



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 08:55 PM BST

PDB ID : 5MDO
Title : Crystal structure of in vitro folded Chitoporin VhChip from *Vibrio harveyi* (crystal form I)
Authors : Zahn, M.; van den Berg, B.
Deposited on : 2016-11-13
Resolution : 1.95 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
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

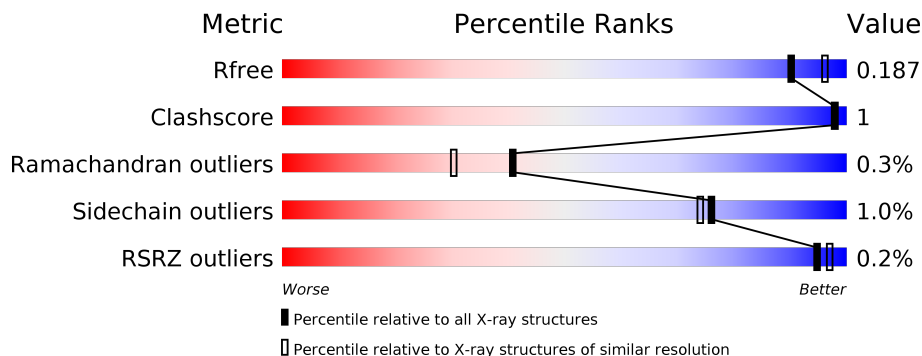
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	352	
1	B	352	
1	C	352	
1	D	352	
1	E	352	
1	F	352	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 18093 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 Chitoporin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	341	2677	1689	439	540	9	0	1	0
1	B	341	2677	1689	439	540	9	0	1	0
1	C	341	2665	1680	438	538	9	0	0	0
1	D	341	2665	1680	438	538	9	0	0	0
1	E	341	2677	1689	439	540	9	0	1	0
1	F	341	2677	1689	439	540	9	0	1	0

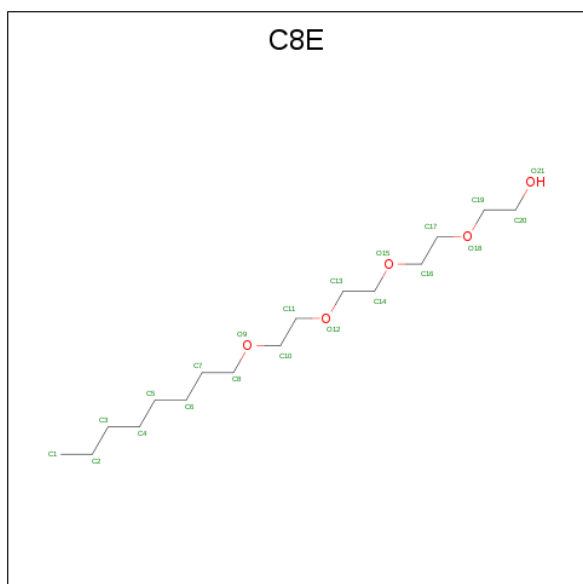
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	initiating methionine	UNP L0RVU0
A	0	GLY	-	expression tag	UNP L0RVU0
B	-1	MSE	-	initiating methionine	UNP L0RVU0
B	0	GLY	-	expression tag	UNP L0RVU0
C	-1	MSE	-	initiating methionine	UNP L0RVU0
C	0	GLY	-	expression tag	UNP L0RVU0
D	-1	MSE	-	initiating methionine	UNP L0RVU0
D	0	GLY	-	expression tag	UNP L0RVU0
E	-1	MSE	-	initiating methionine	UNP L0RVU0
E	0	GLY	-	expression tag	UNP L0RVU0
F	-1	MSE	-	initiating methionine	UNP L0RVU0
F	0	GLY	-	expression tag	UNP L0RVU0

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	3	Total Na 3 3	0	0
2	E	3	Total Na 3 3	0	0
2	B	3	Total Na 3 3	0	0
2	C	3	Total Na 3 3	0	0
2	A	3	Total Na 3 3	0	0
2	F	3	Total Na 3 3	0	0

- Molecule 3 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C₁₆H₃₄O₅).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 12 8 4	0	0
3	A	1	Total C O 9 6 3	0	0
3	A	1	Total C O 10 9 1	0	0
3	A	1	Total C O 14 9 5	0	0
3	A	1	Total C O 12 10 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 9 1	0	0
3	A	1	Total C O 21 16 5	0	0
3	B	1	Total C O 21 16 5	0	0
3	B	1	Total C O 21 16 5	0	0
3	C	1	Total C O 21 16 5	0	0
3	D	1	Total C O 14 12 2	0	0
3	D	1	Total C O 13 11 2	0	0
3	D	1	Total C O 11 10 1	0	0
3	E	1	Total C 8 8	0	0
3	E	1	Total C O 12 10 2	0	0
3	E	1	Total C O 15 12 3	0	0
3	F	1	Total C O 17 14 3	0	0

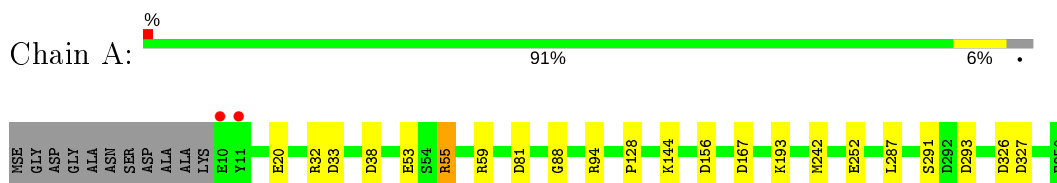
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	326	Total O 326 326	0	0
4	B	281	Total O 281 281	0	0
4	C	293	Total O 293 293	0	0
4	D	290	Total O 290 290	0	0
4	E	293	Total O 293 293	0	0
4	F	313	Total O 313 313	0	0

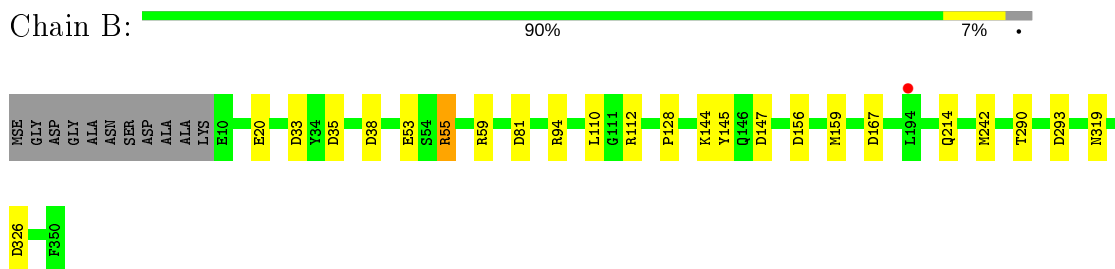
3 Residue-property plots [i](#)

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.

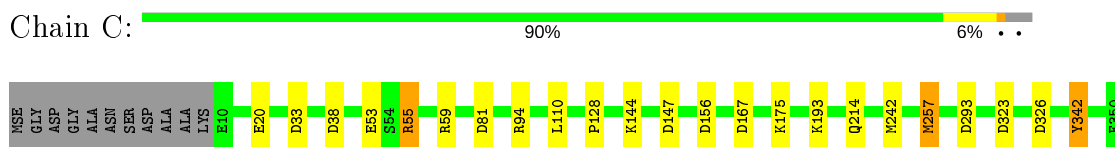
- Molecule 1: Chitoporin



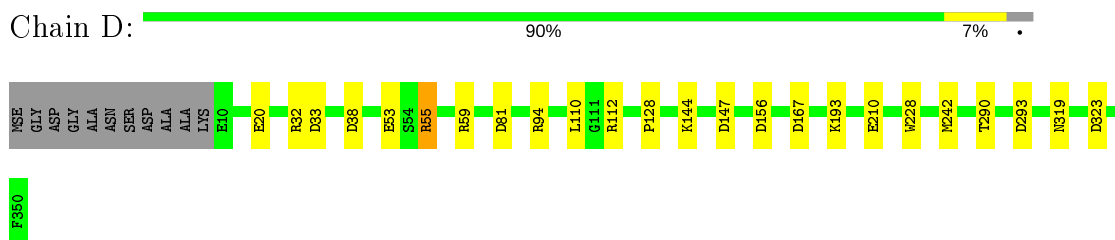
- Molecule 1: Chitoporin



- Molecule 1: Chitoporin



- Molecule 1: Chitoporin



- Molecule 1: Chitoporin





- Molecule 1: Chitoporin

Chain F: 91% 5% . . .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	146.88Å 123.38Å 147.03Å 90.00° 117.89° 90.00°	Depositor
Resolution (Å)	129.94 – 1.95 64.97 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (129.94-1.95) 99.9 (64.97-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.167 , 0.187 0.168 , 0.187	Depositor DCC
R_{free} test set	3124 reflections (0.93%)	wwPDB-VP
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.717	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for -h-l,k,h 0.008 for l,k,-h-l 0.013 for h,-k,-h-l 0.013 for -h-l,-k,l 0.120 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18093	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical 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: NA, C8E

