



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:56 PM UTC

PDB ID : 6H7V / pdb_00006h7v
Title : Crystal structure of BauA, the Ferric preacinetobactin receptor from *Acinetobacter baumannii*
Authors : Moynie, L.; Naismith, J.H.
Deposited on : 2018-07-31
Resolution : 2.54 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

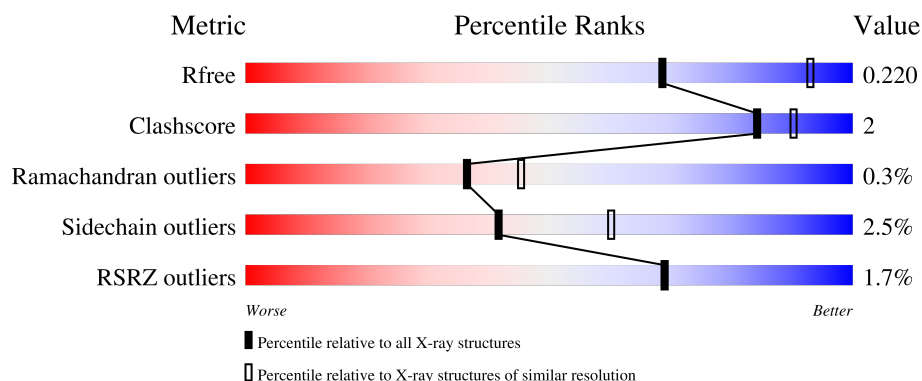
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

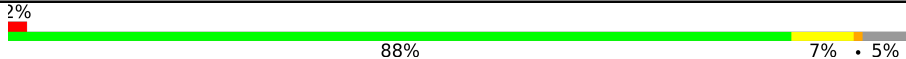
The reported resolution of this entry is 2.54 Å.

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}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	706	
1	B	706	
1	C	706	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15929 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 Ligand-gated channel protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	672	Total	C	N	O	Se	0	0	0
			5144	3248	861	1025	10			
1	B	671	Total	C	N	O	Se	0	0	0
			5136	3244	860	1022	10			
1	C	671	Total	C	N	O	Se	0	1	0
			5144	3250	861	1023	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP D0CC21
A	-1	ALA	-	expression tag	UNP D0CC21
A	0	MSE	-	expression tag	UNP D0CC21
A	377	SER	GLY	conflict	UNP D0CC21
B	-2	GLY	-	expression tag	UNP D0CC21
B	-1	ALA	-	expression tag	UNP D0CC21
B	0	MSE	-	expression tag	UNP D0CC21
B	377	SER	GLY	conflict	UNP D0CC21
C	-2	GLY	-	expression tag	UNP D0CC21
C	-1	ALA	-	expression tag	UNP D0CC21
C	0	MSE	-	expression tag	UNP D0CC21
C	377	SER	GLY	conflict	UNP D0CC21

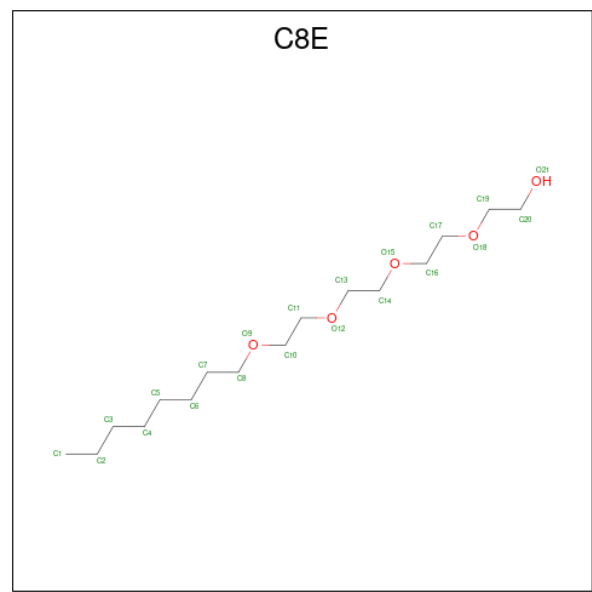
- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 3 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (CCD ID: C8E)

(formula: C₁₆H₃₄O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	10	1		
3	B	1	Total	C	O	0	0
			12	10	2		
3	B	1	Total	C	O	0	0
			12	10	2		
3	B	1	Total	C	O	0	0
			12	10	2		
3	B	1	Total	C	O	0	0
			14	12	2		
3	B	1	Total	C	O	0	0
			9	8	1		
3	B	1	Total	C	O	0	0
			11	10	1		
3	C	1	Total	C	O	0	0
			15	12	3		
3	C	1	Total	C	O	0	0
			15	12	3		
3	C	1	Total	C	O	0	0
			12	10	2		
3	C	1	Total	C	O	0	0
			13	8	5		
3	C	1	Total	C	O	0	0
			14	12	2		

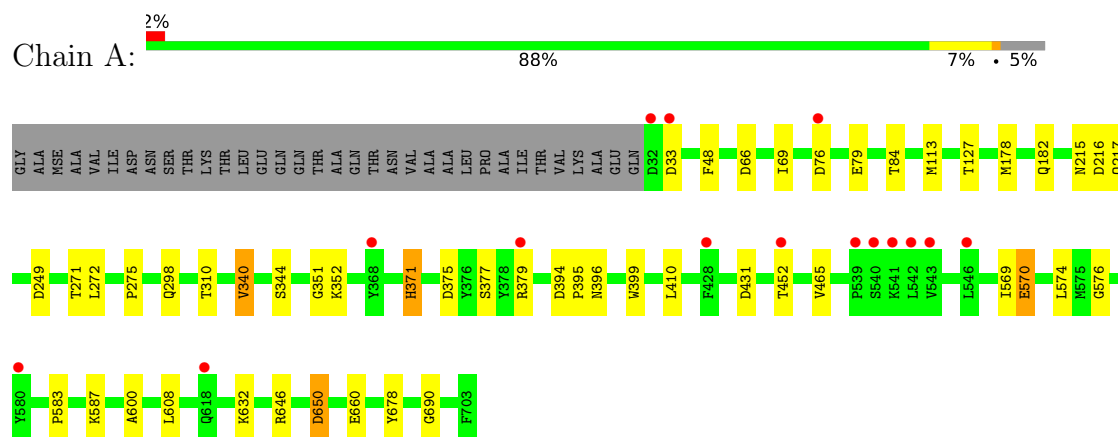
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	87	Total 87	O 87	0	0
4	B	103	Total 103	O 103	0	0
4	C	113	Total 113	O 113	0	0

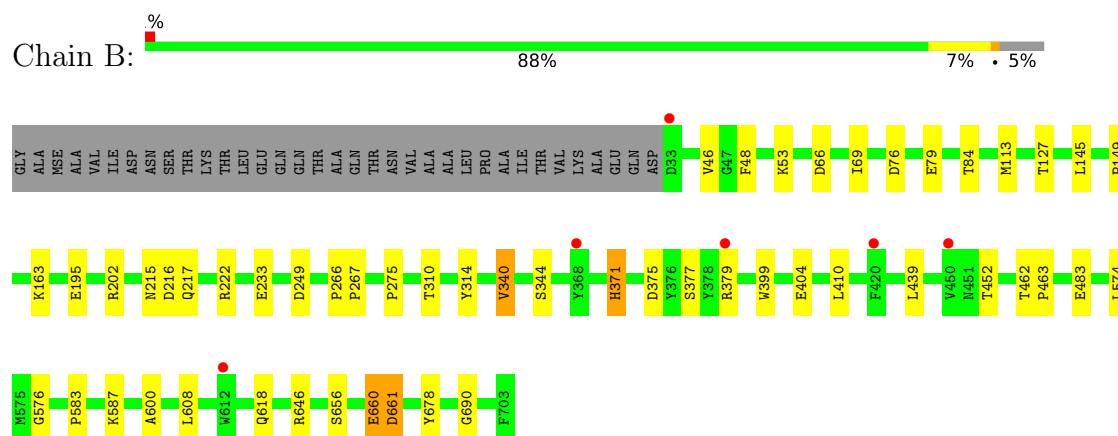
3 Residue-property plots [i](#)

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.

