



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 6, 2020 – 02:10 PM BST

PDB ID : 3SY9
Title : Crystal structure of Pseudomonas aeruginosa OccD2 (OpdC)
Authors : van den Berg, B.; Eren, E.
Deposited on : 2011-07-16
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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

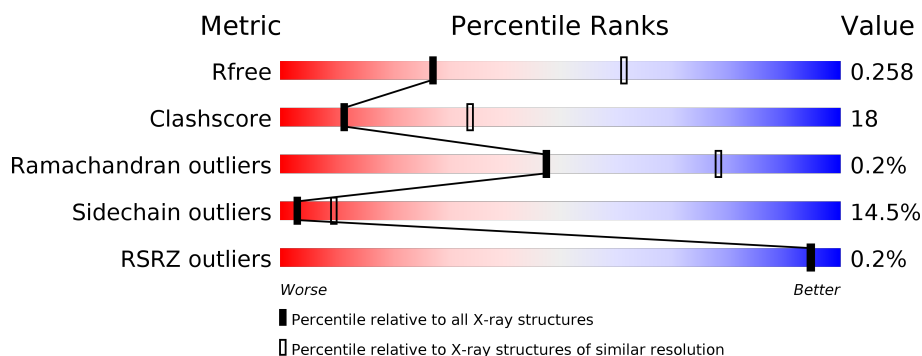
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	430	
1	B	430	
1	C	430	
1	D	430	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BOG	A	506	X	-	-	-
3	BOG	B	507	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11713 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 Histidine porin OpdC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	0	0
			2874	1830	477	565	2			
1	B	372	Total	C	N	O	S	0	0	0
			2886	1838	480	566	2			
1	C	360	Total	C	N	O	S	0	0	0
			2767	1761	459	545	2			
1	D	361	Total	C	N	O	S	0	0	0
			2770	1760	458	550	2			

There are 36 discrepancies between the modelled and reference sequences:

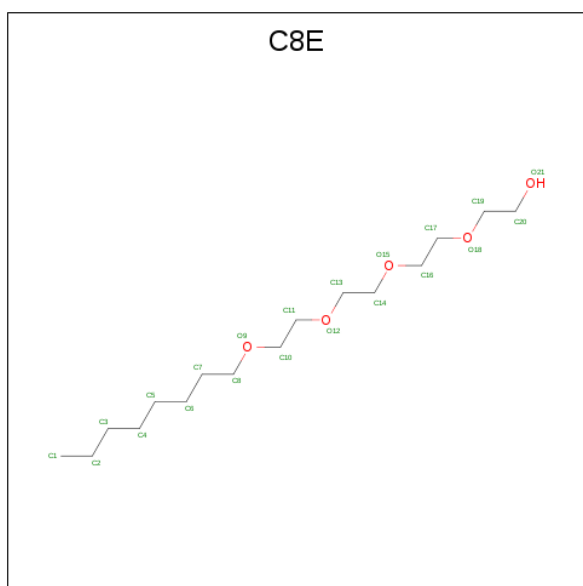
Chain	Residue	Modelled	Actual	Comment	Reference
A	328	VAL	LEU	SEE REMARK 999	UNP Q9I6X0
A	423	GLY	-	expression tag	UNP Q9I6X0
A	424	GLY	-	expression tag	UNP Q9I6X0
A	425	HIS	-	expression tag	UNP Q9I6X0
A	426	HIS	-	expression tag	UNP Q9I6X0
A	427	HIS	-	expression tag	UNP Q9I6X0
A	428	HIS	-	expression tag	UNP Q9I6X0
A	429	HIS	-	expression tag	UNP Q9I6X0
A	430	HIS	-	expression tag	UNP Q9I6X0
B	328	VAL	LEU	SEE REMARK 999	UNP Q9I6X0
B	423	GLY	-	expression tag	UNP Q9I6X0
B	424	GLY	-	expression tag	UNP Q9I6X0
B	425	HIS	-	expression tag	UNP Q9I6X0
B	426	HIS	-	expression tag	UNP Q9I6X0
B	427	HIS	-	expression tag	UNP Q9I6X0
B	428	HIS	-	expression tag	UNP Q9I6X0
B	429	HIS	-	expression tag	UNP Q9I6X0
B	430	HIS	-	expression tag	UNP Q9I6X0
C	328	VAL	LEU	SEE REMARK 999	UNP Q9I6X0
C	423	GLY	-	expression tag	UNP Q9I6X0
C	424	GLY	-	expression tag	UNP Q9I6X0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	425	HIS	-	expression tag	UNP Q9I6X0
C	426	HIS	-	expression tag	UNP Q9I6X0
C	427	HIS	-	expression tag	UNP Q9I6X0
C	428	HIS	-	expression tag	UNP Q9I6X0
C	429	HIS	-	expression tag	UNP Q9I6X0
C	430	HIS	-	expression tag	UNP Q9I6X0
D	328	VAL	LEU	SEE REMARK 999	UNP Q9I6X0
D	423	GLY	-	expression tag	UNP Q9I6X0
D	424	GLY	-	expression tag	UNP Q9I6X0
D	425	HIS	-	expression tag	UNP Q9I6X0
D	426	HIS	-	expression tag	UNP Q9I6X0
D	427	HIS	-	expression tag	UNP Q9I6X0
D	428	HIS	-	expression tag	UNP Q9I6X0
D	429	HIS	-	expression tag	UNP Q9I6X0
D	430	HIS	-	expression tag	UNP Q9I6X0

- Molecule 2 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C₁₆H₃₄O₅).



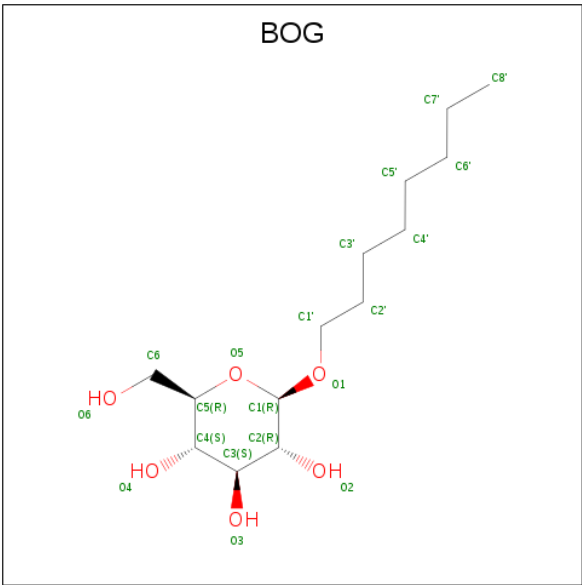
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			14	9	5		
2	A	1	Total	C	O	0	0
			12	10	2		
2	A	1	Total	C	O	0	0
			16	11	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			16	13	3		
2	A	1	Total	C	O	0	0
			21	16	5		
2	B	1	Total	C	O	0	0
			10	9	1		
2	B	1	Total	C	O	0	0
			16	11	5		
2	B	1	Total	C	O	0	0
			15	12	3		
2	B	1	Total	C	O	0	0
			16	13	3		
2	B	1	Total	C	O	0	0
			21	16	5		
2	B	1	Total	C	O	0	0
			11	10	1		
2	C	1	Total	C	O	0	0
			9	6	3		
2	C	1	Total	C	O	0	0
			16	13	3		
2	C	1	Total	C	O	0	0
			18	13	5		
2	C	1	Total	C	O	0	0
			11	10	1		
2	C	1	Total	C		0	0
			8	8			
2	D	1	Total	C	O	0	0
			10	9	1		
2	D	1	Total	C	O	0	0
			12	8	4		

- Molecule 3 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: C₁₄H₂₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			16	10	6		
3	B	1	Total	C	O	0	0
			15	9	6		

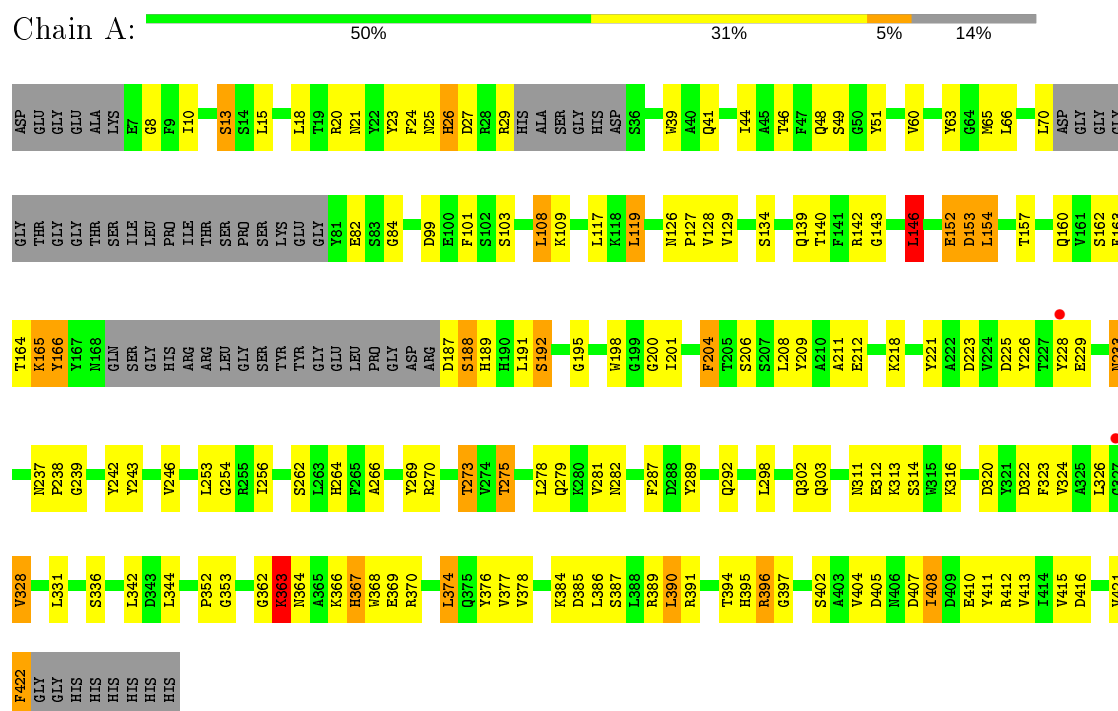
- Molecule 4 is water.