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	1.12	3/2738 (0.1%)	1.04	13/3695 (0.4%)
1	B	1.10	3/2738 (0.1%)	1.01	15/3695 (0.4%)
1	C	1.07	3/2725 (0.1%)	1.02	16/3677 (0.4%)
1	D	1.13	5/2725 (0.2%)	1.03	15/3677 (0.4%)
1	E	1.07	2/2738 (0.1%)	1.01	15/3695 (0.4%)
1	F	1.13	2/2738 (0.1%)	1.02	17/3695 (0.5%)
All	All	1.10	18/16402 (0.1%)	1.02	91/22134 (0.4%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	53	GLU	CD-OE1	-7.88	1.17	1.25
1	B	53	GLU	CD-OE1	-7.79	1.17	1.25
1	F	53	GLU	CD-OE1	-7.48	1.17	1.25
1	A	53	GLU	CD-OE1	-6.93	1.18	1.25
1	B	145	TYR	CE1-CZ	6.46	1.47	1.38
1	D	210	GLU	CD-OE2	-5.87	1.19	1.25
1	B	20	GLU	CB-CG	-5.81	1.41	1.52
1	D	228	TRP	CG-CD1	5.76	1.44	1.36
1	A	252	GLU	CG-CD	5.74	1.60	1.51
1	E	53	GLU	CD-OE1	-5.73	1.19	1.25
1	D	20	GLU	CB-CG	-5.63	1.41	1.52
1	C	53	GLU	CD-OE1	-5.48	1.19	1.25
1	D	53	GLU	CG-CD	5.46	1.60	1.51
1	E	20	GLU	CB-CG	-5.31	1.42	1.52
1	F	20	GLU	CB-CG	-5.21	1.42	1.52
1	C	342	TYR	CG-CD2	5.20	1.46	1.39
1	C	20	GLU	CB-CG	-5.14	1.42	1.52
1	A	20	GLU	CB-CG	-5.02	1.42	1.52

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	257	MSE	CG-SE-CE	-10.76	75.23	98.90
1	C	293	ASP	CB-CG-OD1	8.75	126.18	118.30
1	E	81	ASP	CB-CG-OD1	8.21	125.68	118.30
1	D	293	ASP	CB-CG-OD1	8.04	125.54	118.30
1	A	156	ASP	CB-CG-OD1	7.76	125.28	118.30
1	B	55	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	A	81	ASP	CB-CG-OD1	7.48	125.03	118.30
1	F	293	ASP	CB-CG-OD2	-7.37	111.66	118.30
1	A	55	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	B	55	ARG	NE-CZ-NH2	-7.23	116.68	120.30
1	E	38	ASP	CB-CG-OD1	7.17	124.75	118.30
1	D	81	ASP	CB-CG-OD1	7.15	124.74	118.30
1	D	59	ARG	NE-CZ-NH2	-7.09	116.76	120.30
1	C	81	ASP	CB-CG-OD1	7.03	124.63	118.30
1	E	293	ASP	CB-CG-OD1	7.03	124.63	118.30
1	C	59	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	E	55	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	E	94	ARG	NE-CZ-NH2	-6.79	116.91	120.30
1	D	55	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	F	55	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	E	156	ASP	CB-CG-OD1	6.57	124.22	118.30
1	F	38	ASP	CB-CG-OD1	6.52	124.17	118.30
1	A	33	ASP	CB-CG-OD1	6.50	124.15	118.30
1	B	38	ASP	CB-CG-OD1	6.45	124.11	118.30
1	C	55	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	B	293	ASP	CB-CG-OD2	-6.43	112.51	118.30
1	D	94	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	D	32	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	D	33	ASP	CB-CG-OD1	6.39	124.05	118.30
1	A	38	ASP	CB-CG-OD1	6.38	124.05	118.30
1	F	55	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	F	81	ASP	CB-CG-OD1	6.28	123.95	118.30
1	B	33	ASP	CB-CG-OD1	6.21	123.89	118.30
1	F	33	ASP	CB-CG-OD1	6.18	123.87	118.30
1	B	112	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	E	33	ASP	CB-CG-OD1	6.08	123.78	118.30
1	B	81	ASP	CB-CG-OD1	6.07	123.76	118.30
1	D	38	ASP	CB-CG-OD1	6.07	123.76	118.30
1	B	59	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	E	55	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	C	33	ASP	CB-CG-OD1	5.98	123.68	118.30
1	C	38	ASP	CB-CG-OD1	5.93	123.63	118.30
1	A	55	ARG	NE-CZ-NH2	-5.87	117.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	ASP	CB-CG-OD1	5.87	123.58	118.30
1	C	94	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	F	32	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	B	156	ASP	CB-CG-OD1	5.82	123.54	118.30
1	D	293	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	F	59	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	326	ASP	CB-CG-OD1	5.72	123.45	118.30
1	B	147	ASP	CB-CG-OD1	5.69	123.42	118.30
1	F	156	ASP	CB-CG-OD1	5.63	123.37	118.30
1	B	94	ARG	NE-CZ-NH2	-5.63	117.49	120.30
1	E	94	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	E	20	GLU	CB-CA-C	-5.57	99.27	110.40
1	D	112	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	C	147	ASP	CB-CG-OD1	5.52	123.27	118.30
1	B	293	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	59	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	F	147	ASP	CB-CG-OD1	5.42	123.18	118.30
1	C	55	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	E	68	GLU	OE1-CD-OE2	-5.42	116.80	123.30
1	A	20	GLU	CB-CA-C	-5.40	99.61	110.40
1	C	323	ASP	CB-CG-OD1	5.35	123.11	118.30
1	F	144	LYS	CD-CE-NZ	-5.34	99.42	111.70
1	B	326	ASP	CB-CG-OD1	5.33	123.10	118.30
1	D	147	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	287	LEU	CB-CG-CD1	5.30	120.02	111.00
1	F	326	ASP	CB-CG-OD1	5.30	123.07	118.30
1	D	156	ASP	CB-CG-OD1	5.28	123.05	118.30
1	D	20	GLU	CB-CA-C	-5.28	99.85	110.40
1	E	112	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	E	230	GLU	CG-CD-OE1	-5.26	107.78	118.30
1	C	293	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	E	122	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	F	287	LEU	CB-CG-CD1	5.20	119.84	111.00
1	B	20	GLU	CB-CA-C	-5.19	100.02	110.40
1	D	193	LYS	CB-CA-C	-5.17	100.05	110.40
1	F	94	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	B	35	ASP	CB-CG-OD1	5.17	122.95	118.30
1	C	20	GLU	CB-CA-C	-5.14	100.12	110.40
1	F	81	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	E	326	ASP	CB-CG-OD1	5.11	122.90	118.30
1	F	94	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	D	323	ASP	CB-CG-OD1	5.09	122.88	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	C	156	ASP	CB-CG-OD1	5.06	122.86	118.30
1	C	326	ASP	CB-CG-OD1	5.06	122.85	118.30
1	C	175	LYS	CD-CE-NZ	-5.04	100.11	111.70
1	A	32	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	F	314	ARG	NE-CZ-NH1	5.00	122.80	120.30

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	2677	0	2428	4	0
1	B	2677	0	2428	5	0
1	C	2665	0	2420	4	0
1	D	2665	0	2420	3	0
1	E	2677	0	2428	3	0
1	F	2677	0	2428	2	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
3	A	88	0	132	2	0
3	B	42	0	68	0	0
3	C	21	0	34	0	0
3	D	38	0	63	0	0
3	E	35	0	61	0	0
3	F	17	0	27	0	0
4	A	326	0	0	3	0
4	B	281	0	0	1	0
4	C	293	0	0	1	0
4	D	290	0	0	0	0
4	E	293	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	313	0	0	0	0
All	All	18093	0	14937	22	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 1.