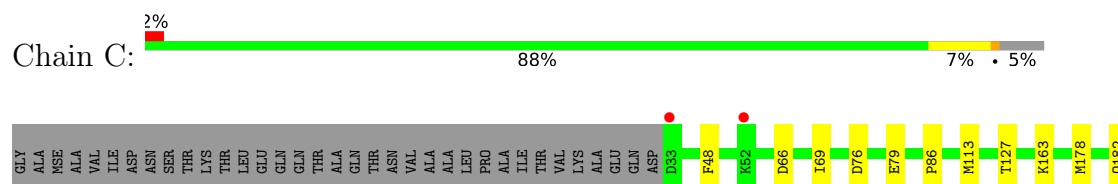
- Molecule 1: Ligand-gated channel protein

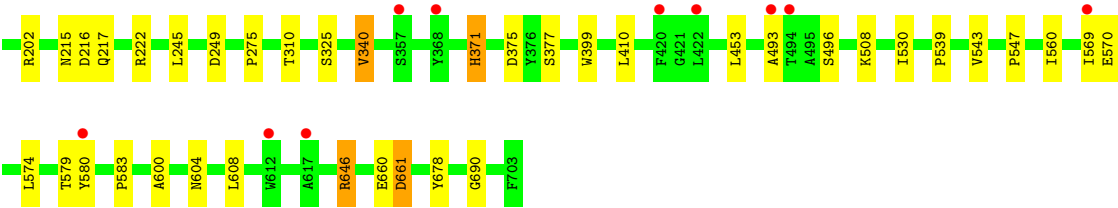


- Molecule 1: Ligand-gated channel protein



- Molecule 1: Ligand-gated channel protein





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	182.31Å 220.42Å 101.67Å 90.00° 98.65° 90.00°	Depositor
Resolution (Å)	139.53 – 2.54 139.53 – 2.54	Depositor EDS
% Data completeness (in resolution range)	99.9 (139.53-2.54) 99.9 (139.53-2.54)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.57 (at 2.55Å)	Xtriage
Refinement program	REFMAC 5.8.0218	Depositor
R, R_{free}	0.183 , 0.213 0.193 , 0.220	Depositor DCC
R_{free} test set	6485 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	41.2	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 28.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15929	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.73	0/5258	0.78	0/7138
1	B	0.74	0/5250	0.78	0/7127
1	C	0.76	0/5258	0.79	0/7138
All	All	0.74	0/15766	0.79	0/21403

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	5144	0	4964	21	0
1	B	5136	0	4960	24	0
1	C	5144	0	4970	27	0
2	A	20	0	30	1	0
2	B	12	0	18	0	0
2	C	20	0	30	0	0
3	A	11	0	19	0	0
3	B	70	0	122	1	0
3	C	69	0	111	4	0
4	A	87	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	103	0	0	1	0
4	C	113	0	0	1	0
All	All	15929	0	15224	71	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 2.

All (71) 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:650:ASP:OD2	4:A:901:HOH:O	2.09	0.71
1:A:33:ASP:OD2	4:A:902:HOH:O	2.12	0.67
1:B:439:LEU:C	1:B:439:LEU:HD12	2.22	0.65
1:C:604:ASN:HB3	3:C:809:C8E:H131	1.84	0.59
1:B:463:PRO:HG3	3:C:806:C8E:H132	1.88	0.56
1:C:310:THR:HB	1:C:340:VAL:HG13	1.88	0.55
1:B:310:THR:HB	1:B:340:VAL:HG13	1.89	0.54
1:A:396:ASN:ND2	1:C:325:SER:O	2.41	0.54
1:A:310:THR:HB	1:A:340:VAL:HG13	1.90	0.53
1:C:574:LEU:HD11	1:C:608:LEU:HD11	1.91	0.53
1:B:618:GLN:HA	1:B:618:GLN:OE1	2.09	0.52
1:C:222:ARG:HB2	1:C:245:LEU:HB3	1.90	0.52
1:B:222:ARG:HD2	3:B:809:C8E:H12	1.89	0.52
1:A:569:ILE:HG22	1:A:570:GLU:N	2.25	0.52
1:C:539:PRO:HA	1:C:547:PRO:HB3	1.93	0.50
1:B:217:GLN:HA	1:B:249:ASP:O	2.12	0.50
1:A:394:ASP:OD1	1:A:395:PRO:HD2	2.12	0.49
1:A:113:MSE:HE1	1:A:127:THR:OG1	2.12	0.49
1:B:215:ASN:O	1:B:216:ASP:HB2	2.13	0.48
1:A:377:SER:HB3	1:A:410:LEU:HD22	1.94	0.48
1:B:76:ASP:OD1	1:B:79:GLU:HG3	2.14	0.47
1:C:215:ASN:O	1:C:216:ASP:HB2	2.13	0.47
1:C:377:SER:HB3	1:C:410:LEU:HD22	1.97	0.47
1:A:215:ASN:O	1:A:216:ASP:HB2	2.13	0.47
1:A:217:GLN:HA	1:A:249:ASP:O	2.15	0.47
1:A:275:PRO:HA	1:A:399:TRP:CD2	2.50	0.47
1:A:574:LEU:HD11	1:A:608:LEU:HD11	1.97	0.47
1:C:178:MSE:HE2	1:C:182:GLN:OE1	2.15	0.47
1:C:222:ARG:HD2	1:C:245:LEU:HD23	1.96	0.47
1:B:574:LEU:HD11	1:B:608:LEU:HD11	1.97	0.46
1:A:76:ASP:OD1	1:A:79:GLU:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ASP:HA	1:A:69:ILE:HD12	1.98	0.45
1:C:660:GLU:O	1:C:661:ASP:HB2	2.17	0.45
1:A:178:MSE:HE2	1:A:182:GLN:OE1	2.16	0.45
1:A:678:TYR:CZ	1:A:690:GLY:HA3	2.51	0.45
1:B:113:MSE:HE1	1:B:127:THR:OG1	2.18	0.44
1:B:371:HIS:CD2	1:B:371:HIS:C	2.96	0.44
1:B:660:GLU:O	1:B:661:ASP:HB2	2.18	0.44
1:B:163:LYS:HD3	1:B:202:ARG:NH2	2.33	0.44
1:B:149:PRO:HD2	4:B:943:HOH:O	2.16	0.44
1:C:76:ASP:OD1	1:C:79:GLU:HG3	2.18	0.43
1:C:163:LYS:HD3	1:C:202:ARG:NH2	2.33	0.43
1:C:604:ASN:HB3	3:C:809:C8E:C13	2.46	0.43
1:C:113:MSE:HE1	1:C:127:THR:OG1	2.17	0.43
1:A:298:GLN:O	1:A:351:GLY:HA2	2.18	0.43
1:B:84:THR:O	1:B:576:GLY:HA2	2.18	0.43
1:A:371:HIS:CD2	1:A:371:HIS:C	2.96	0.43
1:B:678:TYR:CZ	1:B:690:GLY:HA3	2.53	0.42
1:C:646:ARG:HD3	4:C:931:HOH:O	2.19	0.42
1:A:271:THR:HG23	2:A:804:EDO:H11	2.01	0.42
1:B:66:ASP:HA	1:B:69:ILE:HD12	2.01	0.42
1:C:678:TYR:CZ	1:C:690:GLY:HA3	2.54	0.42
1:C:371:HIS:CD2	1:C:371:HIS:C	2.97	0.42
1:C:275:PRO:HA	1:C:399:TRP:CD2	2.54	0.42
1:C:580:TYR:CE2	3:C:809:C8E:O9	2.73	0.41
1:B:275:PRO:HA	1:B:399:TRP:CD2	2.55	0.41
1:C:496:SER:HB2	1:C:543:VAL:HB	2.02	0.41
1:B:439:LEU:C	1:B:439:LEU:CD1	2.92	0.41
1:C:217:GLN:HA	1:C:249:ASP:O	2.20	0.41
1:B:46:VAL:HG12	1:B:145:LEU:HD13	2.03	0.41
1:B:266:PRO:HA	1:B:267:PRO:HD3	1.97	0.41
1:C:66:ASP:HA	1:C:69:ILE:HD12	2.03	0.41
1:A:272:LEU:HA	4:A:921:HOH:O	2.20	0.41
1:C:508:LYS:O	1:C:530:ILE:HA	2.20	0.41
1:A:84:THR:O	1:A:576:GLY:HA2	2.21	0.41
1:B:314:TYR:CD1	1:B:314:TYR:C	2.99	0.40
1:B:377:SER:HB3	1:B:410:LEU:HD22	2.02	0.40
1:B:462:THR:OG1	1:B:483:GLU:HB2	2.21	0.40
1:C:496:SER:CB	1:C:543:VAL:HB	2.51	0.40
1:C:86:PRO:HB2	1:C:579:THR:HG23	2.03	0.40
1:C:453:LEU:HD21	1:C:493:ALA:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	670/706 (95%)	648 (97%)	20 (3%)	2 (0%)	36	45
1	B	669/706 (95%)	645 (96%)	22 (3%)	2 (0%)	36	45
1	C	670/706 (95%)	646 (96%)	22 (3%)	2 (0%)	36	45
All	All	2009/2118 (95%)	1939 (96%)	64 (3%)	6 (0%)	36	45