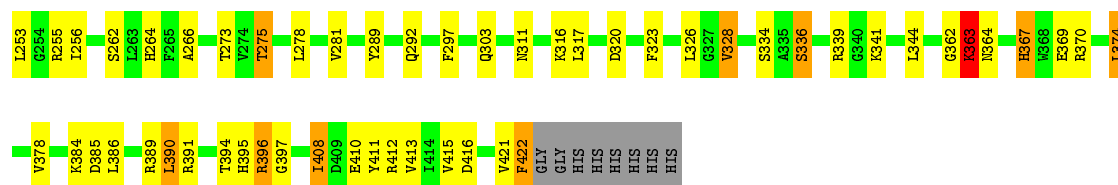
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	42	Total	O	0	0
			42	42		
4	B	32	Total	O	0	0
			32	32		
4	C	32	Total	O	0	0
			32	32		
4	D	27	Total	O	0	0
			27	27		

3 Residue-property plots

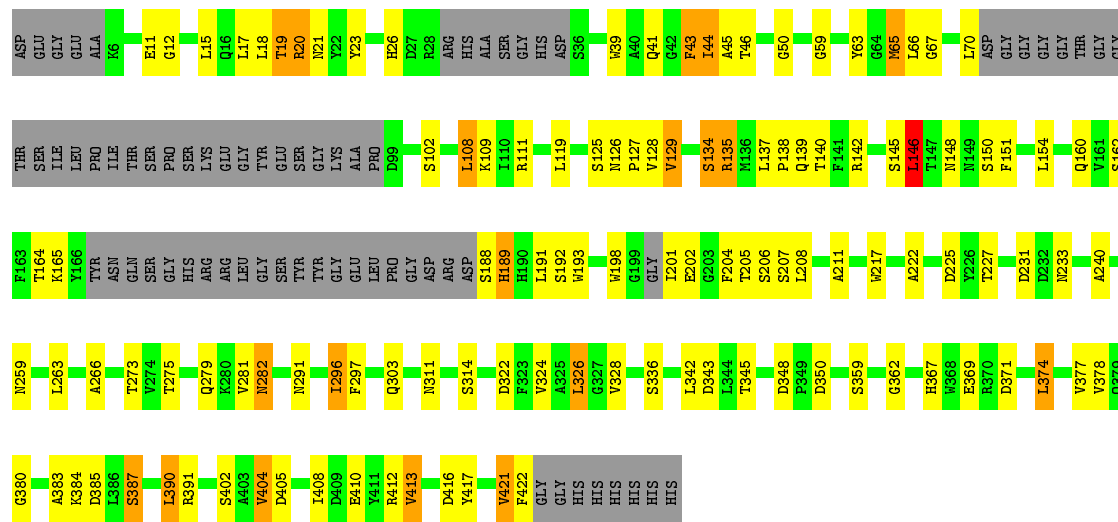
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Histidine porin OpdC

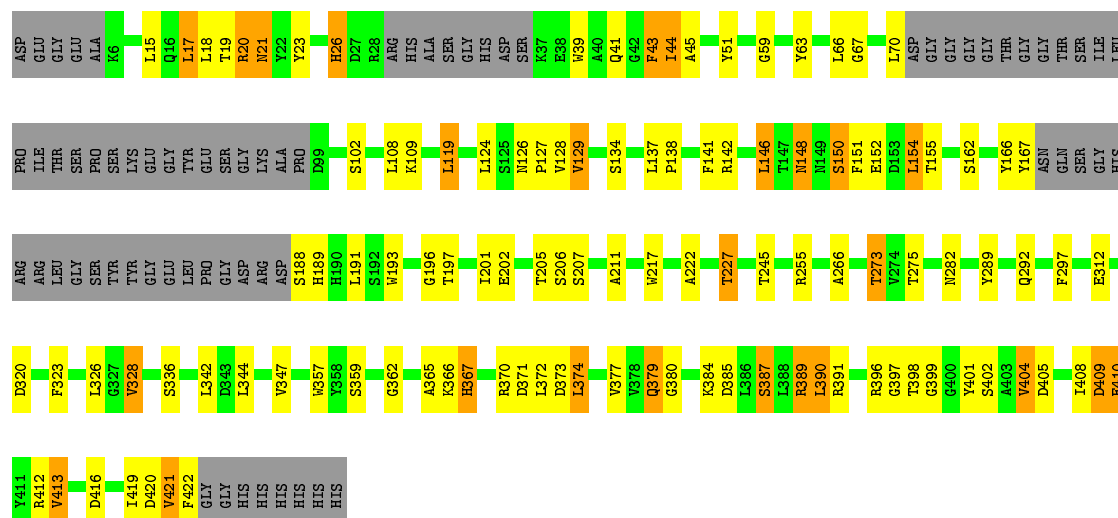




• Molecule 1: Histidine porin OpdC



• Molecule 1: Histidine porin OpdC



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	93.35Å 102.83Å 101.70Å 77.67° 62.57° 62.95°	Depositor
Resolution (Å)	14.96 – 2.80 40.92 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.9 (14.96-2.80) 89.4 (40.92-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.216 , 0.266 0.213 , 0.258	Depositor DCC
R_{free} test set	1992 reflections (2.77%)	wwPDB-VP
Wilson B-factor (Å ²)	56.6	Xtriage
Anisotropy	0.555	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,h-l,k 0.000 for h,l,h-k 0.458 for h,h-k,h-l 0.008 for -h,-k,-h+l 0.008 for -h,-h+k,-l 0.010 for -h,-l,-k 0.011 for -h,-h+l,-h+k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11713	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: C8E, BOG

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	0/2950	0.63	1/4011 (0.0%)
1	B	0.44	0/2962	0.63	0/4026
1	C	0.41	0/2839	0.63	1/3863 (0.0%)
1	D	0.42	0/2843	0.64	0/3871
All	All	0.42	0/11594	0.63	2/15771 (0.0%)

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	A	0	2
1	B	0	3
All	All	0	5

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	146	LEU	CA-CB-CG	5.49	127.94	115.30
1	A	146	LEU	CA-CB-CG	5.45	127.83	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	165	LYS	Peptide
1	A	84	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	B	165	LYS	Peptide
1	B	166	TYR	Peptide
1	B	84	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2874	0	2624	120	0
1	B	2886	0	2642	115	0
1	C	2767	0	2496	78	0
1	D	2770	0	2497	78	0
2	A	79	0	118	2	0
2	B	89	0	141	5	0
2	C	62	0	95	2	0
2	D	22	0	32	1	0
3	A	16	0	17	2	0
3	B	15	0	15	6	0
4	A	42	0	0	6	0
4	B	32	0	0	1	0
4	C	32	0	0	3	0
4	D	27	0	0	0	0
All	All	11713	0	10677	393	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 18.

The worst 5 of 393 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:B:201:ILE:HG21	1:B:204:PHE:HB3	1.17	1.10
1:A:103:SER:HA	3:A:506:BOG:H1	1.32	1.04
1:C:201:ILE:HG22	1:C:202:GLU:H	1.25	0.99
1:A:41:GLN:HG2	1:A:70:LEU:HD11	1.51	0.92
1:D:148:ASN:HD21	1:D:150:SER:HB2	1.37	0.89

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	361/430 (84%)	341 (94%)	19 (5%)	1 (0%)	41	72
1	B	362/430 (84%)	338 (93%)	23 (6%)	1 (0%)	41	72
1	C	350/430 (81%)	335 (96%)	15 (4%)	0	100	100
1	D	353/430 (82%)	338 (96%)	14 (4%)	1 (0%)	41	72
All	All	1426/1720 (83%)	1352 (95%)	71 (5%)	3 (0%)	47	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	363	LYS
1	A	363	LYS
1	D	152	GLU

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	291/349 (83%)	252 (87%)	39 (13%)	4	12
1	B	292/349 (84%)	252 (86%)	40 (14%)	3	11
1	C	275/349 (79%)	233 (85%)	42 (15%)	2	8
1	D	278/349 (80%)	234 (84%)	44 (16%)	2	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1136/1396 (81%)	971 (86%)	165 (14%)	3 9

5 of 165 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	390	LEU
1	C	145	SER
1	D	379	GLN
1	B	408	ILE
1	C	43	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	148	ASN
1	D	282	ASN
1	D	26	HIS
1	C	139	GLN
1	C	303	GLN

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](#)

20 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
2	C8E	A	502	-	11,11,20	0.32	0	10,10,19	0.56	0
2	C8E	B	504	-	15,15,20	0.38	0	14,14,19	0.51	0
2	C8E	B	503	-	14,14,20	0.40	0	13,13,19	0.47	0
2	C8E	C	501	-	8,8,20	0.49	0	7,7,19	0.27	0
2	C8E	D	501	-	9,9,20	0.34	0	8,8,19	0.52	0
2	C8E	A	501	-	13,13,20	0.57	0	12,12,19	0.45	0
2	C8E	B	501	-	9,9,20	0.33	0	8,8,19	0.75	0
2	C8E	C	505	-	7,7,20	0.36	0	6,6,19	0.37	0
3	BOG	A	506	-	16,16,20	1.34	2 (12%)	21,21,25	2.19	8 (38%)
2	C8E	A	505	-	20,20,20	0.46	0	19,19,19	0.38	0
2	C8E	B	505	-	20,20,20	0.43	0	19,19,19	0.45	0
2	C8E	A	504	-	15,15,20	0.42	0	14,14,19	0.31	0
2	C8E	B	502	-	15,15,20	0.55	0	14,14,19	0.55	0
3	BOG	B	507	-	15,15,20	1.54	3 (20%)	19,20,25	2.59	9 (47%)
2	C8E	D	502	-	11,11,20	0.56	0	10,10,19	0.34	0
2	C8E	C	502	-	15,15,20	0.43	0	14,14,19	0.29	0
2	C8E	C	504	-	10,10,20	0.42	0	9,9,19	0.43	0
2	C8E	A	503	-	15,15,20	0.48	0	14,14,19	0.42	0
2	C8E	C	503	-	17,17,20	0.48	0	16,16,19	0.33	0
2	C8E	B	506	-	10,10,20	0.41	0	9,9,19	0.39	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
2	C8E	A	502	-	-	5/9/9/18	-
2	C8E	B	504	-	-	7/13/13/18	-
2	C8E	B	503	-	-	5/12/12/18	-
2	C8E	C	501	-	-	4/6/6/18	-
2	C8E	D	501	-	-	5/7/7/18	-
2	C8E	A	501	-	-	7/11/11/18	-
2	C8E	B	501	-	-	3/7/7/18	-
2	C8E	C	505	-	-	1/5/5/18	-
3	BOG	A	506	-	2/2/5/5	2/7/27/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	C8E	A	505	-	-	8/18/18/18	-
2	C8E	B	505	-	-	13/18/18/18	-
2	C8E	A	504	-	-	4/13/13/18	-
2	C8E	B	502	-	-	8/13/13/18	-
3	BOG	B	507	-	2/2/5/5	5/6/26/31	0/1/1/1
2	C8E	D	502	-	-	7/9/9/18	-
2	C8E	C	502	-	-	8/13/13/18	-
2	C8E	C	504	-	-	3/8/8/18	-
2	C8E	A	503	-	-	9/13/13/18	-
2	C8E	C	503	-	-	5/15/15/18	-
2	C8E	B	506	-	-	4/8/8/18	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	507	BOG	C4-C3	-3.87	1.42	1.52
3	A	506	BOG	C4-C3	-3.56	1.43	1.52
3	B	507	BOG	O3-C3	2.53	1.48	1.43
3	A	506	BOG	O3-C3	2.29	1.48	1.43
3	B	507	BOG	C3-C2	-2.08	1.47	1.52