All (22) 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:327:ASP:OD2	4:A:501:HOH:O	2.10	0.69
1:A:291:SER:OG	3:A:407:C8E:H171	2.02	0.60
1:B:214:GLN:NE2	4:B:504:HOH:O	2.33	0.60
1:E:214:GLN:NE2	4:E:505:HOH:O	2.40	0.50
1:A:144:LYS:HD3	1:A:242:MSE:SE	2.62	0.49
1:E:144:LYS:HD3	1:E:242:MSE:SE	2.63	0.48
3:A:407:C8E:H141	4:A:781:HOH:O	2.14	0.47
1:B:110:LEU:N	1:B:110:LEU:HD12	2.30	0.47
1:C:214:GLN:NE2	4:C:508:HOH:O	2.45	0.47
1:C:110:LEU:HD12	1:C:110:LEU:N	2.30	0.46
1:F:110:LEU:N	1:F:110:LEU:HD12	2.31	0.46
1:C:144:LYS:HD3	1:C:242:MSE:SE	2.66	0.46
1:B:144:LYS:HD3	1:B:242:MSE:SE	2.66	0.45
1:A:88:GLY:O	4:A:502:HOH:O	2.21	0.45
1:D:110:LEU:HD12	1:D:110:LEU:N	2.32	0.45
1:D:144:LYS:HD3	1:D:242:MSE:SE	2.67	0.44
1:E:110:LEU:N	1:E:110:LEU:HD12	2.34	0.43
1:F:144:LYS:HD3	1:F:242:MSE:SE	2.69	0.43
1:C:342:TYR:CD2	1:C:342:TYR:N	2.87	0.42
1:D:290:THR:HA	1:D:319:ASN:HB2	2.02	0.41
1:B:290:THR:HA	1:B:319:ASN:HB2	2.03	0.41
1:B:159:MSE:HB2	1:B:159:MSE:HE2	2.03	0.40

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	340/352 (97%)	334 (98%)	5 (2%)	1 (0%)	41	30
1	B	340/352 (97%)	333 (98%)	6 (2%)	1 (0%)	41	30
1	C	339/352 (96%)	332 (98%)	6 (2%)	1 (0%)	41	30
1	D	339/352 (96%)	332 (98%)	6 (2%)	1 (0%)	41	30
1	E	340/352 (97%)	332 (98%)	7 (2%)	1 (0%)	41	30
1	F	340/352 (97%)	332 (98%)	7 (2%)	1 (0%)	41	30
All	All	2038/2112 (96%)	1995 (98%)	37 (2%)	6 (0%)	41	30

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	PRO
1	D	128	PRO
1	C	128	PRO
1	B	128	PRO
1	E	128	PRO
1	F	128	PRO

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	263/258 (102%)	260 (99%)	3 (1%)	73	71
1	B	263/258 (102%)	261 (99%)	2 (1%)	81	80
1	C	262/258 (102%)	258 (98%)	4 (2%)	65	60
1	D	262/258 (102%)	260 (99%)	2 (1%)	81	80
1	E	263/258 (102%)	260 (99%)	3 (1%)	73	71
1	F	263/258 (102%)	261 (99%)	2 (1%)	81	80
All	All	1576/1548 (102%)	1560 (99%)	16 (1%)	76	74

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ARG
1	A	167	ASP
1	A	193	LYS
1	B	55	ARG
1	B	167	ASP
1	C	55	ARG
1	C	167	ASP
1	C	193	LYS
1	C	257	MSE
1	D	55	ARG
1	D	167	ASP
1	E	55	ARG
1	E	167	ASP
1	E	193	LYS
1	F	55	ARG
1	F	167	ASP

Some 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 35 ligands modelled in this entry, 18 are monoatomic - leaving 17 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
3	C8E	E	405	-	11,11,20	0.32	0	10,10,19	0.56	0
3	C8E	A	405	-	8,8,20	0.46	0	7,7,19	0.63	0
3	C8E	B	405	-	20,20,20	0.47	0	19,19,19	0.66	0
3	C8E	D	406	-	10,10,20	0.46	0	9,9,19	0.63	0
3	C8E	A	404	-	11,11,20	0.57	0	10,10,19	0.72	0
3	C8E	A	409	-	9,9,20	0.43	0	8,8,19	0.41	0
3	C8E	D	405	-	12,12,20	0.55	0	11,11,19	0.89	0
3	C8E	C	404	-	20,20,20	0.66	0	19,19,19	0.60	0
3	C8E	A	410	-	20,20,20	0.61	0	19,19,19	0.82	0
3	C8E	A	407	-	13,13,20	0.56	0	12,12,19	0.81	0
3	C8E	E	404	-	7,7,20	0.53	0	6,6,19	1.16	1 (16%)
3	C8E	F	404	-	16,16,20	0.38	0	15,15,19	0.56	0
3	C8E	D	404	-	13,13,20	0.58	0	12,12,19	1.01	1 (8%)
3	C8E	E	406	-	14,14,20	0.29	0	13,13,19	0.86	0
3	C8E	B	404	-	20,20,20	0.36	0	19,19,19	0.65	0
3	C8E	A	408	-	11,11,20	0.46	0	10,10,19	0.42	0
3	C8E	A	406	-	9,9,20	0.61	0	8,8,19	0.86	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
3	C8E	E	405	-	-	2/9/9/18	-
3	C8E	A	405	-	-	2/6/6/18	-
3	C8E	B	405	-	-	8/18/18/18	-
3	C8E	D	406	-	-	3/8/8/18	-
3	C8E	A	404	-	-	3/9/9/18	-
3	C8E	A	409	-	-	4/7/7/18	-
3	C8E	D	405	-	-	3/10/10/18	-
3	C8E	C	404	-	-	6/18/18/18	-
3	C8E	A	410	-	-	9/18/18/18	-
3	C8E	A	407	-	-	5/11/11/18	-
3	C8E	E	404	-	-	3/5/5/18	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	C8E	F	404	-	-	2/14/14/18	-
3	C8E	D	404	-	-	1/11/11/18	-
3	C8E	E	406	-	-	4/12/12/18	-
3	C8E	B	404	-	-	5/18/18/18	-
3	C8E	A	408	-	-	5/9/9/18	-
3	C8E	A	406	-	-	0/7/7/18	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	404	C8E	C5-C4-C3	2.09	125.03	114.42
3	D	404	C8E	O9-C10-C11	2.08	119.75	110.39

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	410	C8E	O15-C16-C17-O18
3	B	405	C8E	O9-C10-C11-O12
3	C	404	C8E	O9-C10-C11-O12
3	B	404	C8E	O9-C10-C11-O12
3	B	404	C8E	O12-C13-C14-O15
3	A	410	C8E	O9-C10-C11-O12
3	A	410	C8E	O18-C19-C20-O21
3	B	404	C8E	C6-C7-C8-O9
3	A	407	C8E	O12-C13-C14-O15
3	B	404	C8E	O18-C19-C20-O21
3	A	408	C8E	O9-C10-C11-O12
3	A	405	C8E	O15-C16-C17-O18
3	C	404	C8E	C6-C7-C8-O9
3	B	405	C8E	C4-C5-C6-C7
3	A	410	C8E	O12-C13-C14-O15
3	B	405	C8E	O12-C13-C14-O15
3	A	409	C8E	C6-C7-C8-O9
3	E	405	C8E	C6-C7-C8-O9
3	D	405	C8E	O9-C10-C11-O12
3	F	404	C8E	C6-C7-C8-O9
3	B	404	C8E	O15-C16-C17-O18
3	A	408	C8E	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
3	A	405	C8E	O18-C19-C20-O21
3	A	410	C8E	C6-C7-C8-O9
3	E	406	C8E	O9-C10-C11-O12
3	F	404	C8E	O12-C13-C14-O15
3	E	404	C8E	C5-C6-C7-C8
3	A	408	C8E	C4-C5-C6-C7
3	A	409	C8E	C4-C5-C6-C7
3	D	405	C8E	C3-C4-C5-C6
3	B	405	C8E	O18-C19-C20-O21
3	A	407	C8E	C13-C14-O15-C16
3	C	404	C8E	C5-C6-C7-C8
3	A	410	C8E	C13-C14-O15-C16
3	B	405	C8E	C14-C13-O12-C11
3	A	408	C8E	C6-C7-C8-O9
3	E	406	C8E	C6-C7-C8-O9
3	E	404	C8E	C2-C3-C4-C5
3	A	409	C8E	C7-C8-O9-C10
3	E	406	C8E	C14-C13-O12-C11
3	E	405	C8E	C7-C8-O9-C10
3	E	406	C8E	C10-C11-O12-C13
3	D	406	C8E	C5-C6-C7-C8
3	A	410	C8E	C16-C17-O18-C19
3	D	406	C8E	C1-C2-C3-C4
3	B	405	C8E	C20-C19-O18-C17
3	B	405	C8E	C11-C10-O9-C8
3	A	404	C8E	C13-C14-O15-C16
3	A	408	C8E	C1-C2-C3-C4
3	C	404	C8E	C3-C4-C5-C6
3	D	405	C8E	C5-C6-C7-C8
3	A	407	C8E	C14-C13-O12-C11
3	D	406	C8E	C11-C10-O9-C8
3	B	405	C8E	C16-C17-O18-C19
3	A	404	C8E	O15-C16-C17-O18
3	A	410	C8E	C20-C19-O18-C17
3	E	404	C8E	C3-C4-C5-C6
3	C	404	C8E	C1-C2-C3-C4
3	A	409	C8E	C1-C2-C3-C4
3	C	404	C8E	C7-C8-O9-C10
3	A	410	C8E	C7-C8-O9-C10
3	A	407	C8E	O9-C10-C11-O12
3	D	404	C8E	O9-C10-C11-O12
3	A	404	C8E	O12-C13-C14-O15

