



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 04:51 PM BST

PDB ID : 4MT4  
Title : Crystal structure of the Campylobacter jejuni CmeC outer membrane channel  
Authors : Su, C.-C.; Yu, E.W.  
Deposited on : 2013-09-19  
Resolution : 2.37 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](mailto: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.

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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

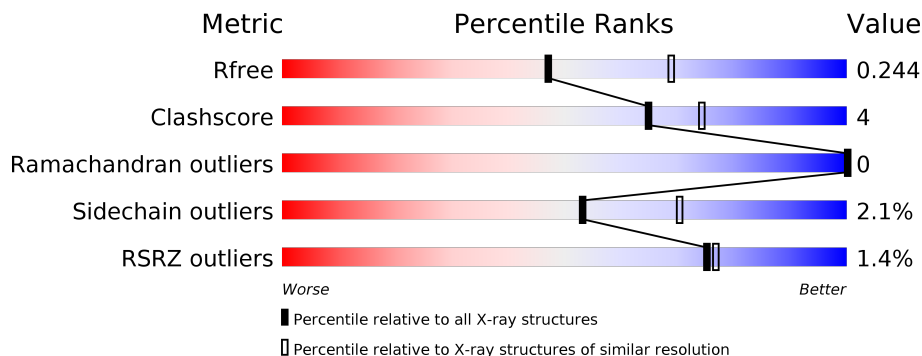
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.37 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	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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  $\geq 3$ , 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	479	 2% 88% 10%
1	B	479	 2% 88% 10%
1	C	479	 2% 88% 10%

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 12304 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.

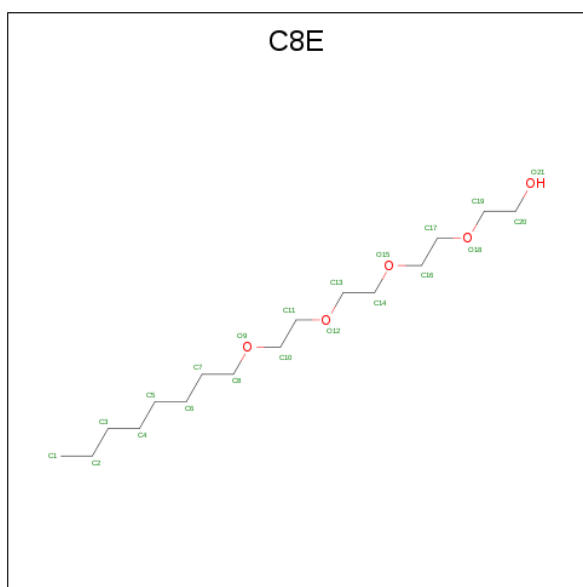
- Molecule 1 is a protein called CmeC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	472	Total	C	N	O	S	0	0	0
			3765	2384	630	745	6			
1	B	473	Total	C	N	O	S	0	0	0
			3774	2389	631	748	6			
1	C	472	Total	C	N	O	S	0	1	0
			3772	2389	632	745	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	474	HIS	-	EXPRESSION TAG	UNP Q8RTE3
A	475	HIS	-	EXPRESSION TAG	UNP Q8RTE3
A	476	HIS	-	EXPRESSION TAG	UNP Q8RTE3
A	477	HIS	-	EXPRESSION TAG	UNP Q8RTE3
A	478	HIS	-	EXPRESSION TAG	UNP Q8RTE3
A	479	HIS	-	EXPRESSION TAG	UNP Q8RTE3
B	474	HIS	-	EXPRESSION TAG	UNP Q8RTE3
B	475	HIS	-	EXPRESSION TAG	UNP Q8RTE3
B	476	HIS	-	EXPRESSION TAG	UNP Q8RTE3
B	477	HIS	-	EXPRESSION TAG	UNP Q8RTE3
B	478	HIS	-	EXPRESSION TAG	UNP Q8RTE3
B	479	HIS	-	EXPRESSION TAG	UNP Q8RTE3
C	474	HIS	-	EXPRESSION TAG	UNP Q8RTE3
C	475	HIS	-	EXPRESSION TAG	UNP Q8RTE3
C	476	HIS	-	EXPRESSION TAG	UNP Q8RTE3
C	477	HIS	-	EXPRESSION TAG	UNP Q8RTE3
C	478	HIS	-	EXPRESSION TAG	UNP Q8RTE3
C	479	HIS	-	EXPRESSION TAG	UNP Q8RTE3

- Molecule 2 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C<sub>16</sub>H<sub>34</sub>O<sub>5</sub>).



