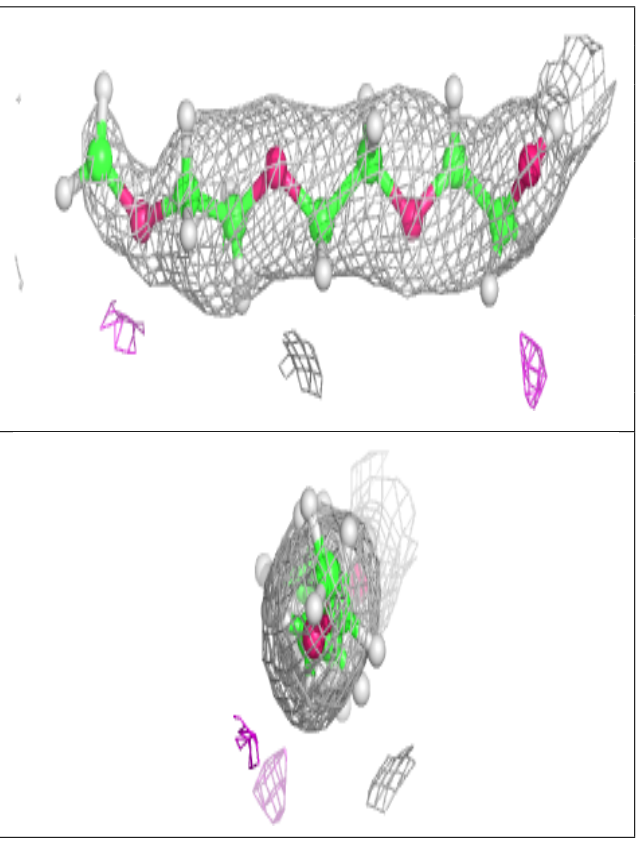
Electron density around C8E A 508:

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



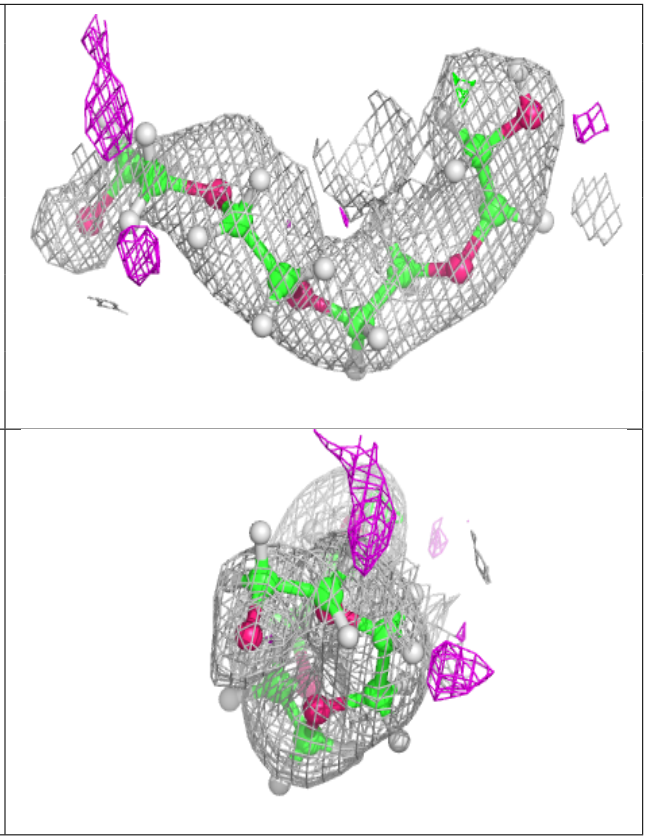
Electron density around C8E A 509:

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



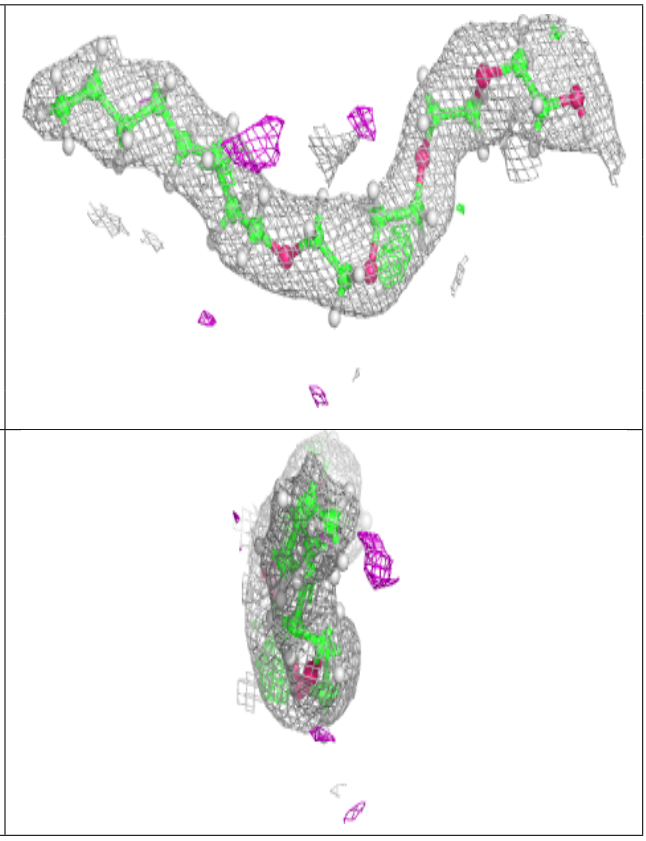
Electron density around C8E A 510:

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



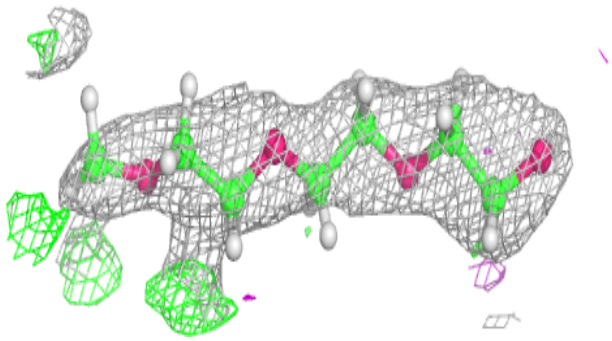
Electron density around C8E A 516:

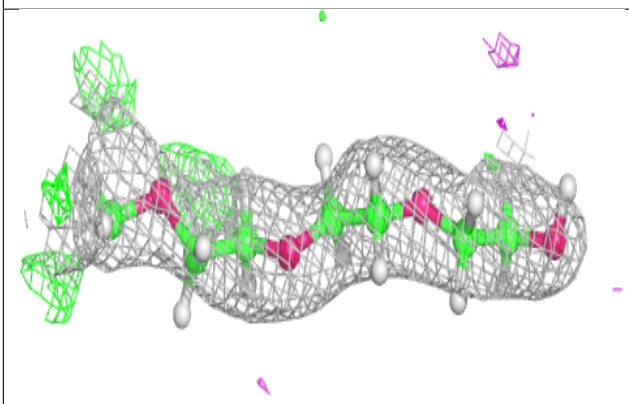
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

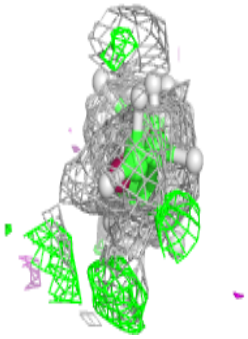


Electron density around C8E A 513:

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

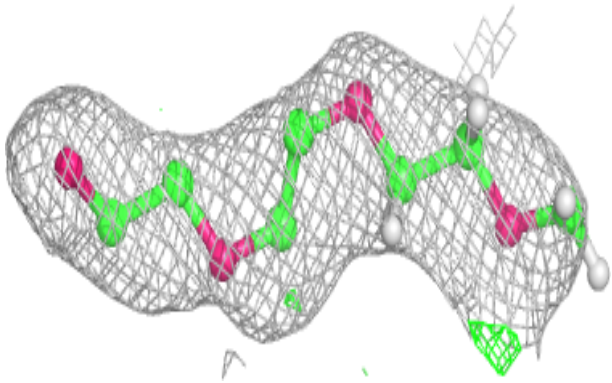


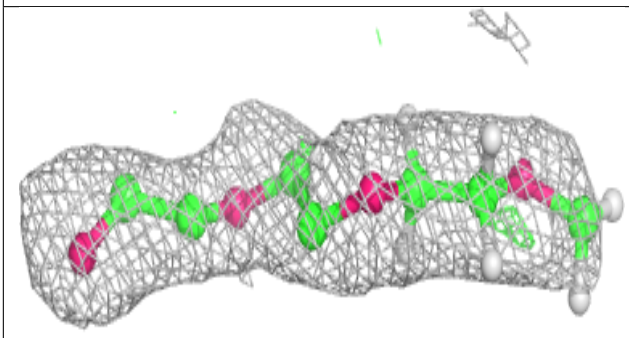


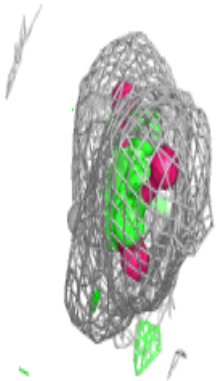


Electron density around C8E A 507:

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

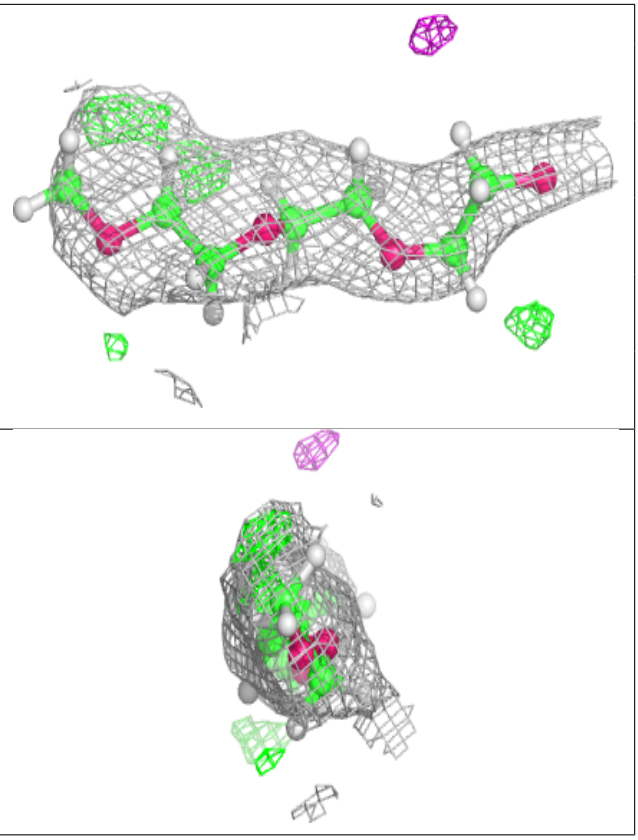






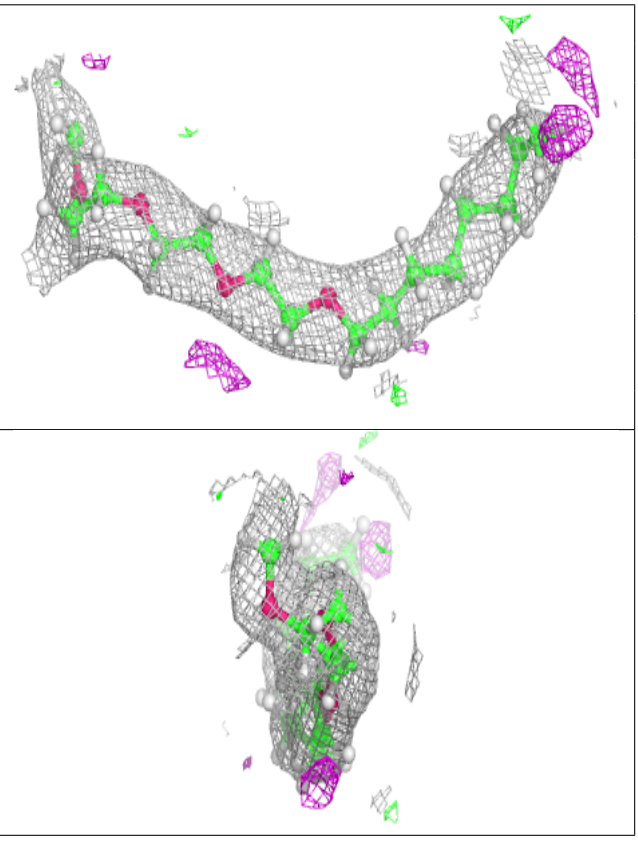
Electron density around C8E A 515:

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



Electron density around C8E A 512:

$2mF_o$-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.