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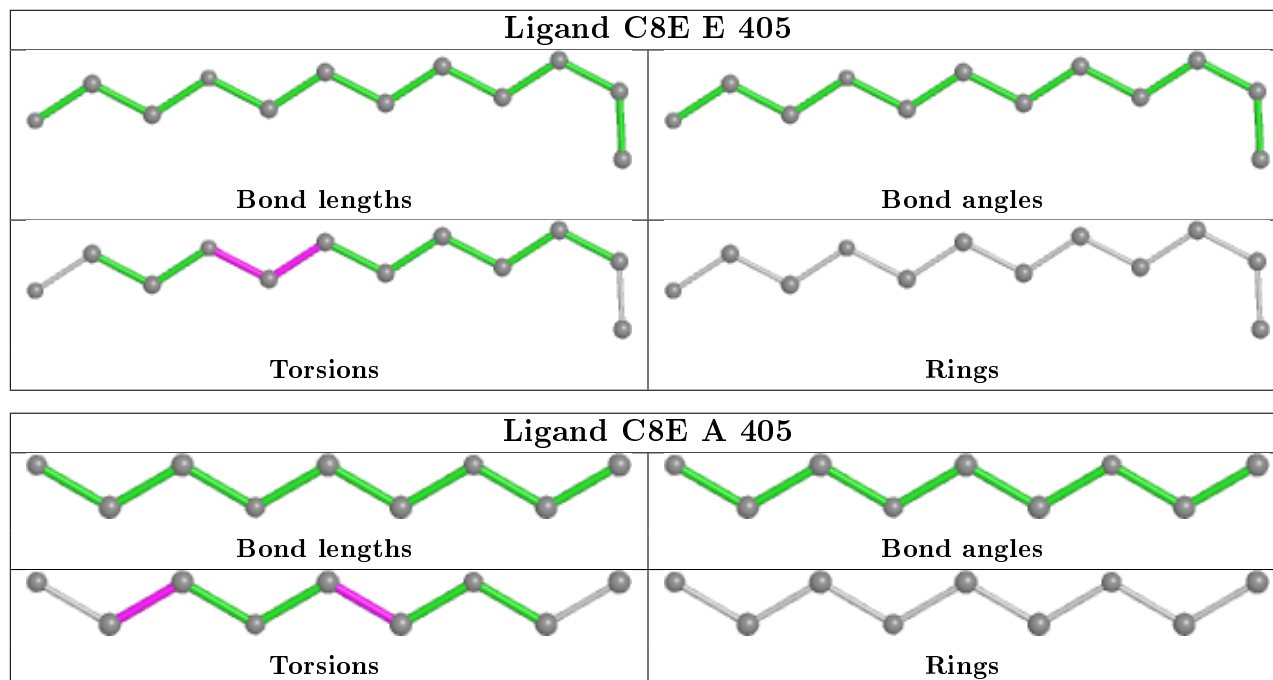
Mol	Chain	Res	Type	Atoms
3	A	407	C8E	O15-C16-C17-O18

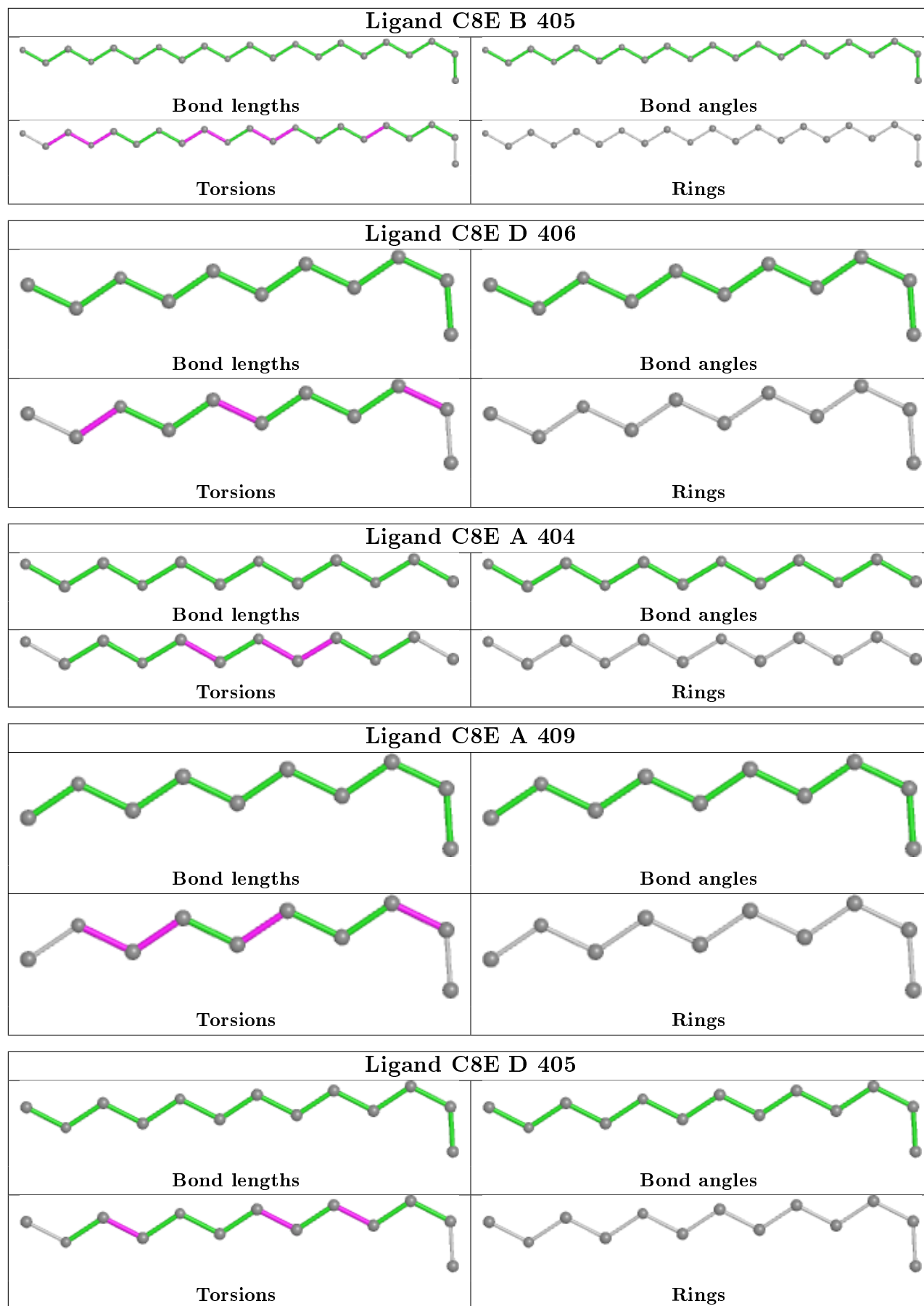
There are no ring outliers.