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	600	ALA
1	A	600	ALA
1	C	600	ALA
1	B	583	PRO
1	C	583	PRO
1	A	583	PRO

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	552/567 (97%)	536 (97%)	16 (3%)	37	55
1	B	551/567 (97%)	535 (97%)	16 (3%)	37	55
1	C	552/567 (97%)	543 (98%)	9 (2%)	55	73
All	All	1655/1701 (97%)	1614 (98%)	41 (2%)	42	60

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	PHE
1	A	340	VAL
1	A	344	SER
1	A	352	LYS
1	A	371	HIS
1	A	375	ASP
1	A	379	ARG
1	A	431	ASP
1	A	452	THR
1	A	465	VAL
1	A	570	GLU
1	A	587	LYS
1	A	632	LYS
1	A	646	ARG
1	A	650	ASP
1	A	660	GLU
1	B	48	PHE
1	B	53	LYS
1	B	195	GLU
1	B	233	GLU
1	B	340	VAL
1	B	344	SER
1	B	371	HIS
1	B	375	ASP
1	B	379	ARG
1	B	404	GLU
1	B	452	THR
1	B	587	LYS
1	B	646	ARG
1	B	656	SER
1	B	660	GLU
1	B	661	ASP
1	C	48	PHE
1	C	340	VAL
1	C	371	HIS
1	C	375	ASP
1	C	560	ILE
1	C	569	ILE
1	C	570	GLU
1	C	646	ARG
1	C	661	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	ASN
1	A	204	ASN
1	A	247	HIS
1	A	298	GLN
1	A	370	ASN
1	A	434	GLN
1	A	544	ASN
1	A	604	ASN
1	A	683	GLN
1	B	111	ASN
1	B	146	ASN
1	B	215	ASN
1	B	247	HIS
1	B	605	GLN
1	B	683	GLN
1	C	73	GLN
1	C	100	ASN
1	C	111	ASN
1	C	298	GLN
1	C	370	ASN
1	C	434	GLN
1	C	544	ASN
1	C	669	ASN
1	C	683	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 oligosaccharides in this entry.