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	507	BOG	C1'-O1-C1	5.81	123.48	113.84
3	A	506	BOG	O5-C5-C4	4.78	118.37	109.69
3	B	507	BOG	O5-C5-C4	4.46	117.78	109.69
3	A	506	BOG	C3-C4-C5	4.40	118.09	110.24
3	B	507	BOG	C1-C2-C3	4.07	118.47	110.00

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	506	BOG	C5
3	A	506	BOG	C3
3	B	507	BOG	C5
3	B	507	BOG	C3

5 of 113 torsion outliers are listed below:

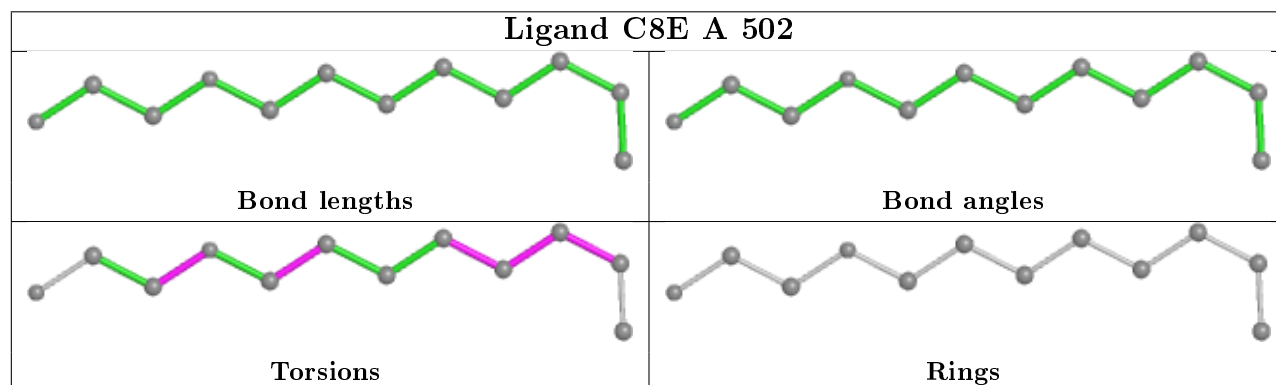
Mol	Chain	Res	Type	Atoms
3	A	506	BOG	C2'-C1'-O1-C1
3	B	507	BOG	C2'-C1'-O1-C1
2	B	503	C8E	C7-C8-O9-C10
2	B	502	C8E	C7-C8-O9-C10
2	C	503	C8E	C14-C13-O12-C11

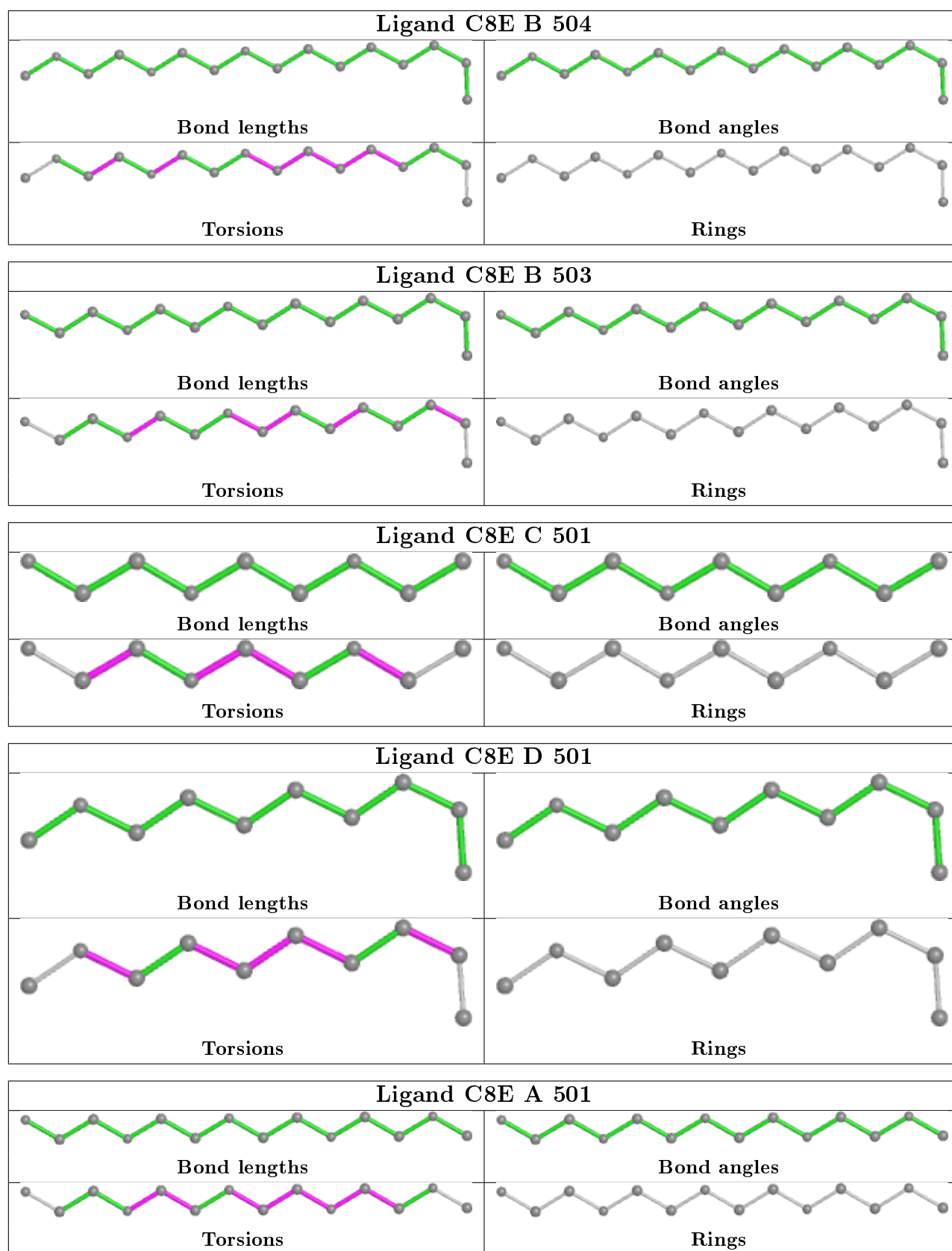
There are no ring outliers.

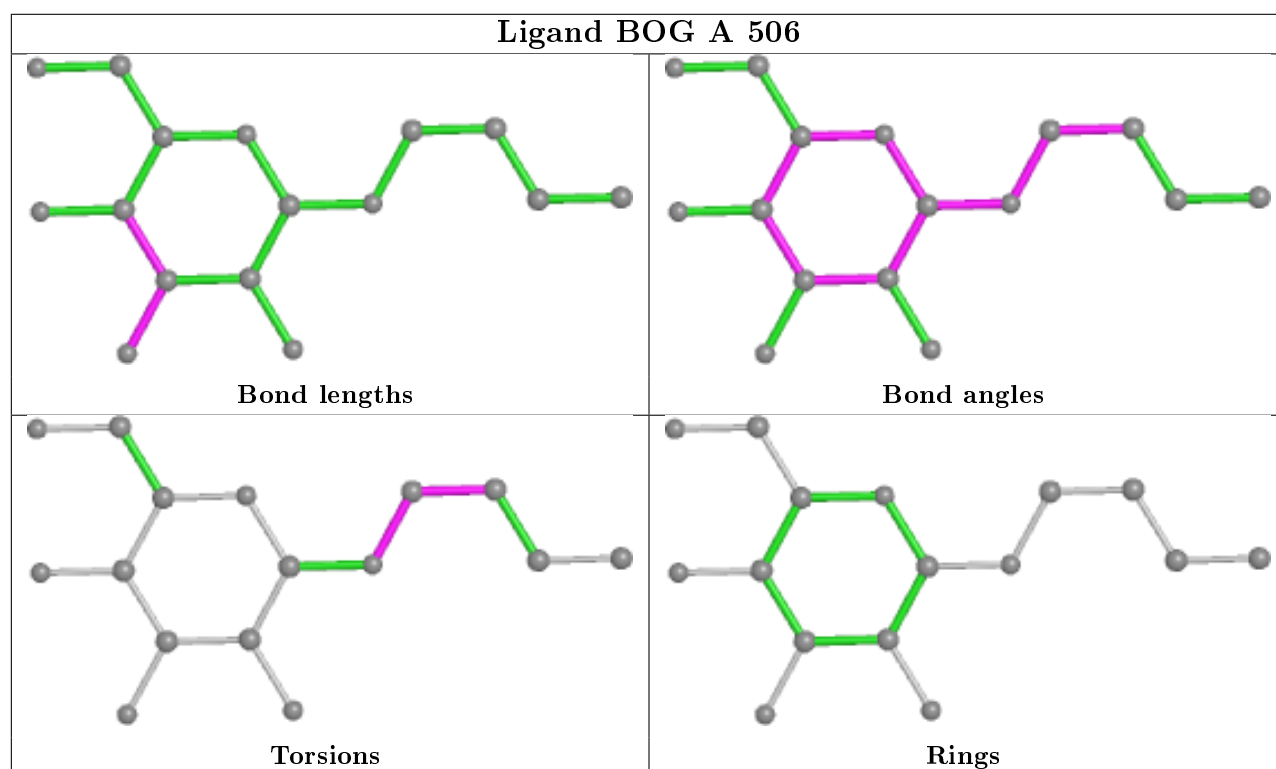
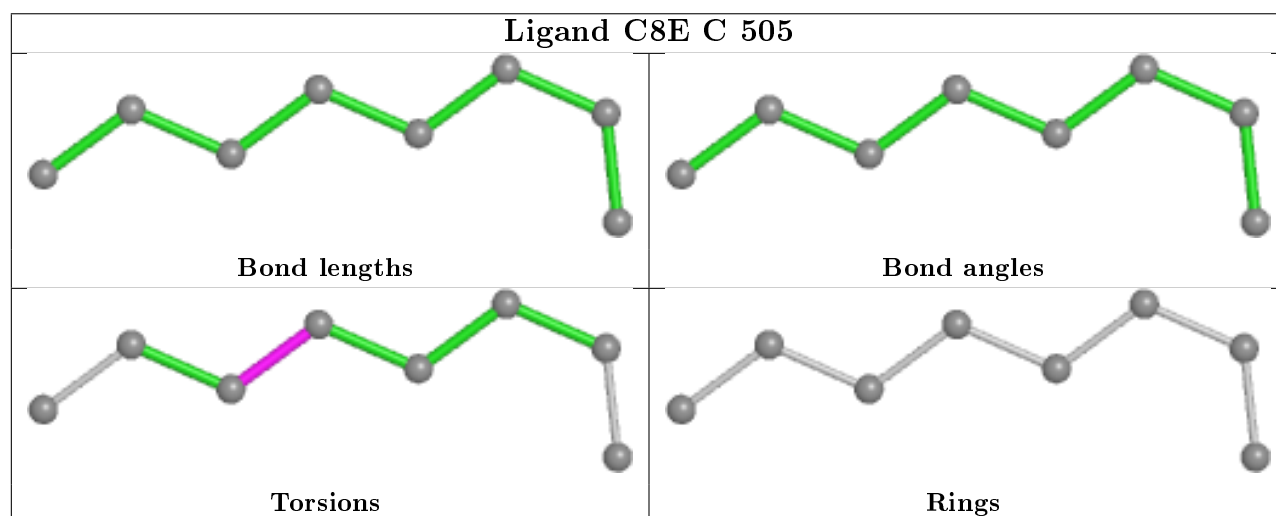
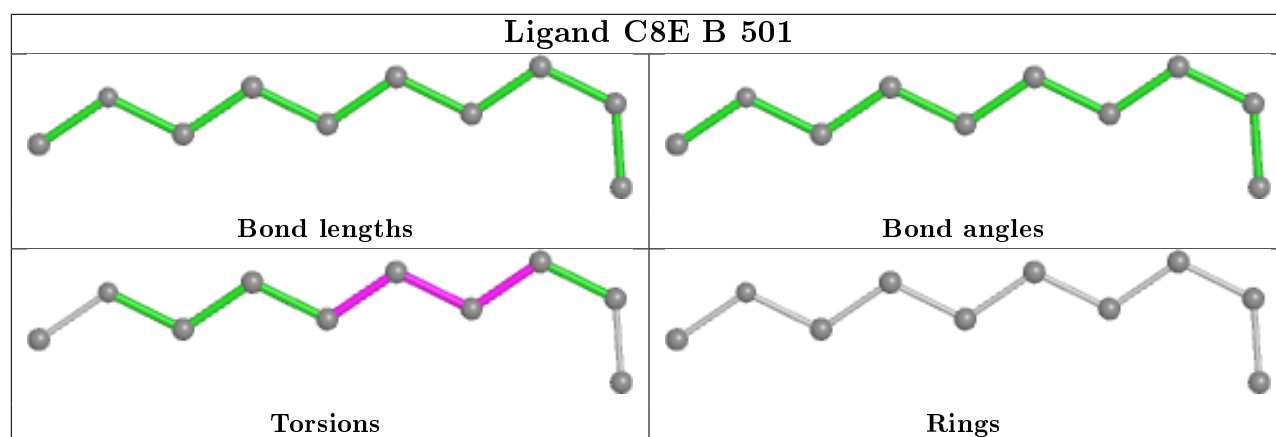
9 monomers are involved in 18 short contacts:

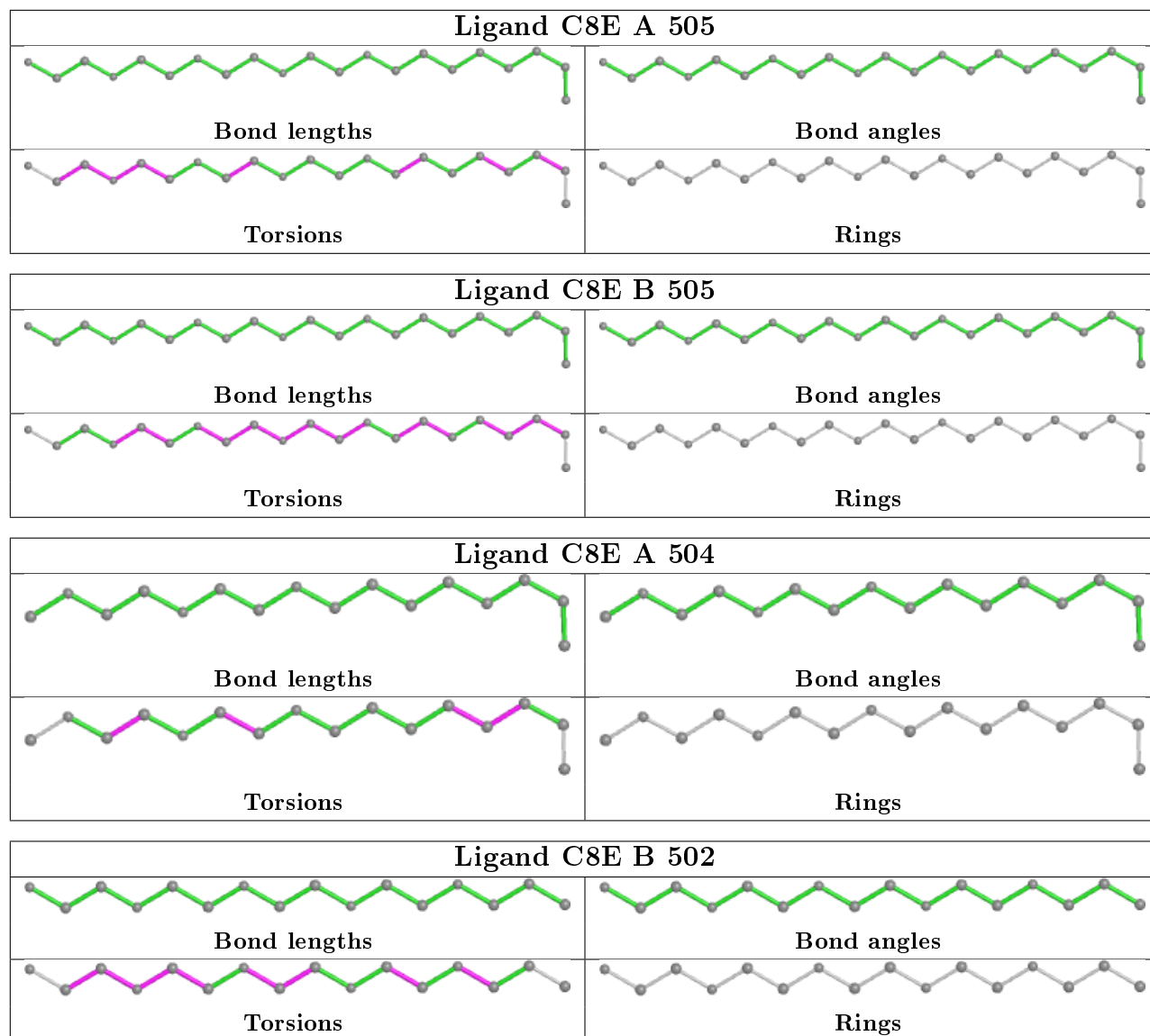
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	502	C8E	1	0
2	B	504	C8E	1	0
2	B	503	C8E	3	0
2	D	501	C8E	1	0
3	A	506	BOG	2	0
2	A	504	C8E	1	0
2	B	502	C8E	1	0
3	B	507	BOG	6	0
2	C	502	C8E	2	0

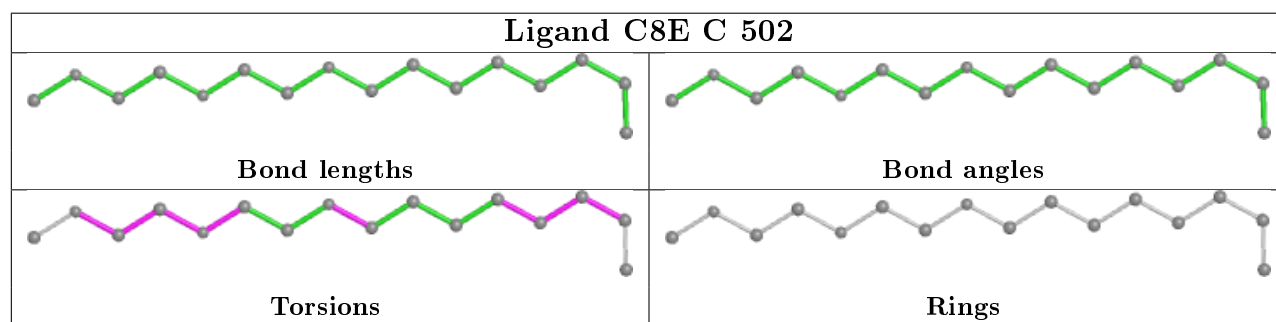
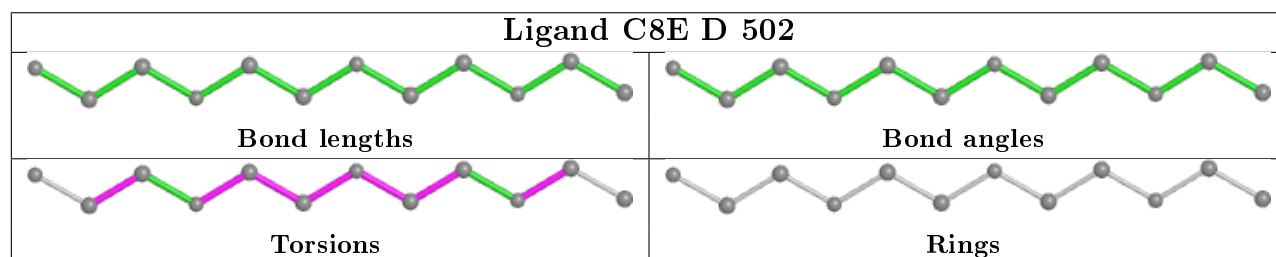
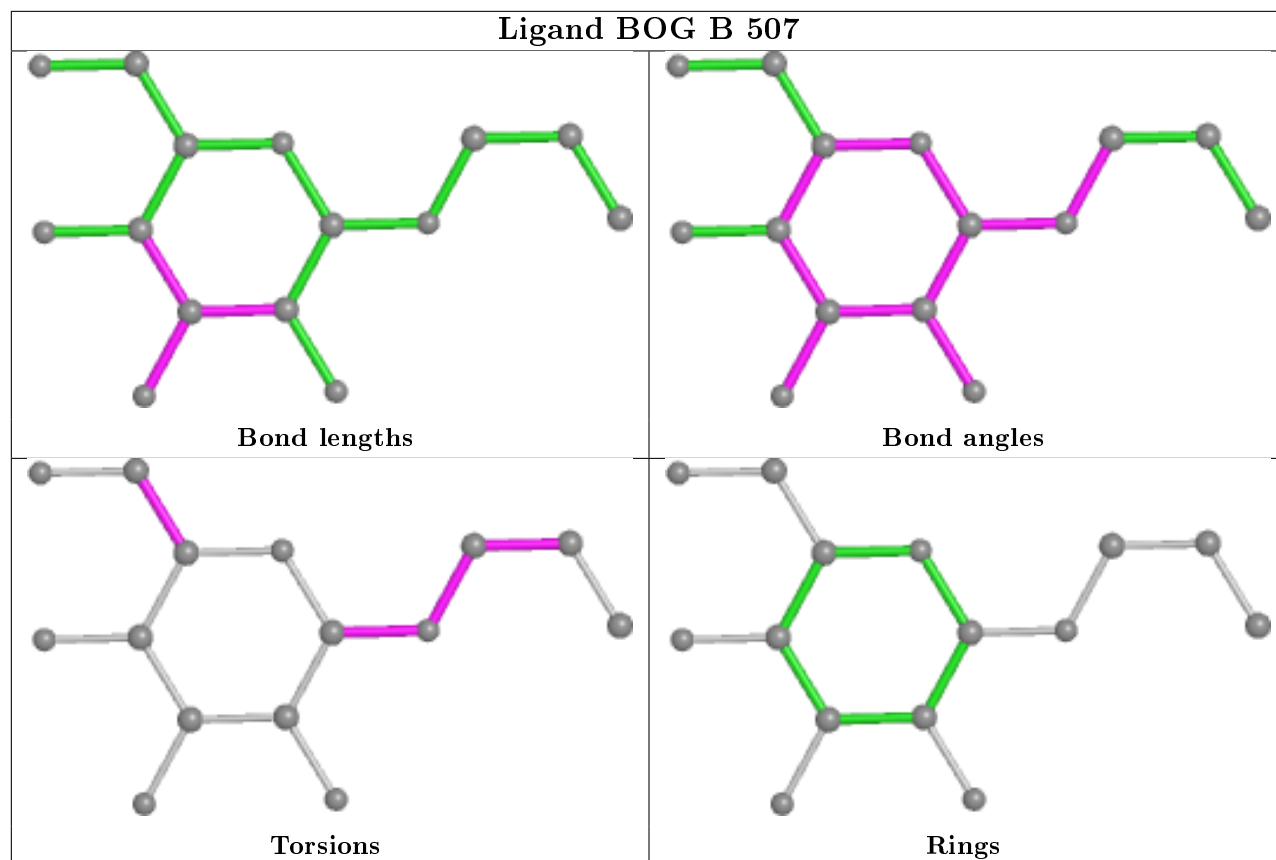
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