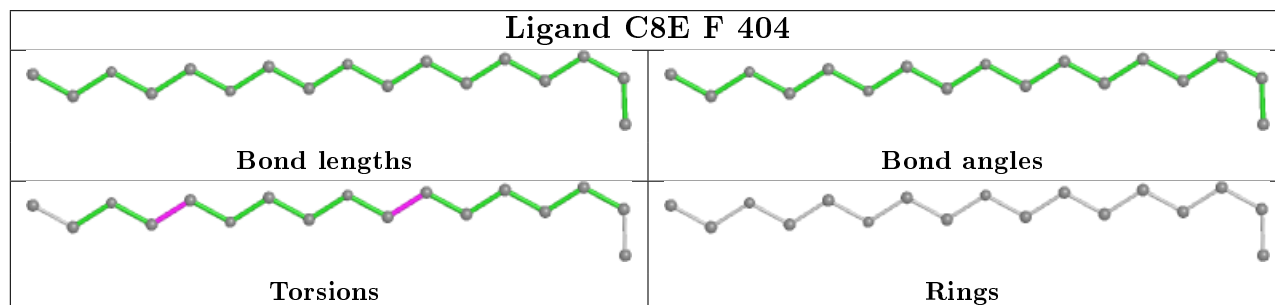
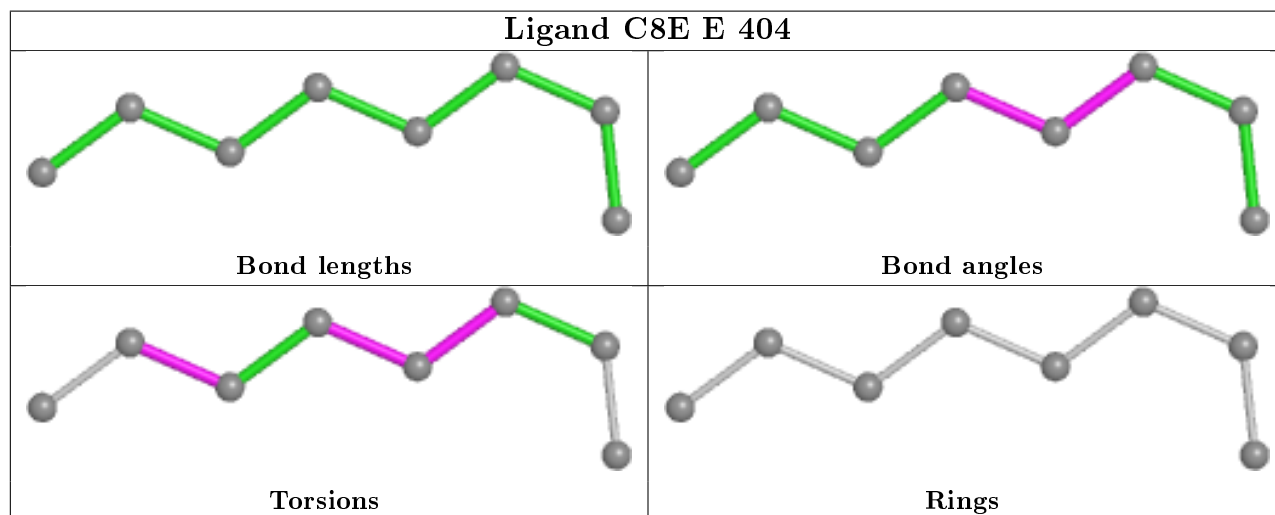
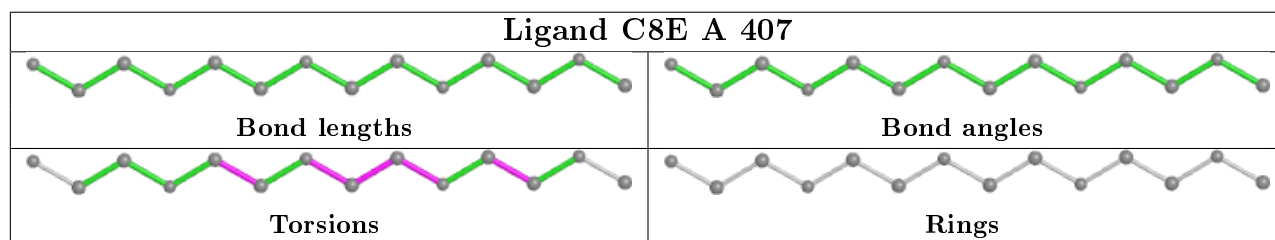
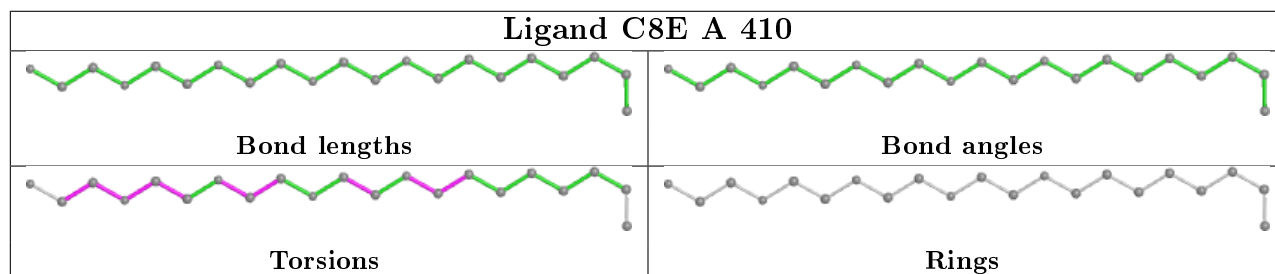
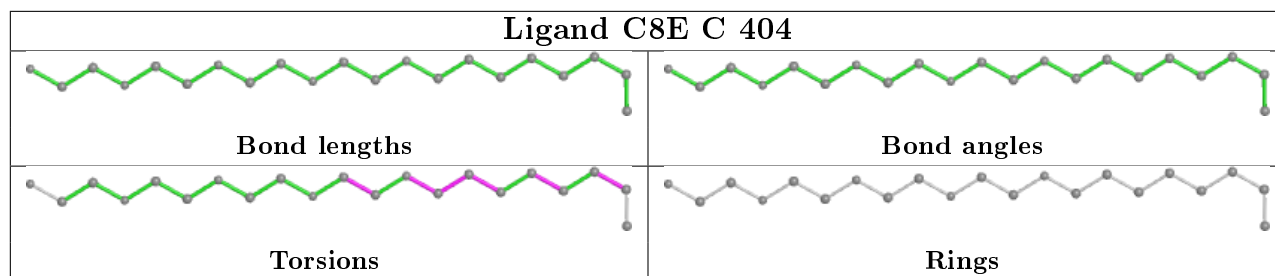
1 monomer is involved in 2 short contacts:

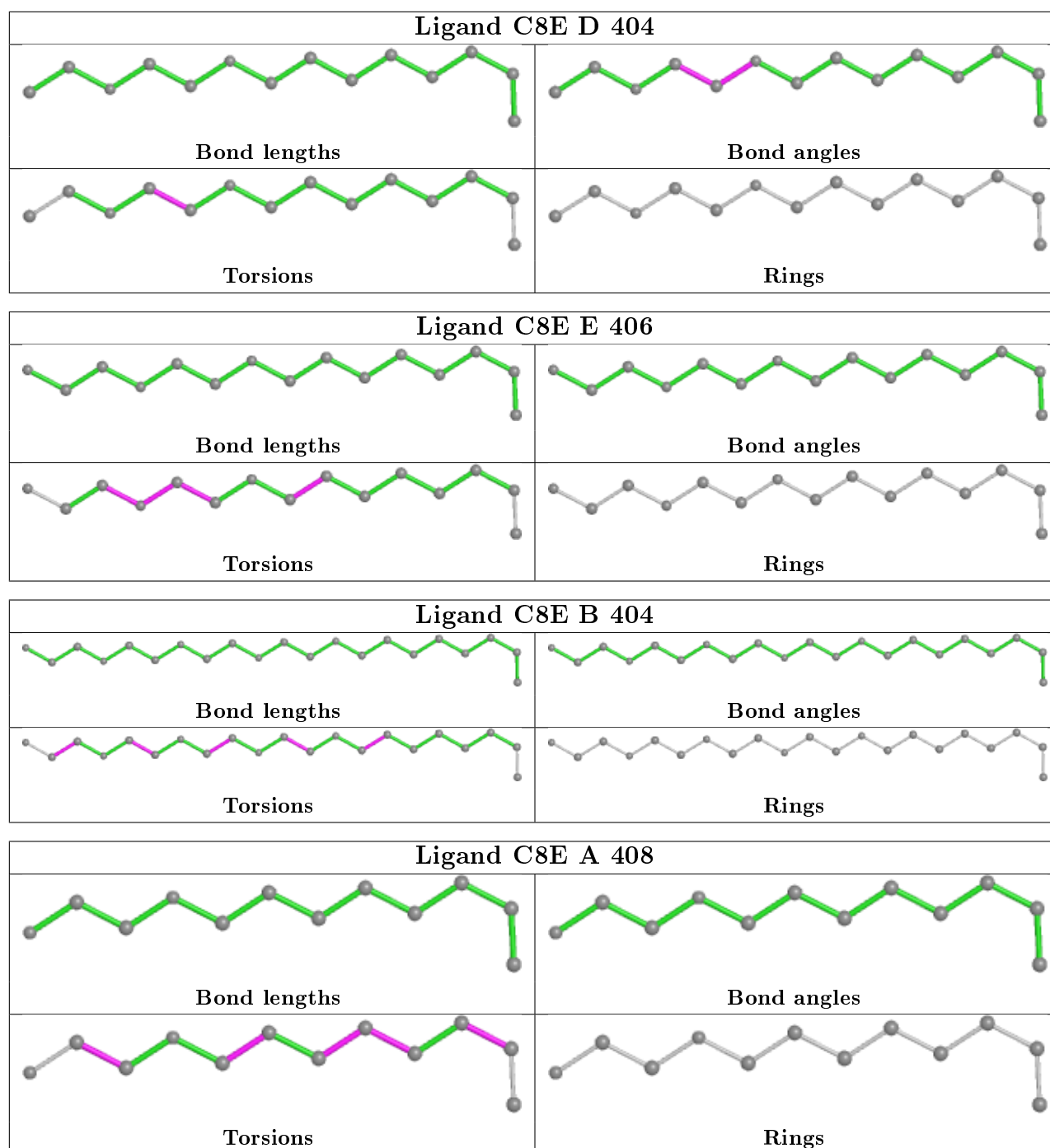
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	407	C8E	2	0

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](#)

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	332/352 (94%)	-0.39	2 (0%) 89 93	25, 33, 51, 97	0
1	B	332/352 (94%)	-0.49	1 (0%) 94 96	25, 35, 52, 91	0
1	C	332/352 (94%)	-0.49	0 100 100	25, 36, 52, 86	0
1	D	332/352 (94%)	-0.55	0 100 100	25, 34, 51, 87	0
1	E	332/352 (94%)	-0.49	1 (0%) 94 96	25, 35, 52, 97	0
1	F	332/352 (94%)	-0.41	0 100 100	24, 33, 50, 94	0
All	All	1992/2112 (94%)	-0.47	4 (0%) 95 97	24, 34, 52, 97	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	10	GLU	2.5
1	E	161	ALA	2.2
1	A	11	TYR	2.2
1	B	194	LEU	2.1