5.6 Ligand geometry

25 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	EDO	C	803	-	3,3,3	0.40	0	2,2,2	0.55	0
3	C8E	C	810	-	13,13,20	0.58	0	12,12,19	0.43	0
3	C8E	A	806	-	10,10,20	0.47	0	9,9,19	0.28	0
2	EDO	C	801	-	3,3,3	0.45	0	2,2,2	0.19	0
3	C8E	B	808	-	8,8,20	0.33	0	7,7,19	0.38	0
2	EDO	C	804	-	3,3,3	0.34	0	2,2,2	0.46	0
3	C8E	C	806	-	14,14,20	0.49	0	13,13,19	0.33	0
3	C8E	B	805	-	11,11,20	0.48	0	10,10,19	0.20	0
3	C8E	B	809	-	10,10,20	0.56	0	9,9,19	0.26	0
2	EDO	B	802	-	3,3,3	0.43	0	2,2,2	0.43	0
2	EDO	A	805	-	3,3,3	0.38	0	2,2,2	0.33	0
3	C8E	B	806	-	11,11,20	0.41	0	10,10,19	0.42	0
3	C8E	C	807	-	14,14,20	0.46	0	13,13,19	0.61	0
2	EDO	C	802	-	3,3,3	0.45	0	2,2,2	0.30	0
2	EDO	C	805	-	3,3,3	0.42	0	2,2,2	0.55	0
2	EDO	B	801	-	3,3,3	0.43	0	2,2,2	0.32	0
3	C8E	B	807	-	13,13,20	0.54	0	12,12,19	0.30	0
3	C8E	C	808	-	11,11,20	0.49	0	10,10,19	0.41	0
2	EDO	A	802	-	3,3,3	0.58	0	2,2,2	0.07	0
2	EDO	B	803	-	3,3,3	0.35	0	2,2,2	0.50	0
3	C8E	B	804	-	11,11,20	0.41	0	10,10,19	0.39	0
2	EDO	A	804	-	3,3,3	0.31	0	2,2,2	0.59	0
2	EDO	A	801	-	3,3,3	0.43	0	2,2,2	0.41	0
2	EDO	A	803	-	3,3,3	0.49	0	2,2,2	0.36	0
3	C8E	C	809	-	12,12,20	0.58	0	11,11,19	0.27	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	EDO	C	803	-	-	0/1/1/1	-
3	C8E	C	810	-	-	4/11/11/18	-
3	C8E	A	806	-	-	4/8/8/18	-
2	EDO	C	801	-	-	0/1/1/1	-
3	C8E	B	808	-	-	4/6/6/18	-
2	EDO	C	804	-	-	1/1/1/1	-
3	C8E	C	806	-	-	6/12/12/18	-
3	C8E	B	805	-	-	3/9/9/18	-
3	C8E	B	809	-	-	1/8/8/18	-
2	EDO	B	802	-	-	1/1/1/1	-
2	EDO	A	805	-	-	0/1/1/1	-
3	C8E	B	806	-	-	6/9/9/18	-
3	C8E	C	807	-	-	4/12/12/18	-
2	EDO	C	802	-	-	1/1/1/1	-
2	EDO	C	805	-	-	1/1/1/1	-
2	EDO	B	801	-	-	0/1/1/1	-
3	C8E	B	807	-	-	5/11/11/18	-
3	C8E	C	808	-	-	4/9/9/18	-
2	EDO	A	802	-	-	0/1/1/1	-
2	EDO	B	803	-	-	0/1/1/1	-
3	C8E	B	804	-	-	6/9/9/18	-
2	EDO	A	804	-	-	1/1/1/1	-
2	EDO	A	801	-	-	1/1/1/1	-
2	EDO	A	803	-	-	0/1/1/1	-
3	C8E	C	809	-	-	5/10/10/18	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	806	C8E	O9-C10-C11-O12
3	C	809	C8E	O18-C19-C20-O21
3	B	807	C8E	C6-C7-C8-O9
3	C	807	C8E	C6-C7-C8-O9
3	B	807	C8E	O9-C10-C11-O12
3	C	806	C8E	O12-C13-C14-O15
3	C	808	C8E	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	A	806	C8E	C2-C3-C4-C5
3	C	808	C8E	C6-C7-C8-O9
2	B	802	EDO	O1-C1-C2-O2
3	B	807	C8E	C5-C6-C7-C8
3	C	808	C8E	C5-C6-C7-C8
3	B	809	C8E	C2-C3-C4-C5
3	C	806	C8E	C4-C5-C6-C7
3	B	805	C8E	C3-C4-C5-C6
3	B	808	C8E	C5-C6-C7-C8
3	A	806	C8E	C3-C4-C5-C6
3	B	806	C8E	C4-C5-C6-C7
3	B	804	C8E	O9-C10-C11-O12
3	B	808	C8E	C6-C7-C8-O9
3	A	806	C8E	C6-C7-C8-O9
3	C	809	C8E	O12-C13-C14-O15
3	C	809	C8E	O9-C10-C11-O12
3	C	809	C8E	O15-C16-C17-O18
3	B	804	C8E	C2-C3-C4-C5
3	C	807	C8E	O9-C10-C11-O12
3	A	806	C8E	C1-C2-C3-C4
2	C	804	EDO	O1-C1-C2-O2
3	C	810	C8E	O9-C10-C11-O12
3	C	806	C8E	C14-C13-O12-C11
3	B	804	C8E	C1-C2-C3-C4
3	C	806	C8E	O9-C10-C11-O12
3	B	806	C8E	C11-C10-O9-C8
3	B	806	C8E	C3-C4-C5-C6
2	A	804	EDO	O1-C1-C2-O2
3	C	806	C8E	C10-C11-O12-C13
3	C	810	C8E	C6-C7-C8-O9
3	C	809	C8E	C10-C11-O12-C13
3	B	806	C8E	C7-C8-O9-C10
3	C	807	C8E	O12-C13-C14-O15
3	B	804	C8E	C4-C5-C6-C7
3	C	808	C8E	C1-C2-C3-C4
2	A	801	EDO	O1-C1-C2-O2
3	B	804	C8E	C3-C4-C5-C6
3	B	807	C8E	C7-C8-O9-C10
3	C	810	C8E	C2-C3-C4-C5
3	B	805	C8E	C6-C7-C8-O9
3	B	805	C8E	C2-C3-C4-C5
3	C	807	C8E	C7-C8-O9-C10

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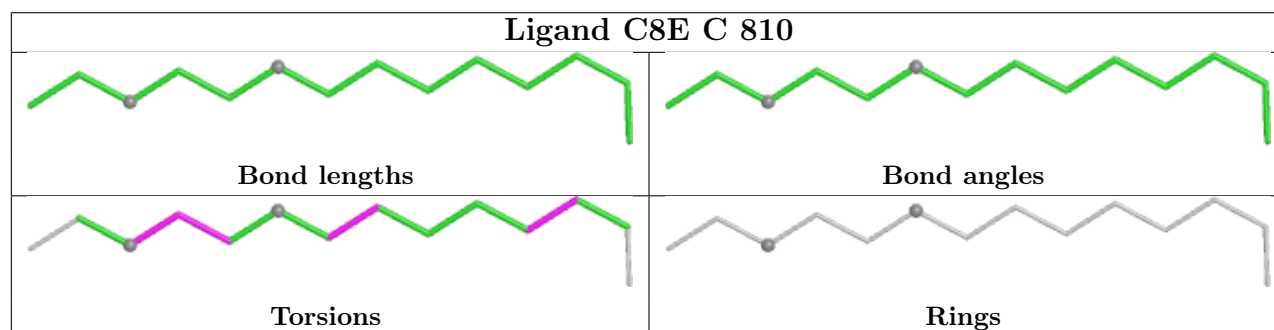
Mol	Chain	Res	Type	Atoms
3	B	807	C8E	C14-C13-O12-C11
3	C	810	C8E	C10-C11-O12-C13
3	B	808	C8E	C2-C3-C4-C5
3	B	804	C8E	C6-C7-C8-O9
2	C	802	EDO	O1-C1-C2-O2
2	C	805	EDO	O1-C1-C2-O2
3	B	808	C8E	C1-C2-C3-C4
3	C	806	C8E	C7-C8-O9-C10
3	B	806	C8E	C2-C3-C4-C5