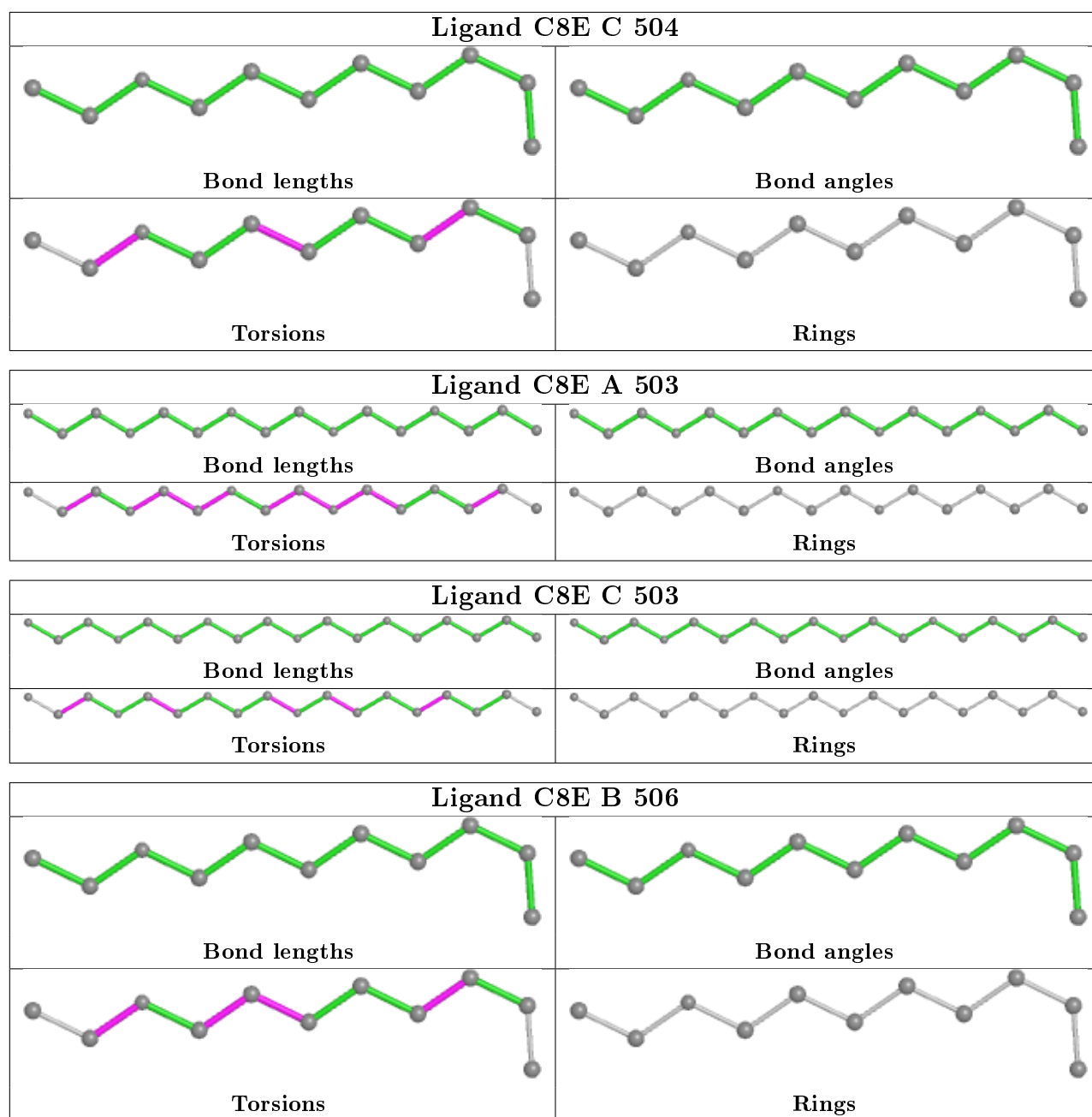












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	86:ALA	C	98:PRO	N	10.04
1	B	86:ALA	C	98:PRO	N	9.84

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	371/430 (86%)	-0.28	2 (0%) 91 88	41, 63, 111, 145	0
1	B	372/430 (86%)	-0.35	1 (0%) 94 93	38, 64, 109, 136	0
1	C	360/430 (83%)	-0.38	0 100 100	38, 71, 111, 135	0
1	D	361/430 (83%)	-0.35	0 100 100	38, 70, 111, 130	0
All	All	1464/1720 (85%)	-0.34	3 (0%) 95 94	38, 67, 111, 145	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	327	GLY	3.8
1	B	228	TYR	2.3
1	A	228	TYR	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](#)

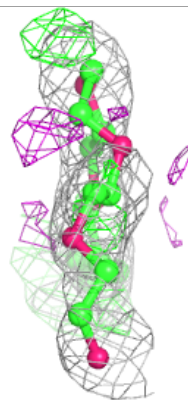
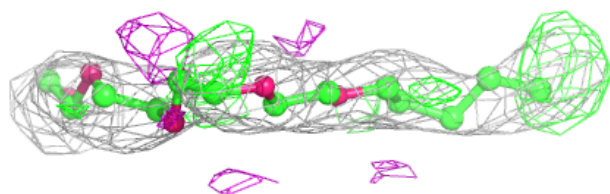
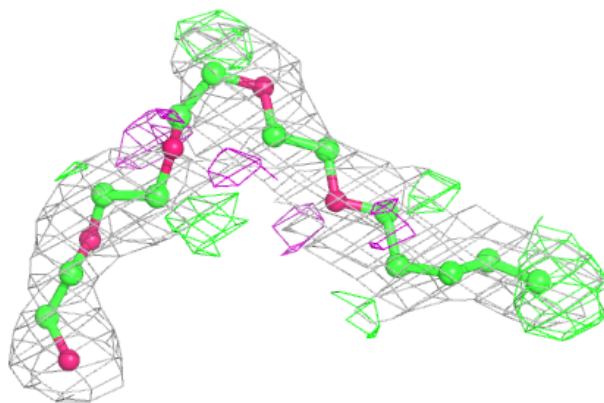
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	C8E	C	503	18/21	0.67	0.27	82,99,113,114	0
2	C8E	A	501	14/21	0.77	0.37	49,82,90,90	0
2	C8E	A	503	16/21	0.83	0.33	65,73,84,90	0
3	BOG	B	507	15/20	0.84	0.15	49,92,113,116	0
2	C8E	A	505	21/21	0.85	0.30	42,67,94,98	0
2	C8E	C	504	11/21	0.85	0.28	54,67,101,102	0
2	C8E	C	505	8/21	0.86	0.24	60,68,84,88	0
2	C8E	A	504	16/21	0.87	0.33	60,79,91,91	0
2	C8E	B	503	15/21	0.88	0.32	53,69,107,108	0
2	C8E	D	502	12/21	0.89	0.22	60,74,97,100	0
2	C8E	B	501	10/21	0.89	0.20	52,61,72,72	0
2	C8E	B	506	11/21	0.90	0.30	54,67,88,91	0
3	BOG	A	506	16/20	0.90	0.16	67,81,93,104	0
2	C8E	C	501	9/21	0.91	0.24	67,78,85,85	0
2	C8E	C	502	16/21	0.91	0.25	55,75,95,96	0
2	C8E	A	502	12/21	0.92	0.24	58,65,68,71	0
2	C8E	B	502	16/21	0.92	0.25	51,71,90,93	0
2	C8E	B	504	16/21	0.93	0.24	60,73,101,104	0
2	C8E	D	501	10/21	0.94	0.21	69,76,79,79	0
2	C8E	B	505	21/21	0.94	0.30	52,79,90,93	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.