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,

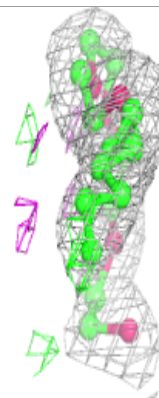
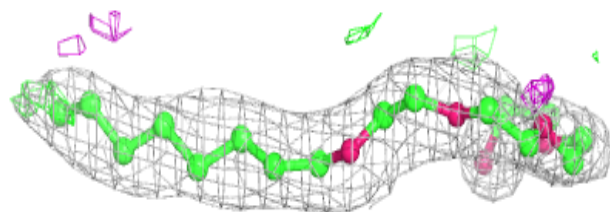
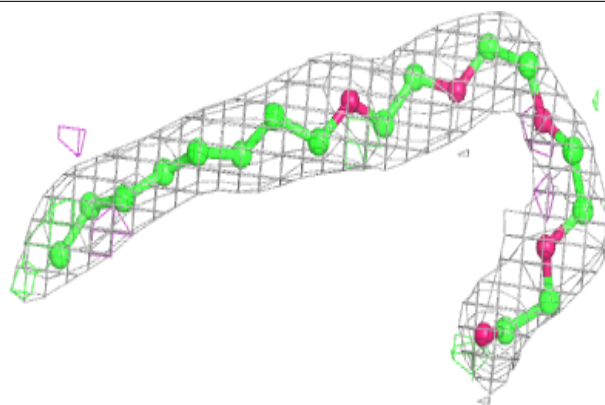
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	C8E	C	404	21/21	0.80	0.16	52,64,74,75	0
3	C8E	A	408	12/21	0.85	0.19	54,67,86,86	0
3	C8E	D	404	14/21	0.86	0.12	43,46,57,59	0
3	C8E	D	405	13/21	0.86	0.12	59,62,76,81	0
3	C8E	A	406	10/21	0.87	0.17	40,50,68,70	0
3	C8E	A	409	10/21	0.88	0.12	58,64,78,80	0
3	C8E	A	410	21/21	0.88	0.15	48,62,71,72	0
3	C8E	D	406	11/21	0.89	0.17	51,64,69,72	0
3	C8E	A	405	9/21	0.89	0.12	60,64,69,72	0
3	C8E	B	405	21/21	0.90	0.13	52,60,72,75	0
3	C8E	A	407	14/21	0.91	0.16	42,56,78,79	0
3	C8E	B	404	21/21	0.91	0.12	48,59,66,69	0
3	C8E	E	406	15/21	0.92	0.10	44,51,59,74	0
3	C8E	E	404	8/21	0.92	0.16	40,48,58,59	0
3	C8E	A	404	12/21	0.93	0.10	41,53,64,68	0
3	C8E	E	405	12/21	0.94	0.11	39,46,63,70	0
3	C8E	F	404	17/21	0.94	0.12	43,49,56,58	0
2	NA	F	402	1/1	0.95	0.07	33,33,33,33	0
2	NA	F	403	1/1	0.97	0.05	37,37,37,37	0
2	NA	D	403	1/1	0.97	0.06	35,35,35,35	0
2	NA	B	403	1/1	0.97	0.07	36,36,36,36	0
2	NA	C	401	1/1	0.98	0.05	33,33,33,33	0
2	NA	E	401	1/1	0.98	0.06	33,33,33,33	0
2	NA	F	401	1/1	0.98	0.05	30,30,30,30	0
2	NA	C	402	1/1	0.98	0.05	36,36,36,36	0
2	NA	E	403	1/1	0.98	0.05	37,37,37,37	0
2	NA	E	402	1/1	0.98	0.05	33,33,33,33	0
2	NA	A	401	1/1	0.98	0.09	30,30,30,30	0
2	NA	D	401	1/1	0.99	0.04	29,29,29,29	0
2	NA	A	403	1/1	0.99	0.05	34,34,34,34	0
2	NA	C	403	1/1	0.99	0.05	37,37,37,37	0
2	NA	D	402	1/1	0.99	0.05	34,34,34,34	0
2	NA	B	401	1/1	0.99	0.06	29,29,29,29	0
2	NA	B	402	1/1	0.99	0.11	35,35,35,35	0
2	NA	A	402	1/1	0.99	0.09	31,31,31,31	0

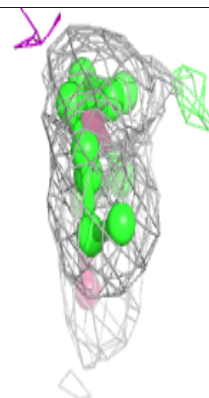
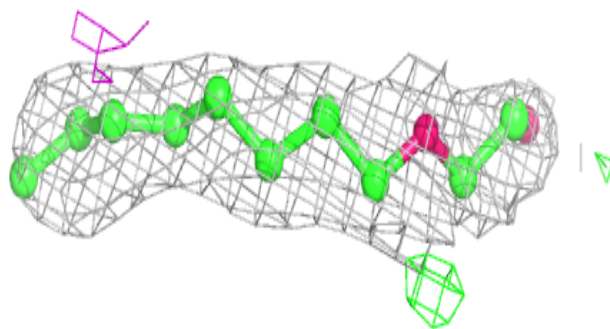
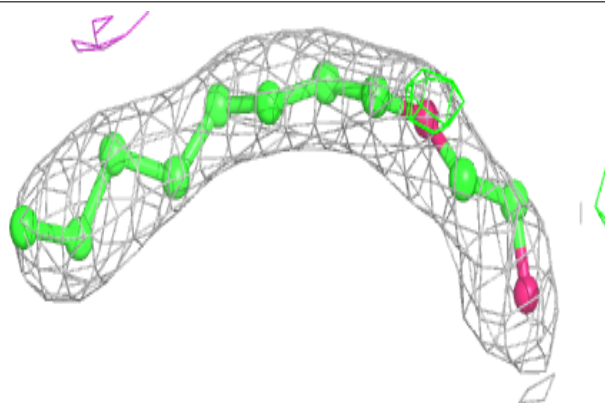
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around C8E C 404:

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

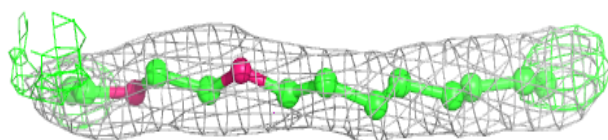
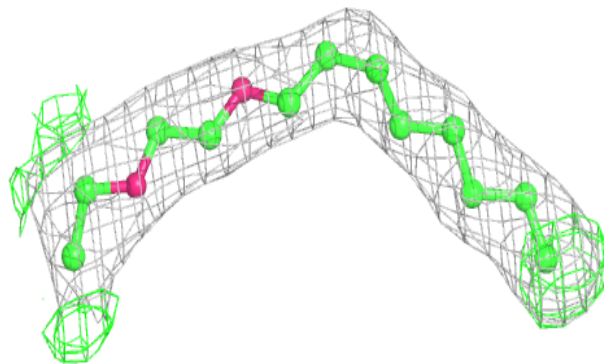
**Electron density around C8E A 408:**

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

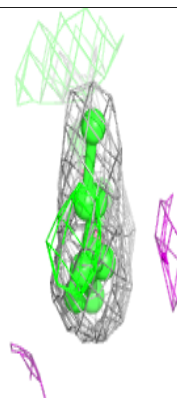
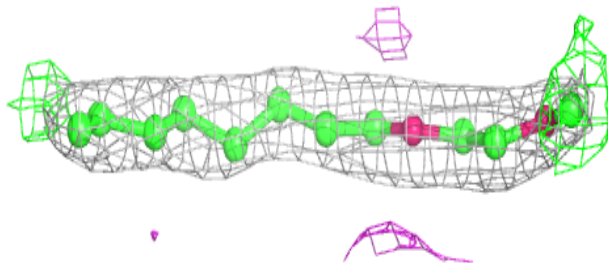
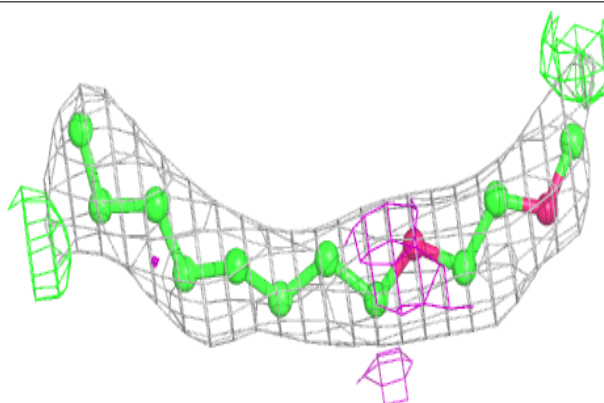


Electron density around C8E D 404:

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

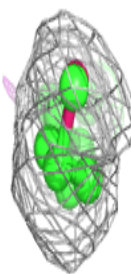
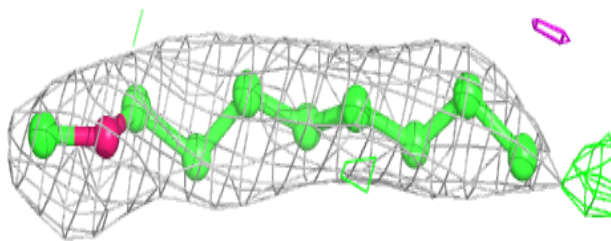
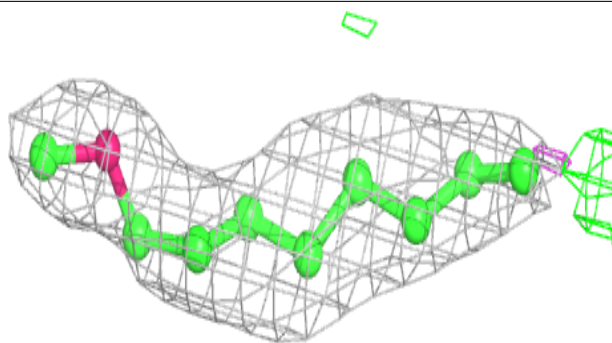
**Electron density around C8E D 405:**

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

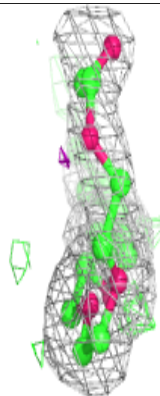
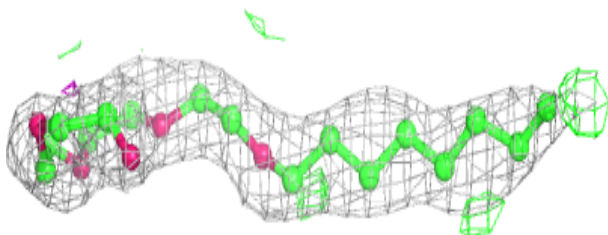
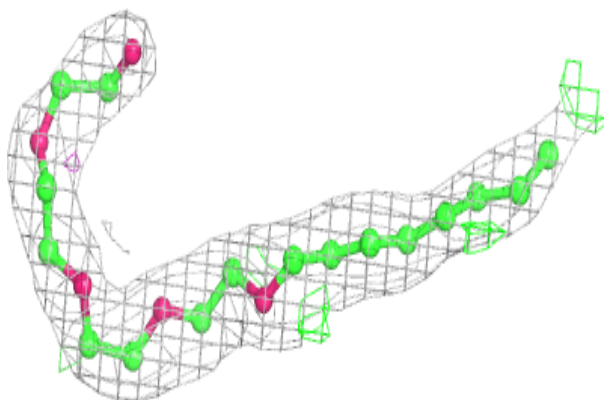


Electron density around C8E A 409:

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

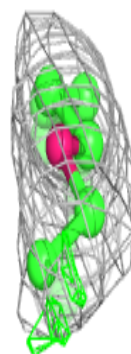
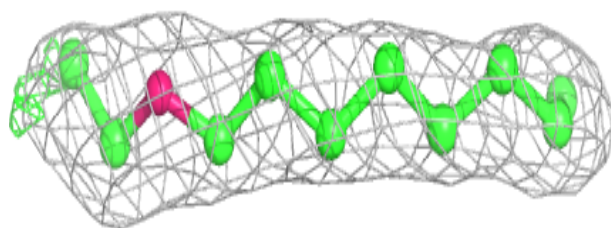
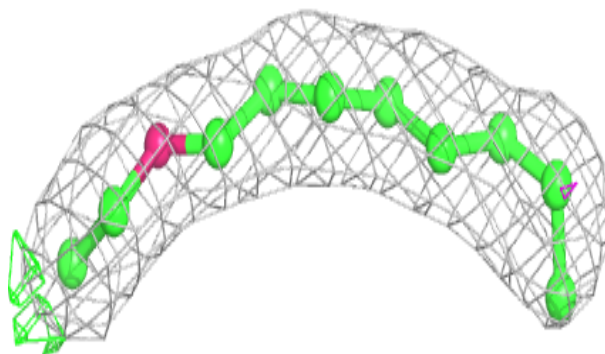
**Electron density around C8E A 410:**

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

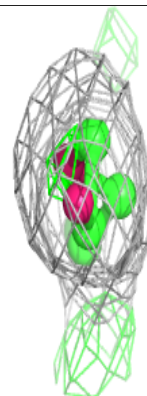
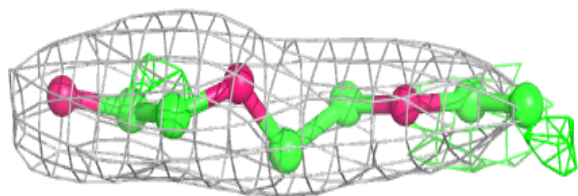
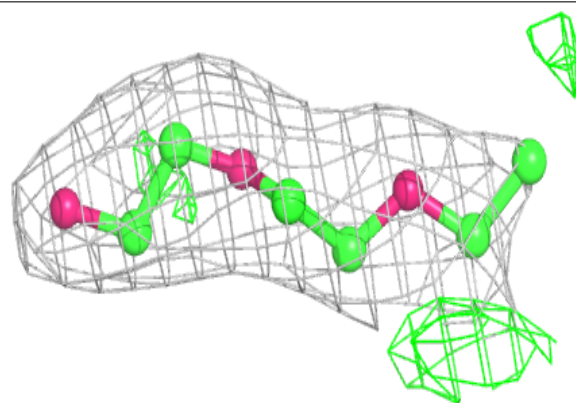


Electron density around C8E D 406:

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

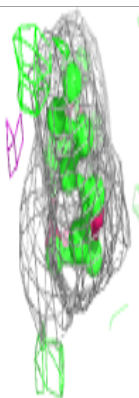
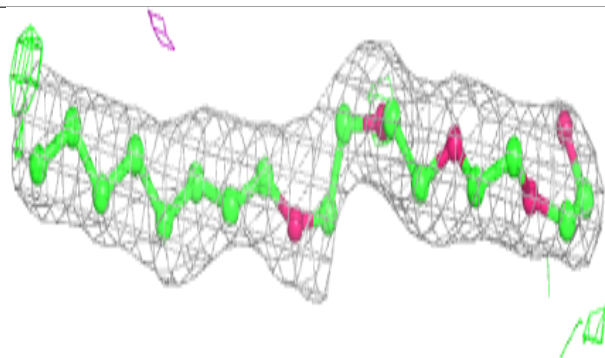
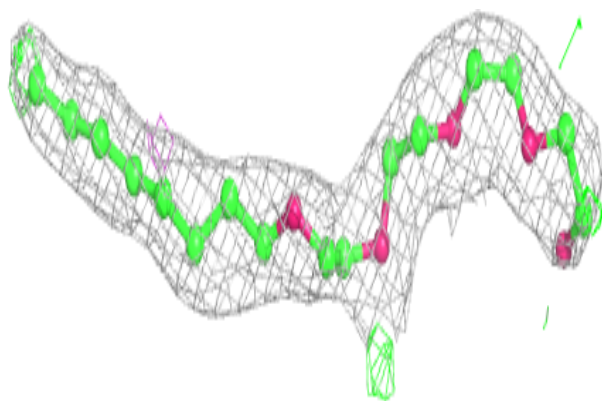
**Electron density around C8E A 405:**

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

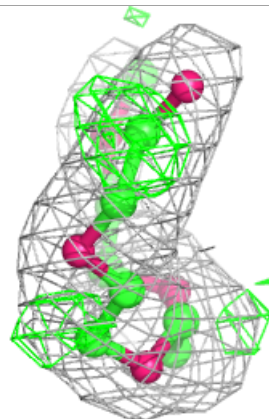
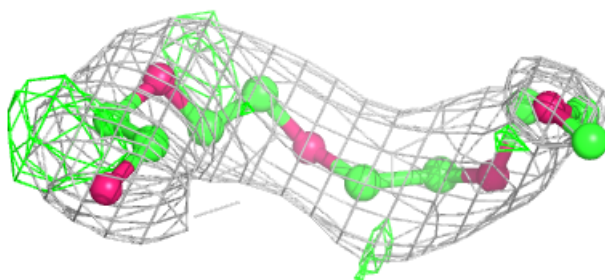
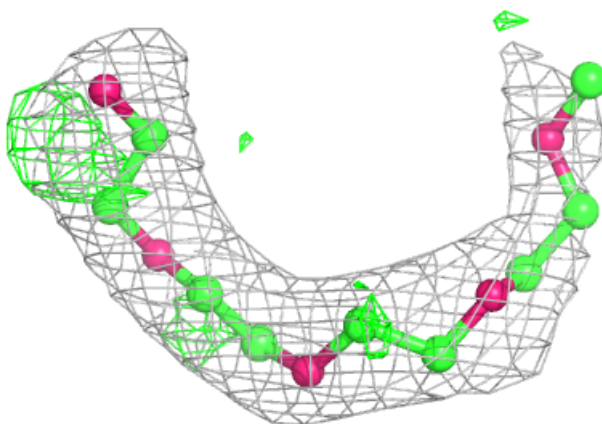


Electron density around C8E B 405:

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

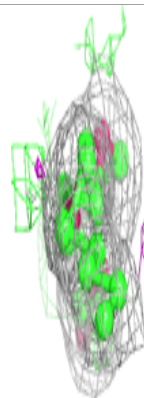
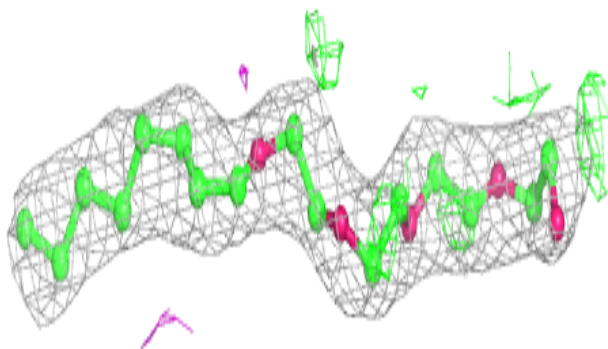
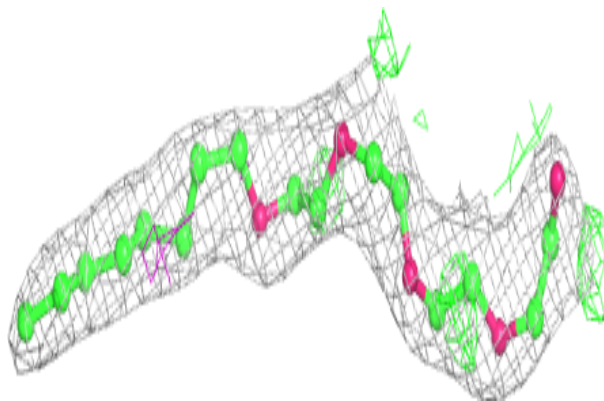
**Electron density around C8E A 407:**

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

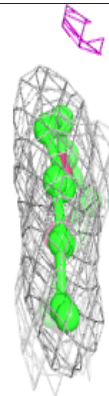
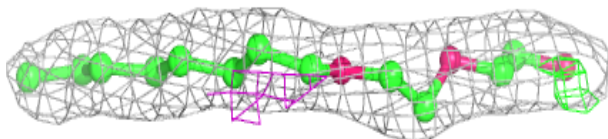
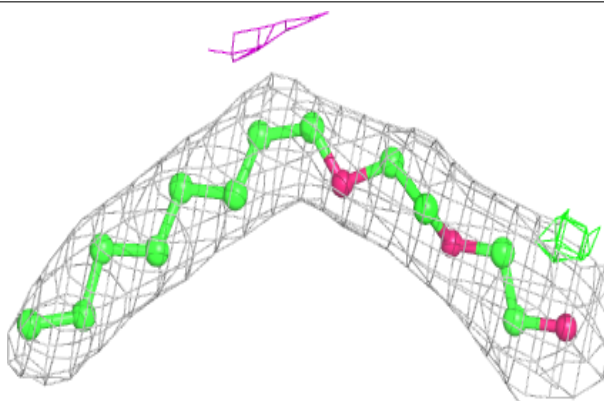


Electron density around C8E B 404:

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

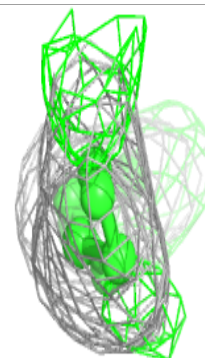
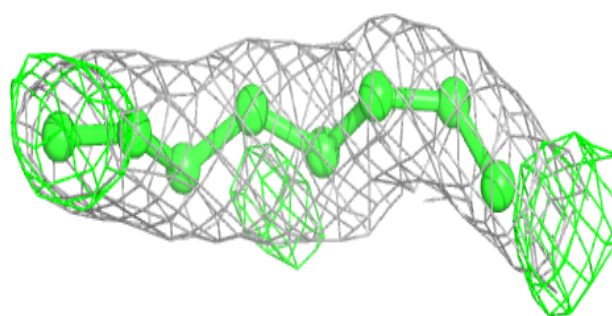
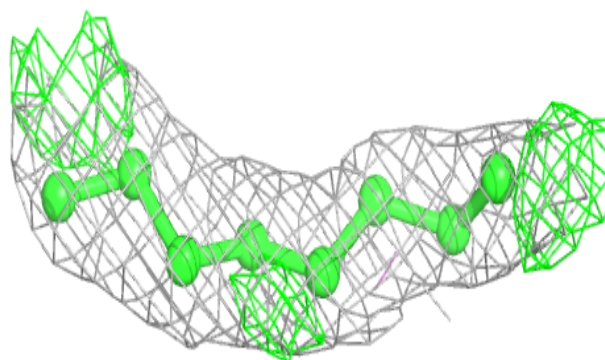
**Electron density around C8E E 406:**

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

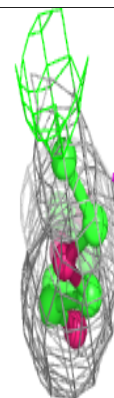
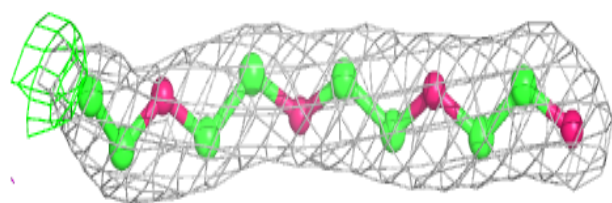
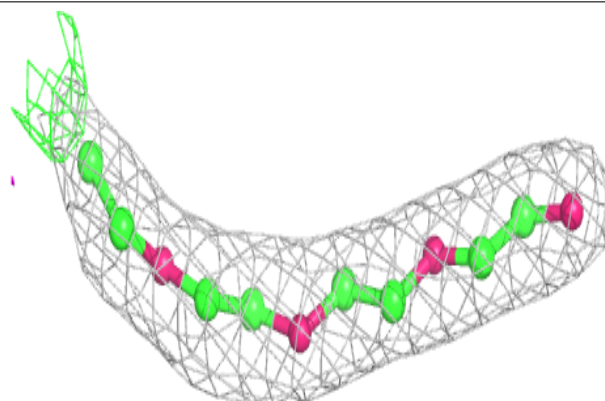


Electron density around C8E E 404:

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

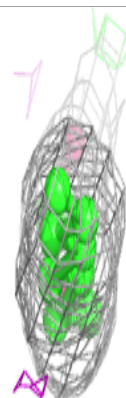
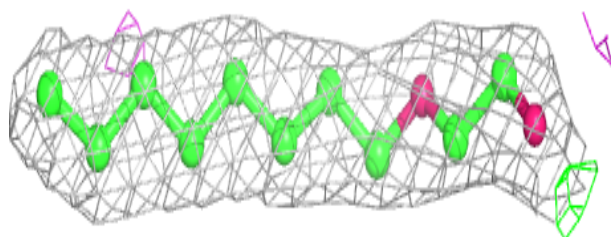
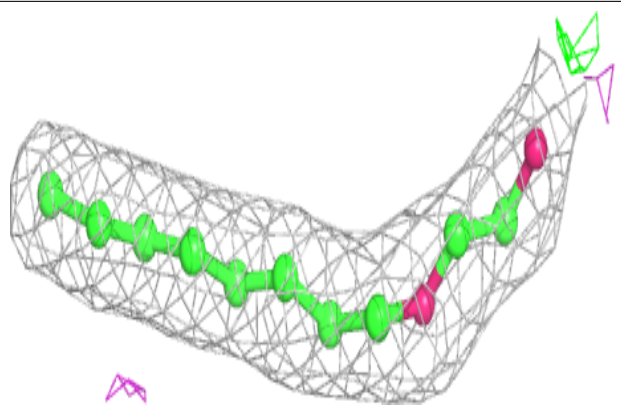
**Electron density around C8E A 404:**

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

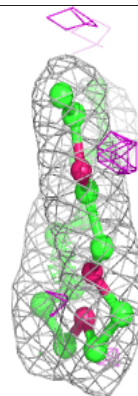
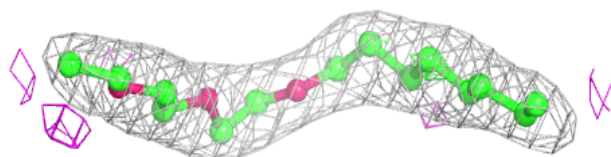
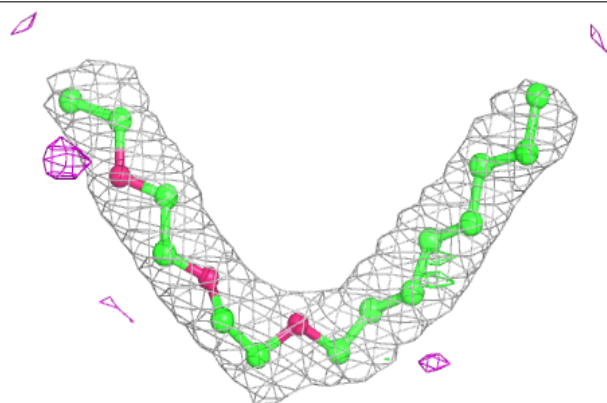


Electron density around C8E E 405:

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

**Electron density around C8E F 404:**

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



6.5 Other polymers

There are no such residues in this entry.