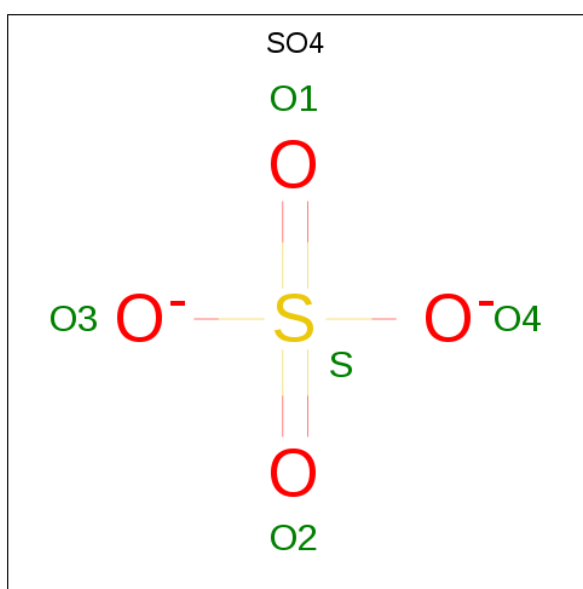
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			21	16	5		
2	A	1	Total	C	O	0	0
			21	16	5		
2	A	1	Total	C	O	0	0
			21	16	5		
2	A	1	Total	C	O	0	0
			21	16	5		
2	A	1	Total	C	O	0	0
			21	16	5		
2	A	1	Total	C	O	0	0
			21	16	5		
2	B	1	Total	C	O	0	0
			21	16	5		
2	B	1	Total	C	O	0	0
			21	16	5		
2	B	1	Total	C	O	0	0
			21	16	5		
2	B	1	Total	C	O	0	0
			21	16	5		
2	C	1	Total	C	O	0	0
			21	16	5		
2	C	1	Total	C	O	0	0
			21	16	5		

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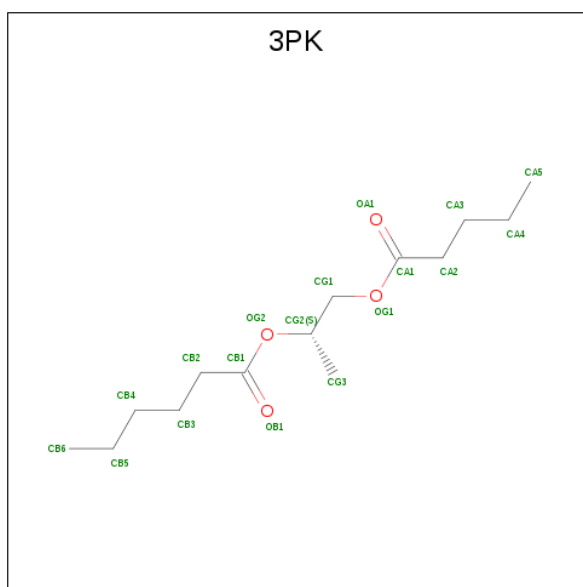
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			21	16	5		
2	C	1	Total	C	O	0	0
			21	16	5		
2	C	1	Total	C	O	0	0
			21	16	5		
2	C	1	Total	C	O	0	0
			21	16	5		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 4 is (2S)-1-(pentanoyloxy)propan-2-yl hexanoate (three-letter code: 3PK) (formula: C<sub>14</sub>H<sub>26</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C O	0	0
			17	13 4		
4	B	1	Total	C O	0	0
			14	10 4		
4	C	1	Total	C O	0	0
			15	11 4		