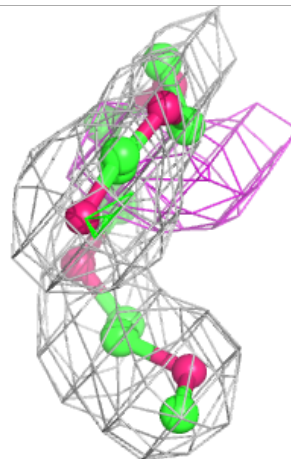
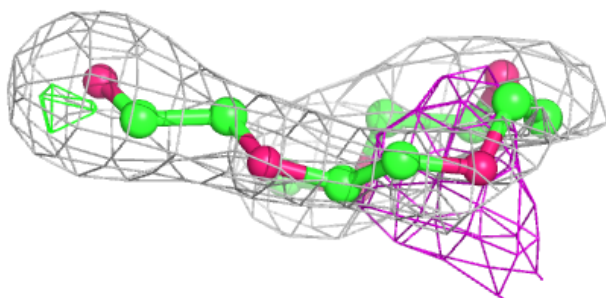
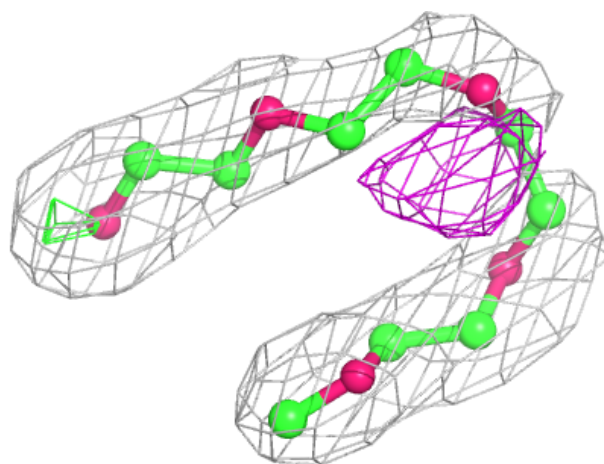
Electron density around C8E C 503:

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



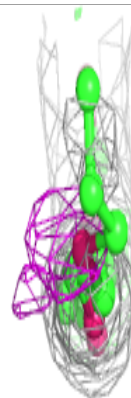
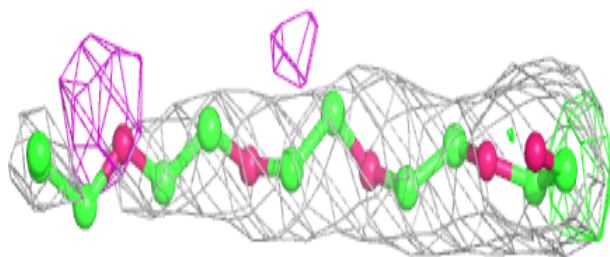
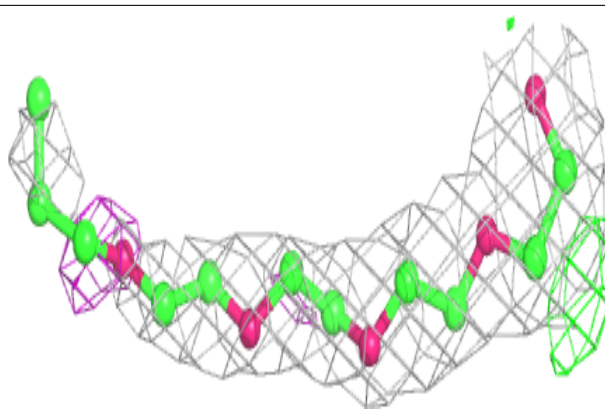
Electron density around C8E A 501:

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

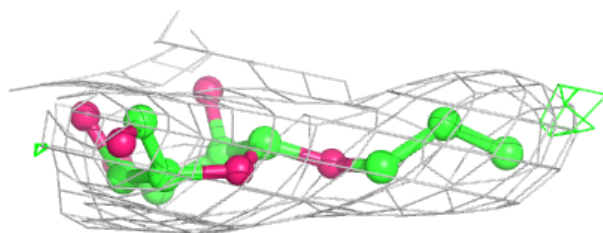
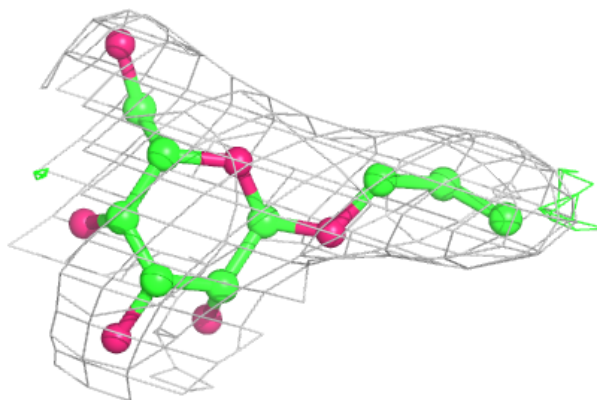


Electron density around C8E A 503:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

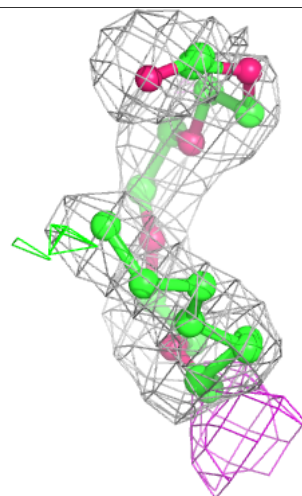
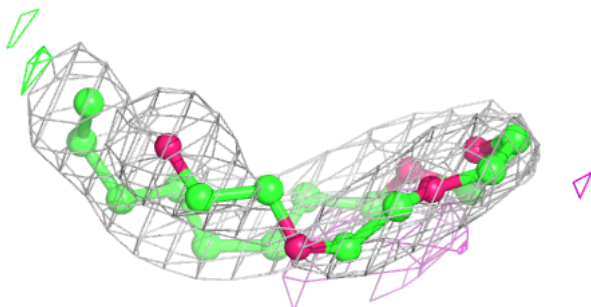
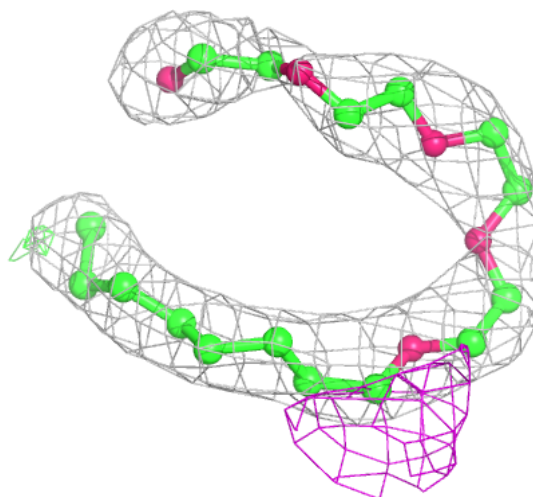
**Electron density around BOG B 507:**

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



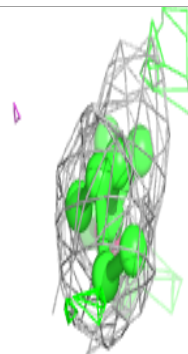
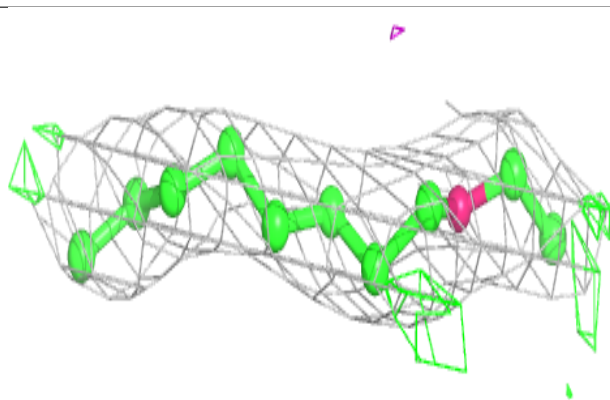
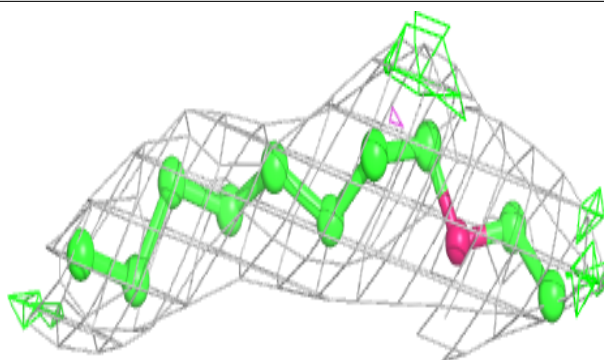
Electron density around C8E A 505:

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and green (positive)

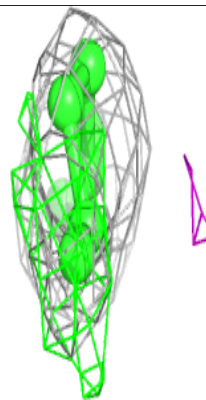
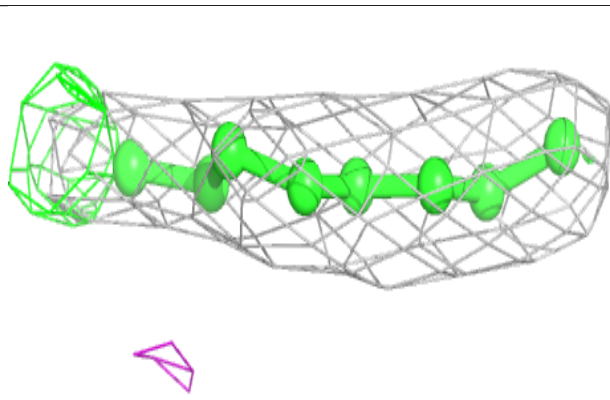
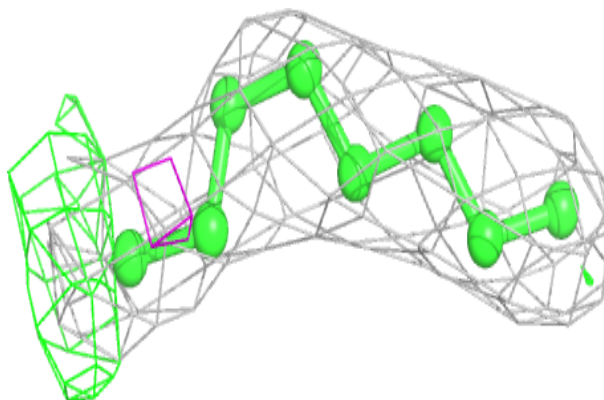


Electron density around C8E C 504:

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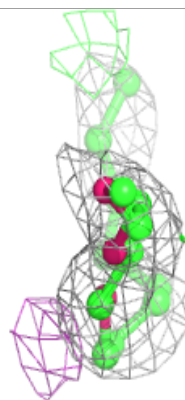
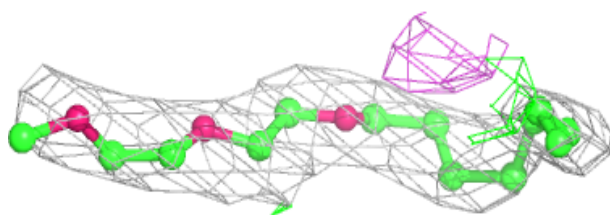
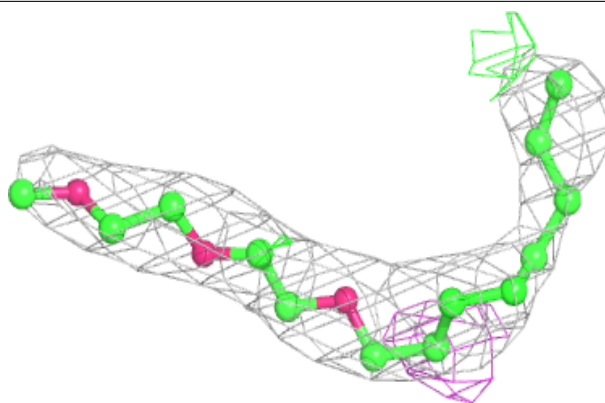
**Electron density around C8E C 505:**

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and green (positive)

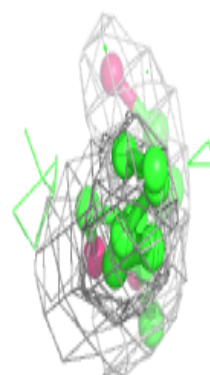
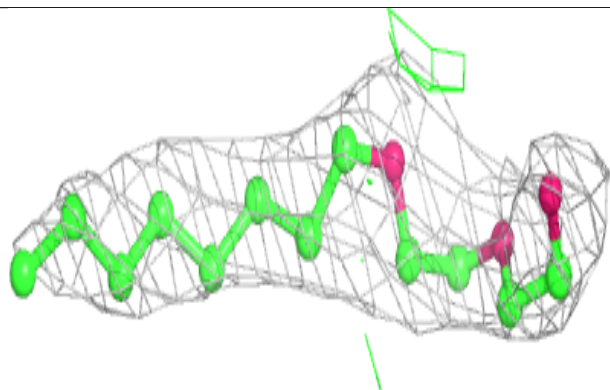
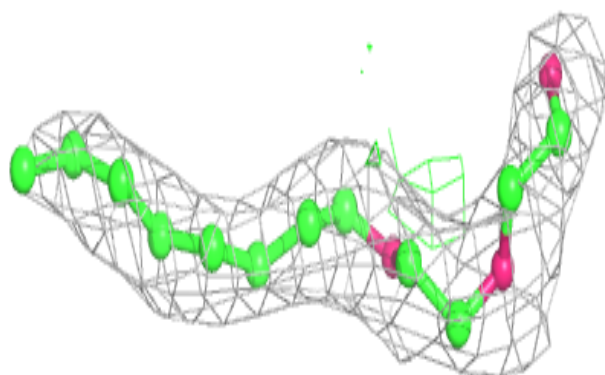


Electron density around C8E A 504:

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and green (positive)

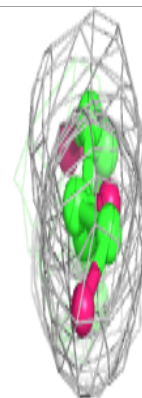
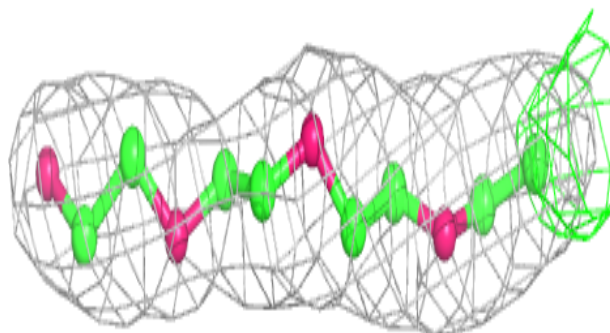
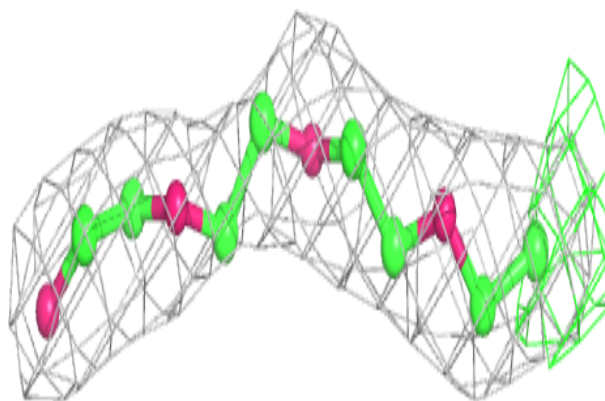
**Electron density around C8E B 503:**

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and green (positive)

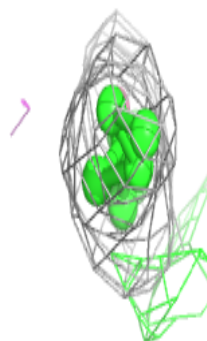
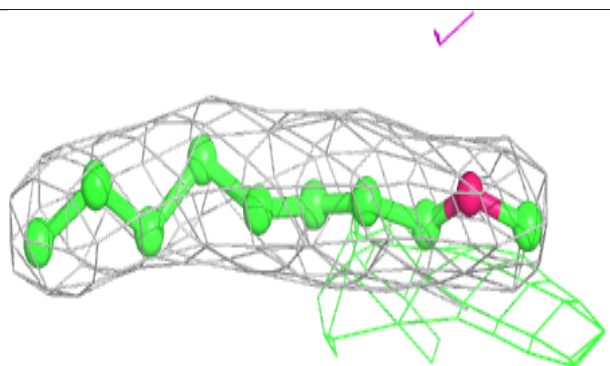
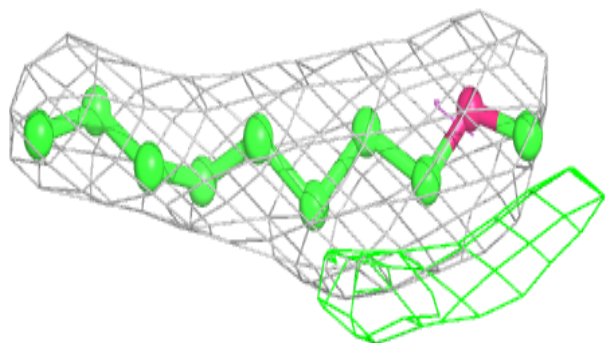


Electron density around C8E D 502:

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and green (positive)

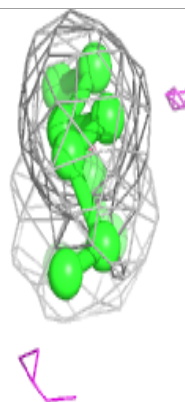
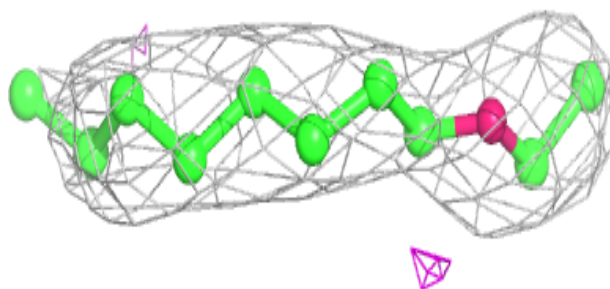
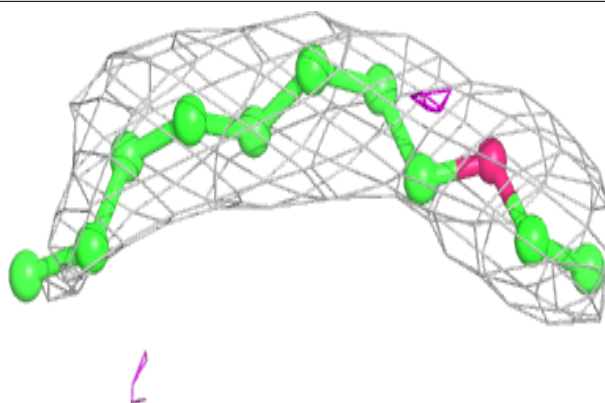
**Electron density around C8E B 501:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

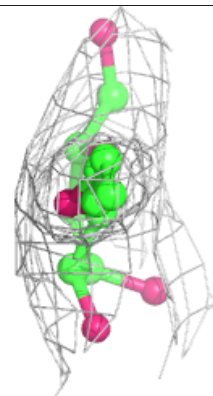
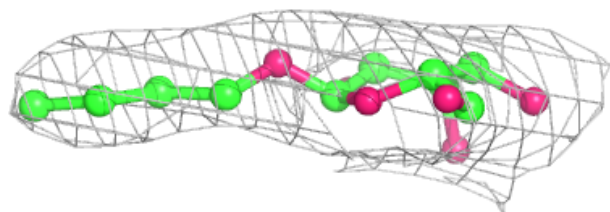
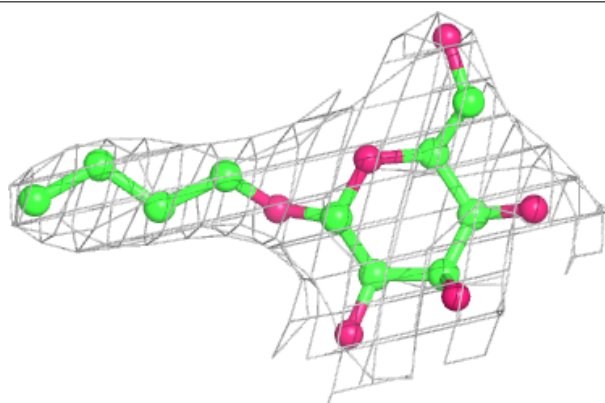


Electron density around C8E B 506:

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and green (positive)