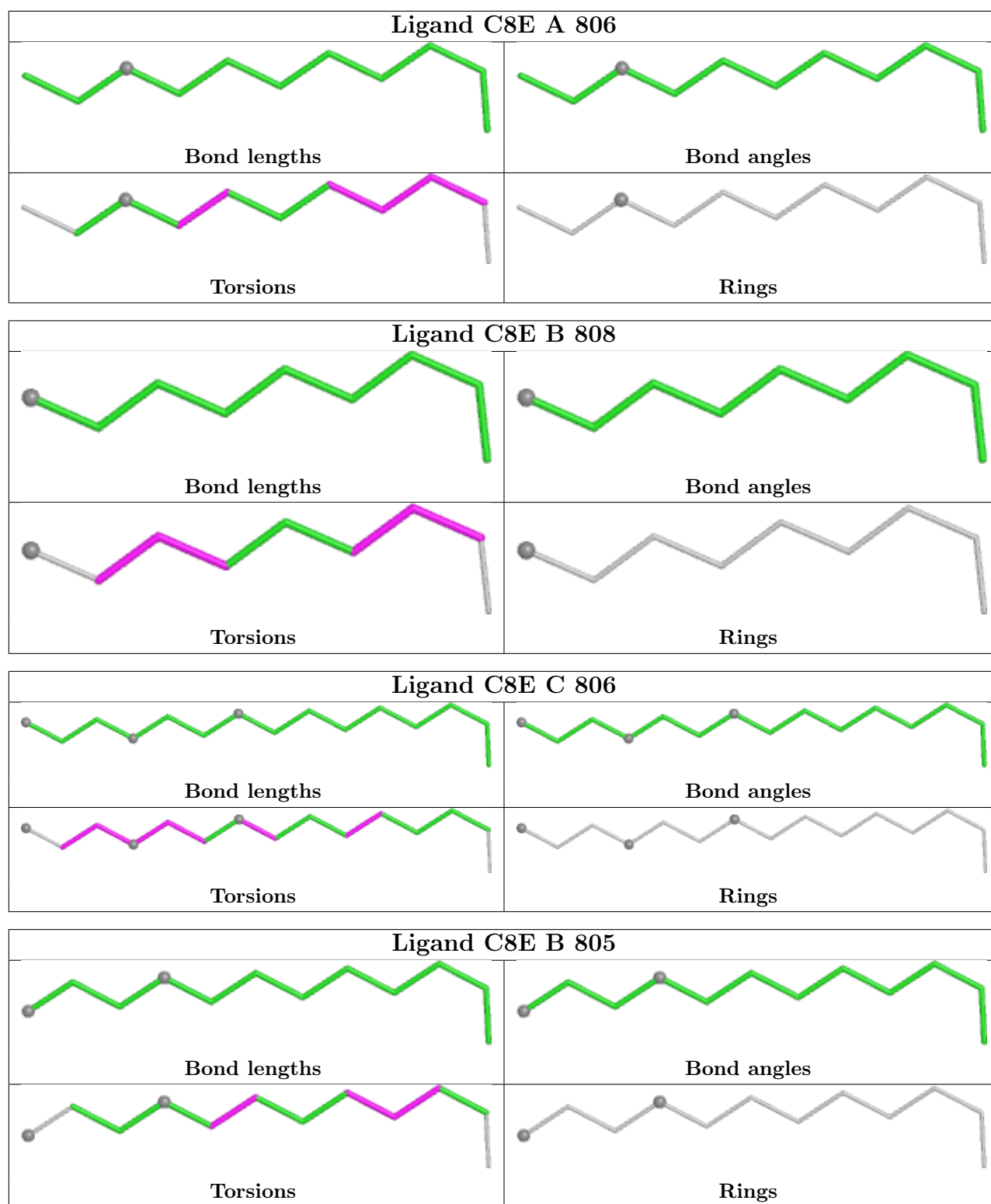
There are no ring outliers.

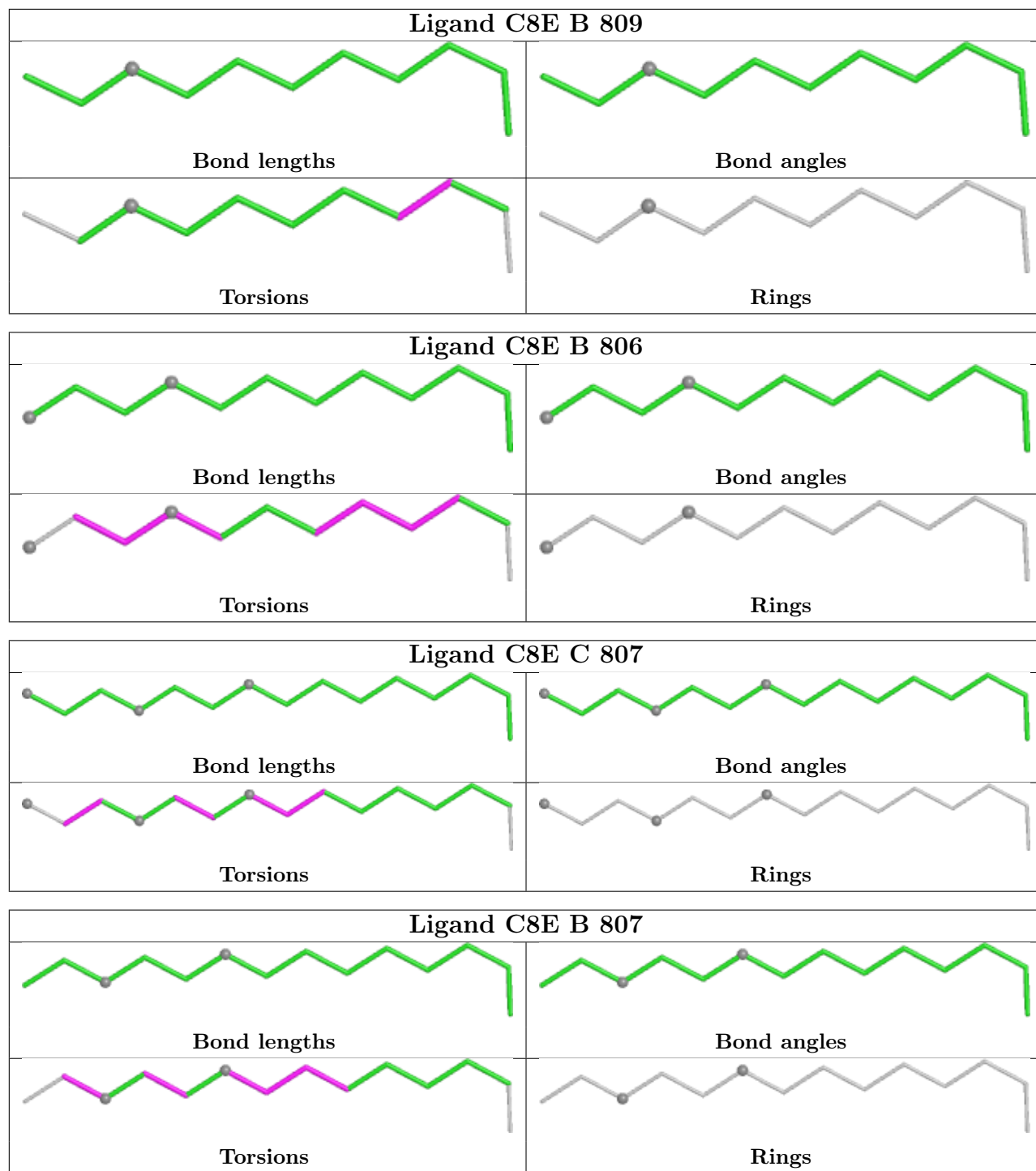
4 monomers are involved in 6 short contacts:

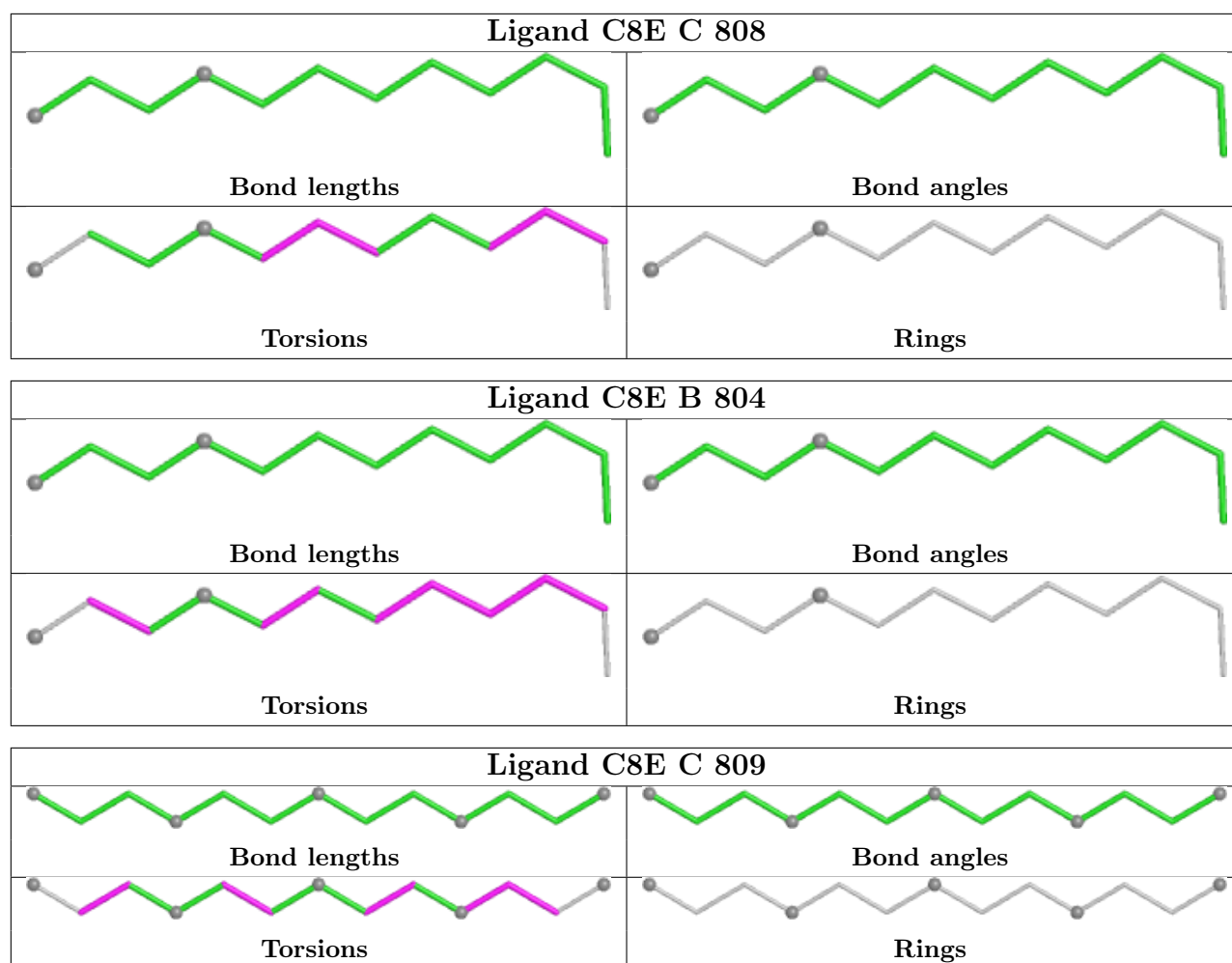
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	806	C8E	1	0
3	B	809	C8E	1	0
2	A	804	EDO	1	0
3	C	809	C8E	3	0

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

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	662/706 (93%)	-0.16	15 (2%) 61 62	27, 43, 69, 110	0
1	B	661/706 (93%)	-0.22	6 (0%) 81 83	28, 42, 63, 92	0
1	C	661/706 (93%)	-0.24	12 (1%) 67 68	23, 40, 63, 86	1 (0%)
All	All	1984/2118 (93%)	-0.21	33 (1%) 69 69	23, 41, 66, 110	1 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	33	ASP	5.2
1	C	612	TRP	5.1
1	C	493	ALA	4.0
1	A	452	THR	3.6
1	A	32	ASP	3.6
1	C	33	ASP	3.6
1	B	450	VAL	3.5
1	A	379	ARG	3.4
1	C	494	THR	3.2
1	B	379	ARG	3.2
1	A	33	ASP	3.2
1	C	420	PHE	3.1
1	A	542	LEU	3.1
1	A	428	PHE	3.0
1	B	612	TRP	3.0
1	C	617	ALA	2.7
1	A	618	GLN	2.5
1	A	539	PRO	2.5
1	C	580	TYR	2.5
1	C	422[A]	LEU	2.5
1	C	368	TYR	2.4
1	A	543	VAL	2.4
1	A	541	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	52	LYS	2.4
1	B	368	TYR	2.4
1	A	540	SER	2.3
1	C	569	ILE	2.3
1	C	357	SER	2.2
1	A	546	LEU	2.1
1	A	368	TYR	2.1
1	A	76	ASP	2.1
1	A	580	TYR	2.0
1	B	420	PHE	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 oligosaccharides 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
3	C8E	B	805	12/21	0.84	0.26	49,54,71,73	0
2	EDO	C	803	4/4	0.85	0.25	56,67,67,68	0
3	C8E	B	807	14/21	0.85	0.27	65,72,84,85	0
3	C8E	B	808	9/21	0.86	0.22	46,54,62,64	0
3	C8E	C	810	14/21	0.87	0.25	56,62,82,89	0
3	C8E	B	809	11/21	0.88	0.21	54,67,69,69	0
3	C8E	C	807	15/21	0.88	0.20	45,50,86,86	0
3	C8E	C	808	12/21	0.88	0.20	54,56,64,65	0
3	C8E	A	806	11/21	0.88	0.22	54,62,67,69	0
3	C8E	B	804	12/21	0.90	0.17	43,48,68,72	0
3	C8E	C	809	13/21	0.91	0.16	48,59,74,76	0
2	EDO	A	801	4/4	0.92	0.23	59,64,67,71	0
2	EDO	A	804	4/4	0.92	0.24	53,54,67,67	0