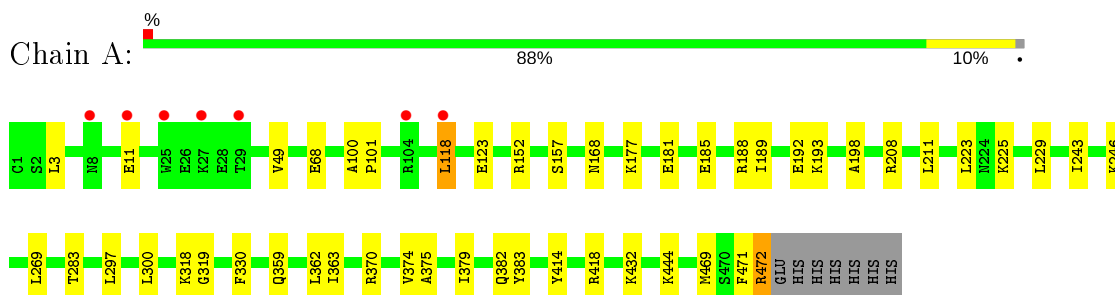
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	194	Total	O	0	0
			194	194		
5	B	185	Total	O	0	0
			185	185		
5	C	180	Total	O	0	0
			180	180		

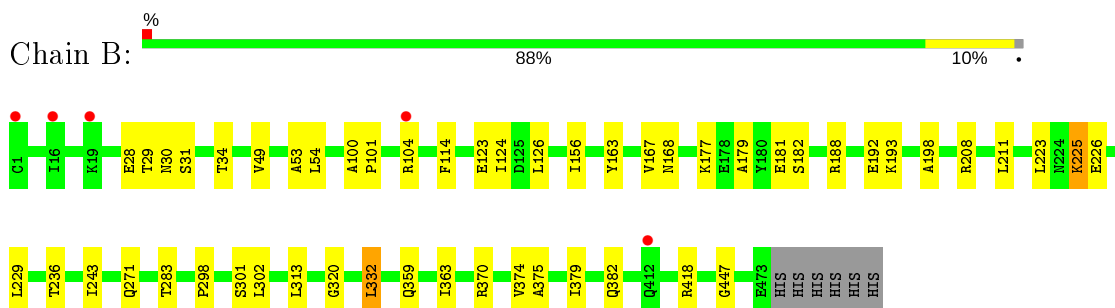
### 3 Residue-property plots [i](#)

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.

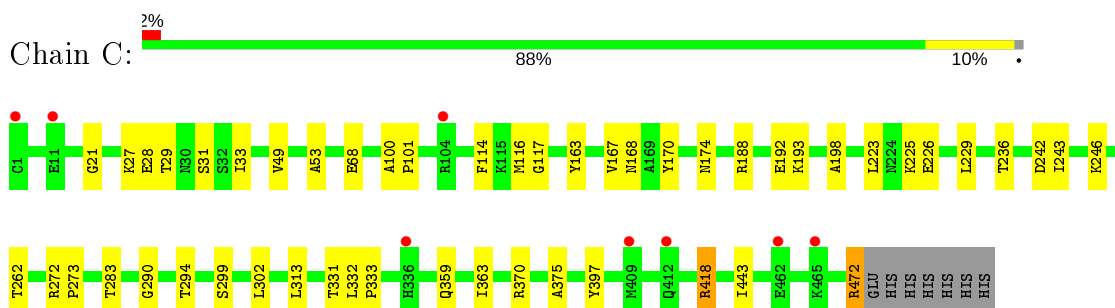
- Molecule 1: CmeC



- Molecule 1: CmeC



- Molecule 1: CmeC



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.83Å 146.32Å 418.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.37 104.72 – 2.37	Depositor EDS
% Data completeness (in resolution range)	98.2 (100.00-2.37) 98.4 (104.72-2.37)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 2.37Å)	Xtrriage
Refinement program	PHENIX dev_1439	Depositor
R, $R_{free}$	0.210 , 0.243 0.211 , 0.244	Depositor DCC
$R_{free}$ test set	5631 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.1	Xtrriage
Anisotropy	0.732	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 51.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12304	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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: 3PK, C8E, SO4

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	0.23	0/3835	0.35	0/5184
1	B	0.21	0/3844	0.35	0/5196
1	C	0.22	0/3846	0.35	0/5199
All	All	0.22	0/11525	0.35	0/15579

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	3765	0	3675	31	0
1	B	3774	0	3681	31	0
1	C	3772	0	3682	31	0
2	A	147	0	238	9	0
2	B	105	0	170	6	0
2	C	126	0	204	5	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	17	0	18	0	0
4	B	14	0	12	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	15	0	14	0	0
5	A	194	0	0	2	0
5	B	185	0	0	1	0
5	C	180	0	0	0	0
All	All	12304	0	11694	97	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 4.