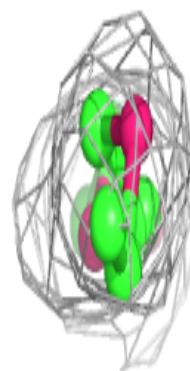
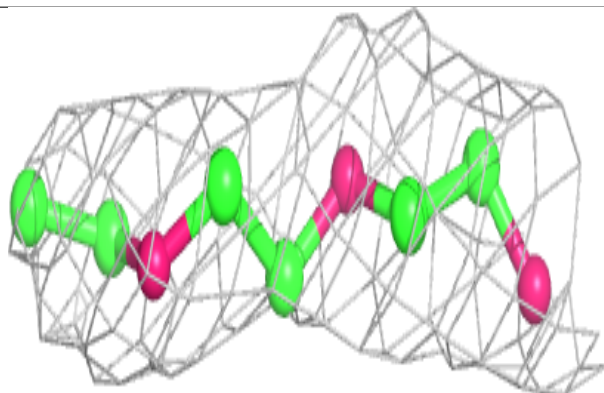
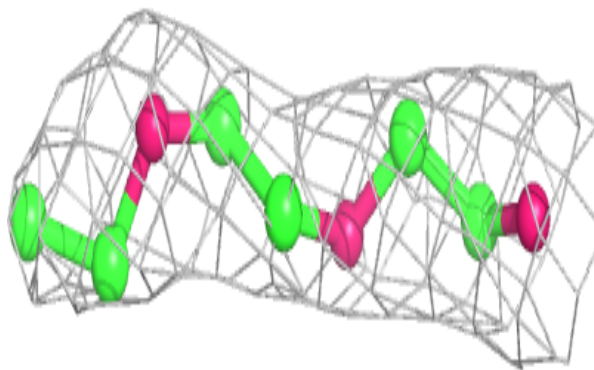
**Electron density around BOG A 506:**

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and green (positive)

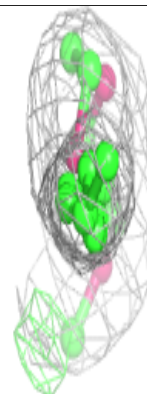
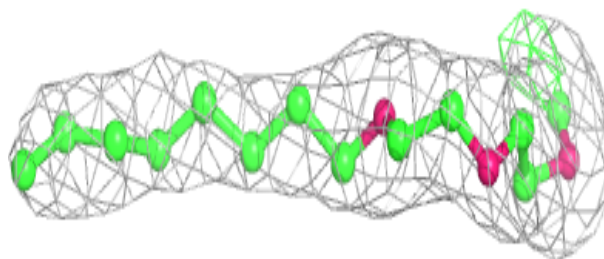
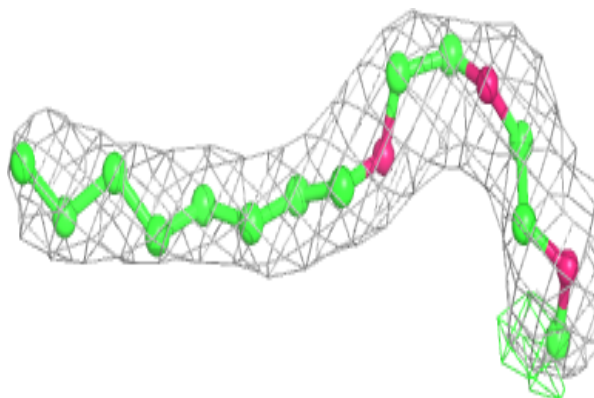


Electron density around C8E C 501:

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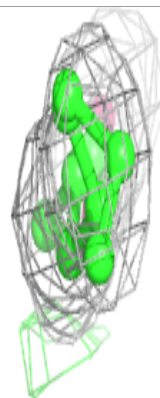
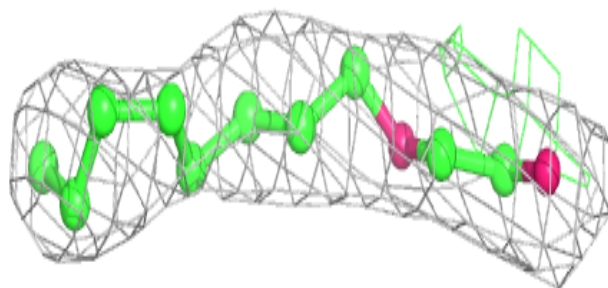
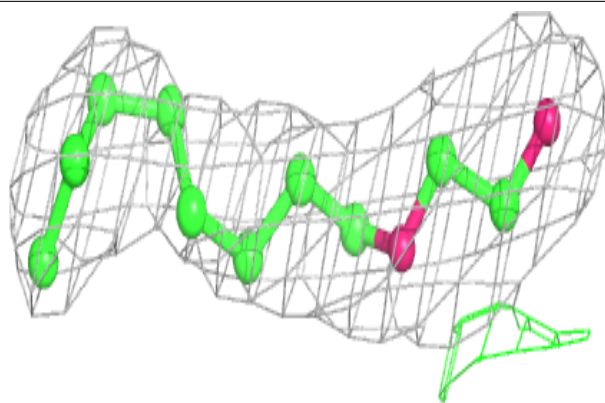
**Electron density around C8E C 502:**

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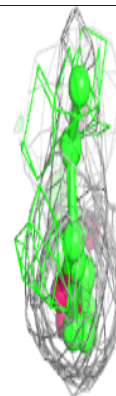
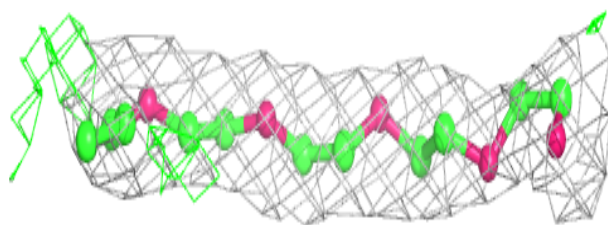
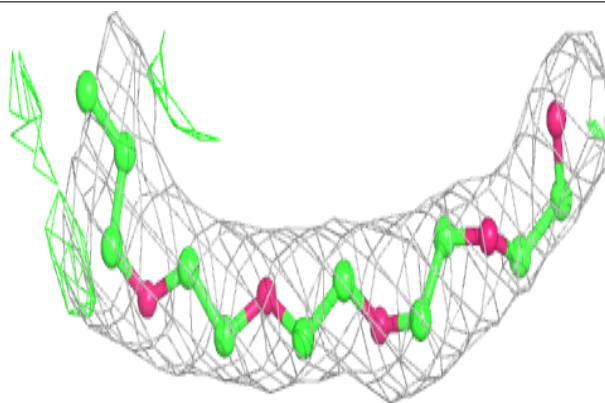


Electron density around C8E A 502:

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

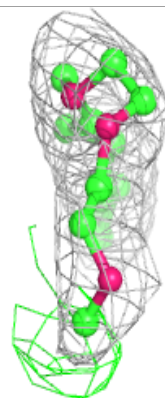
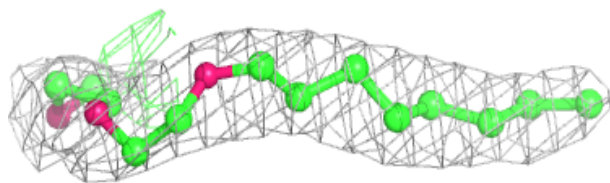
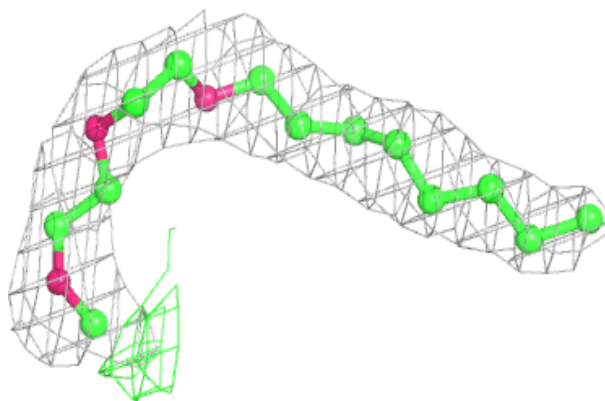
**Electron density around C8E B 502:**

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

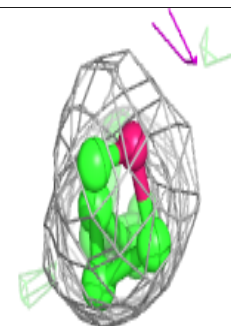
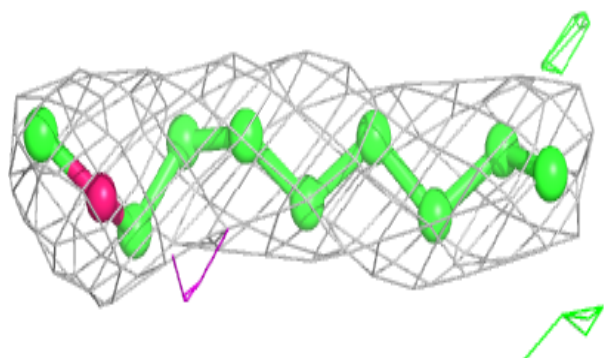
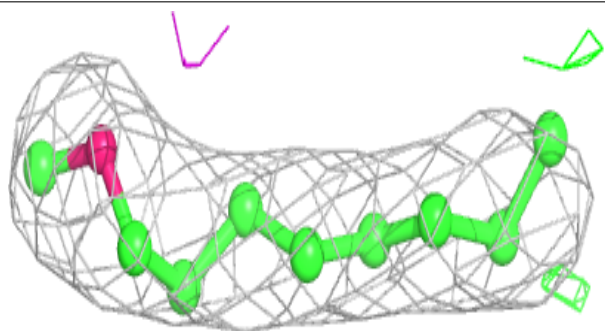


Electron density around C8E B 504:

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

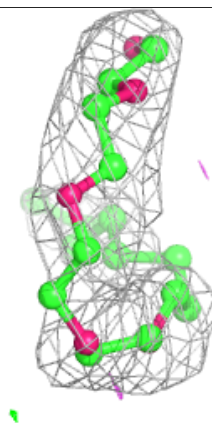
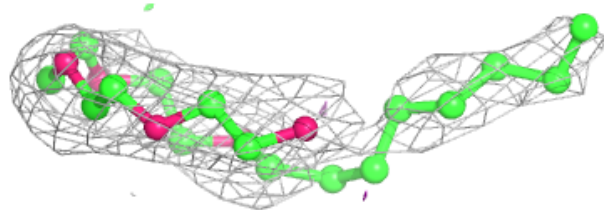
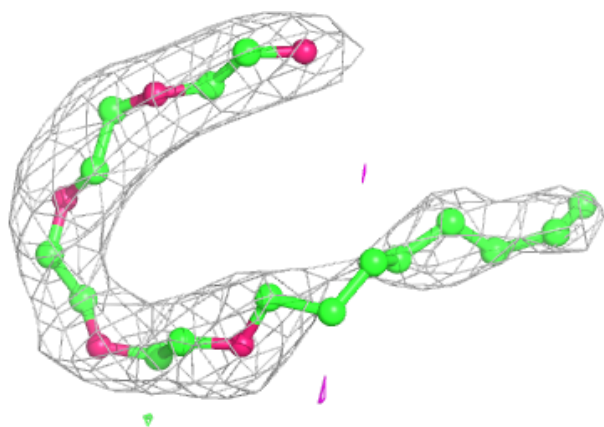
**Electron density around C8E D 501:**

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



Electron density around C8E 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.