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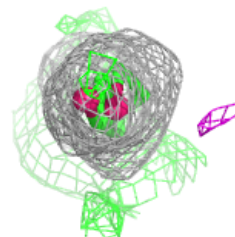
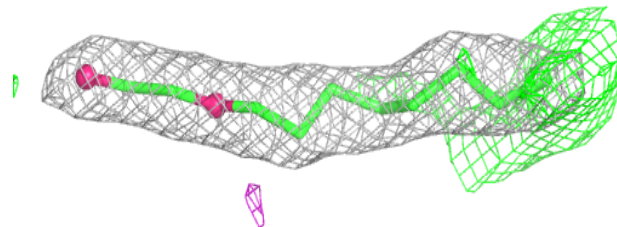
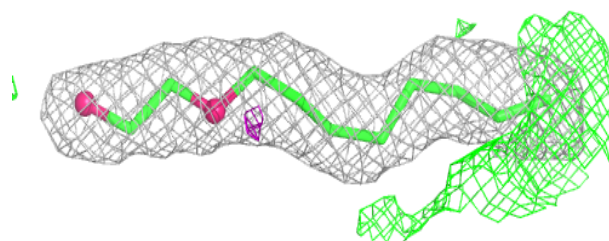
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	C8E	B	806	12/21	0.92	0.17	56,60,72,73	0
3	C8E	C	806	15/21	0.92	0.16	45,56,87,93	0
2	EDO	A	802	4/4	0.93	0.14	41,49,50,52	0
2	EDO	C	804	4/4	0.93	0.14	50,50,56,62	0
2	EDO	B	803	4/4	0.94	0.15	56,56,60,65	0
2	EDO	C	802	4/4	0.94	0.12	41,41,43,52	0
2	EDO	A	803	4/4	0.94	0.16	51,56,59,61	0
2	EDO	B	802	4/4	0.94	0.13	43,50,52,60	0
2	EDO	A	805	4/4	0.96	0.12	45,45,46,54	0
2	EDO	C	805	4/4	0.97	0.11	54,54,55,57	0
2	EDO	B	801	4/4	0.98	0.08	47,49,51,54	0
2	EDO	C	801	4/4	0.98	0.08	41,52,59,62	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.

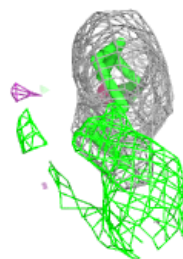
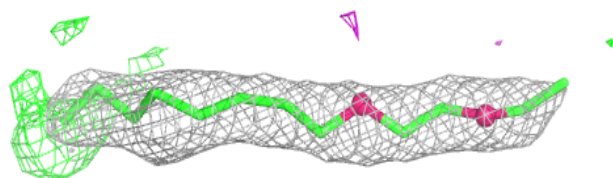
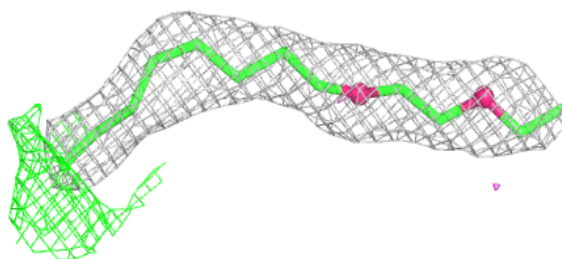
Electron density around C8E B 805:

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

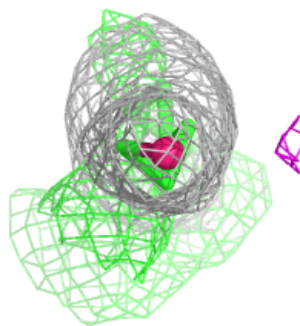
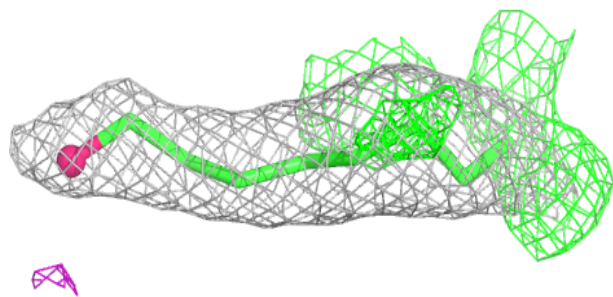
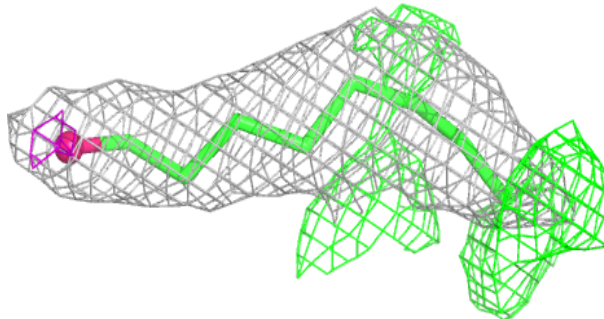


Electron density around C8E B 807:

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

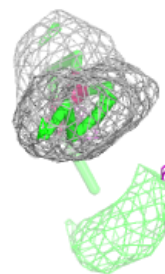
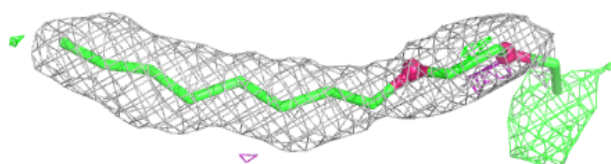
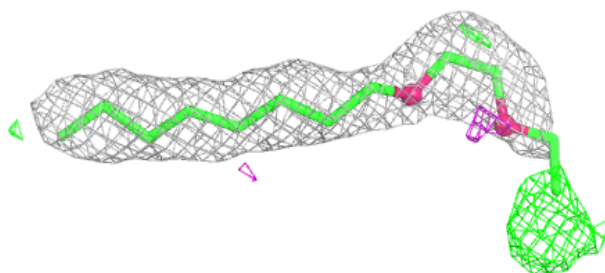
**Electron density around C8E B 808:**

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

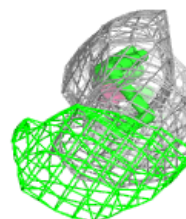
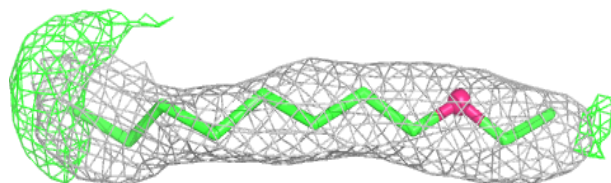
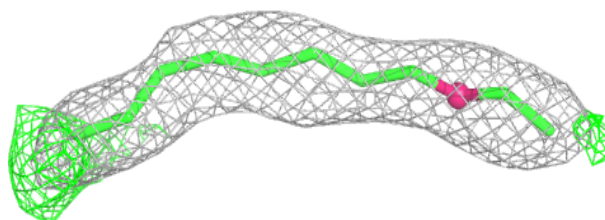


Electron density around C8E C 810:

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

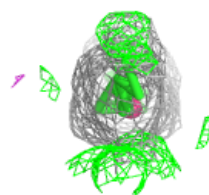
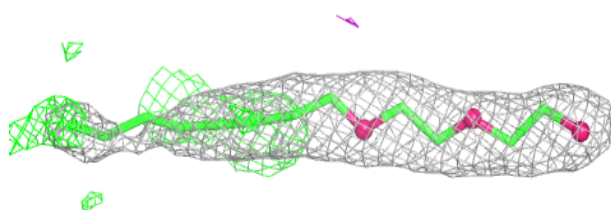
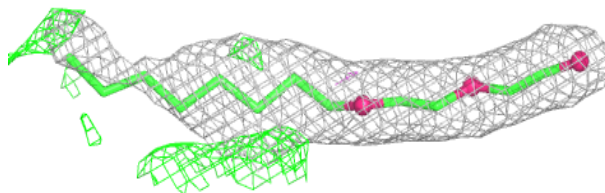
**Electron density around C8E B 809:**

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

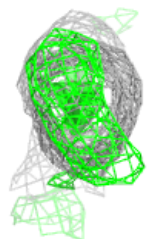
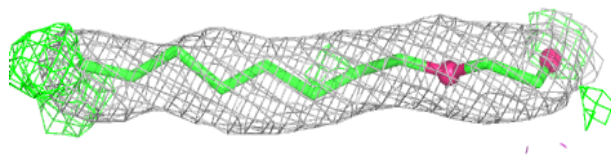
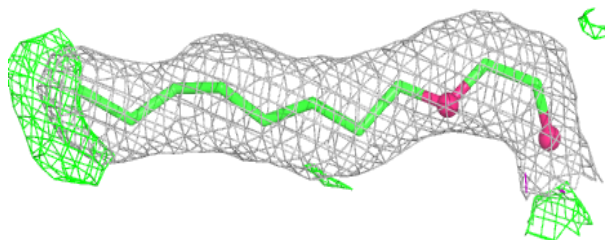


Electron density around C8E C 807:

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

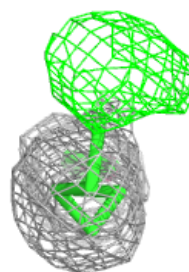
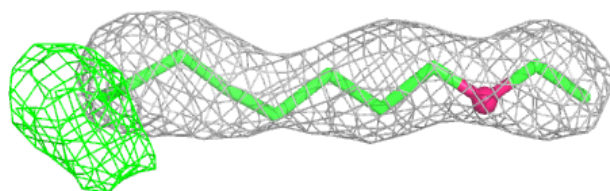
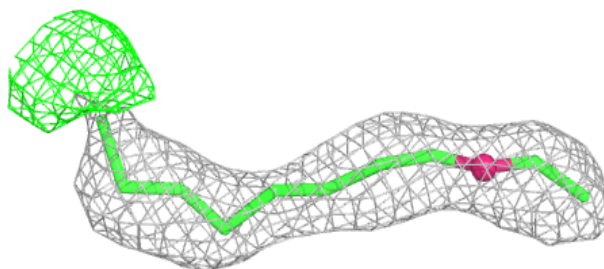
**Electron density around C8E C 808:**

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

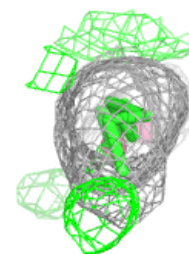
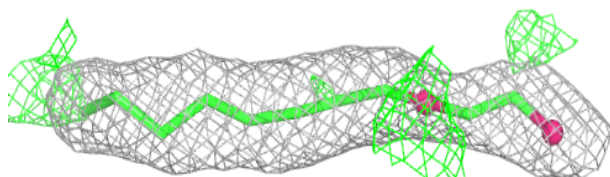
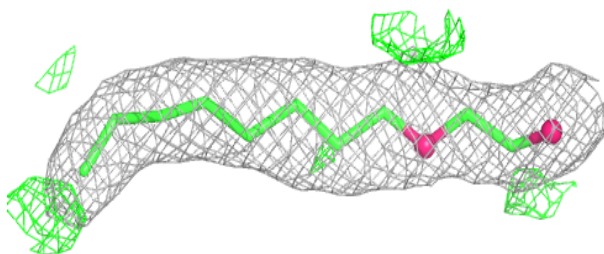


Electron density around C8E A 806:

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

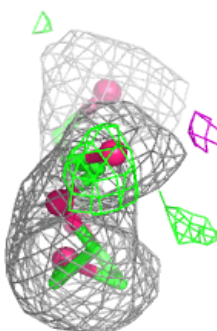
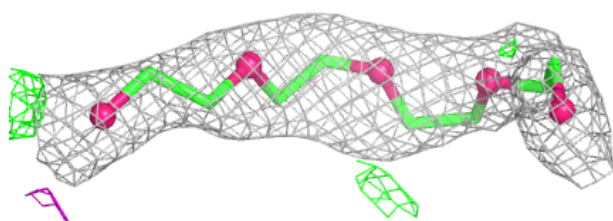
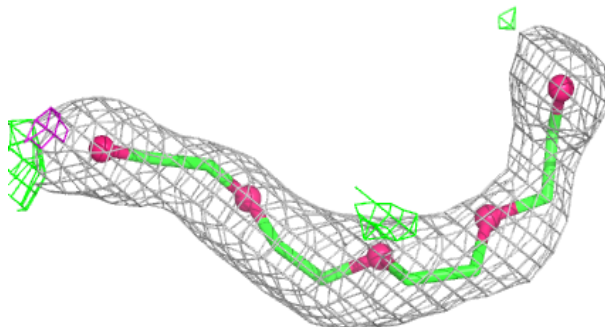
**Electron density around C8E B 804:**

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

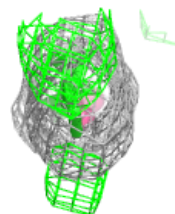
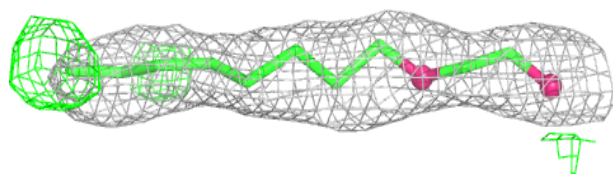
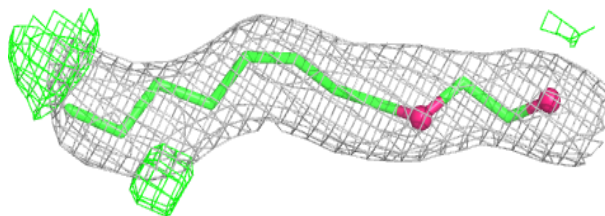


Electron density around C8E C 809:

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

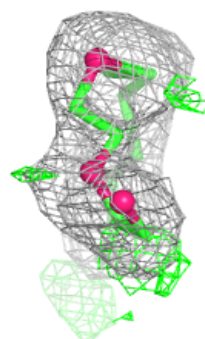
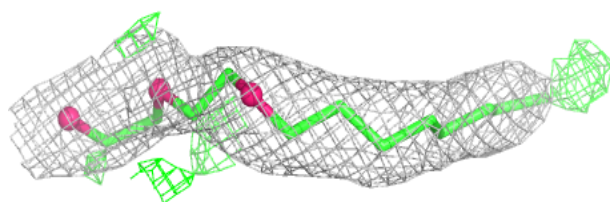
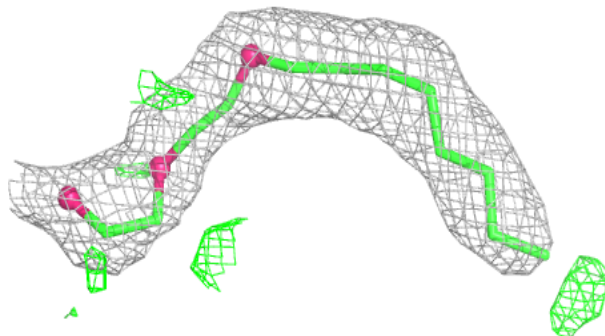
**Electron density around C8E B 806:**

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



Electron density around C8E C 806:

$2mF_o-DF_c$ (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.