All (97) 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)
4:B:507:3PK:H1A2	4:B:507:3PK:CB2	1.43	1.47
4:B:507:3PK:CB2	4:B:507:3PK:CA2	2.30	1.09
2:A:1005:C8E:H82	2:A:1006:C8E:H31	1.49	0.94
4:B:507:3PK:OG1	4:B:507:3PK:CB2	2.30	0.79
4:B:507:3PK:CG1	4:B:507:3PK:CB2	2.66	0.74
1:B:298:PRO:HG3	1:B:332:LEU:HG	1.73	0.70
4:B:507:3PK:CA1	4:B:507:3PK:CB2	2.71	0.68
1:A:375:ALA:HA	1:B:223:LEU:HD11	1.76	0.67
1:A:471:PHE:CD1	1:A:472:ARG:N	2.65	0.65
1:A:319:GLY:H	2:A:1007:C8E:H171	1.62	0.65
1:B:182:SER:HB2	1:B:418:ARG:HH22	1.63	0.64
2:A:1004:C8E:H171	2:B:503:C8E:H171	1.80	0.61
2:A:1009:C8E:H31	1:C:302:LEU:HD21	1.83	0.60
1:B:49:VAL:HG22	1:B:236:THR:HG21	1.84	0.60
1:C:27:LYS:NZ	1:C:28:GLU:O	2.30	0.60
1:C:313:LEU:H	2:C:504:C8E:H191	1.68	0.59
1:A:223:LEU:HD11	1:C:375:ALA:HA	1.85	0.58
1:B:320:GLY:H	2:B:506:C8E:H202	1.67	0.58
1:C:29:THR:HG22	1:C:31:SER:H	1.70	0.57
1:B:375:ALA:HA	1:C:223:LEU:HD11	1.88	0.55
1:B:126:LEU:HD23	4:B:507:3PK:H2A2	1.88	0.55
1:A:188:ARG:NH1	1:A:192:GLU:OE2	2.39	0.55
1:A:469:MET:O	1:A:472:ARG:HG3	2.07	0.54
1:C:116:MET:HG2	2:C:502:C8E:H141	1.90	0.54
1:B:379:ILE:HA	1:B:382:GLN:HE21	1.73	0.53
1:A:118:LEU:HD22	2:A:1006:C8E:H131	1.91	0.53
1:A:68:GLU:OE1	1:A:472:ARG:NH2	2.39	0.53
1:B:313:LEU:H	2:B:502:C8E:H192	1.74	0.53
1:C:188:ARG:NH1	1:C:192:GLU:OE2	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:ILE:HD11	1:B:302:LEU:HD22	1.91	0.52
1:A:300:LEU:HD13	1:A:330:PHE:HD1	1.74	0.52
1:A:370:ARG:HD2	1:B:243:ILE:O	2.10	0.51
1:A:193:LYS:HB3	1:A:198:ALA:HB3	1.91	0.51
1:B:123:GLU:OE2	1:B:301:SER:OG	2.28	0.51
1:B:29:THR:HG22	1:B:31:SER:H	1.75	0.50
1:A:374:VAL:HG11	1:B:226:GLU:HG3	1.94	0.50
1:C:193:LYS:HB3	1:C:198:ALA:HB3	1.93	0.50
1:C:299:SER:OG	1:C:331:THR:OG1	2.30	0.50
1:B:182:SER:HB2	1:B:418:ARG:NH2	2.27	0.50
1:A:243:ILE:O	1:C:370:ARG:HD2	2.12	0.49
1:A:3:LEU:HD11	1:A:297:LEU:HD12	1.94	0.49
1:B:114:PHE:HZ	2:B:502:C8E:H162	1.79	0.48
1:A:359:GLN:O	1:A:363:ILE:HG12	2.14	0.48
1:B:193:LYS:HB3	1:B:198:ALA:HB3	1.96	0.48
2:A:1002:C8E:H71	2:C:501:C8E:H82	1.97	0.47
1:A:208:ARG:NH2	5:A:1267:HOH:O	2.48	0.47
1:B:370:ARG:HD2	1:C:243:ILE:O	2.14	0.47
1:C:33:ILE:HG21	1:C:443:ILE:HG23	1.97	0.47
1:B:53:ALA:HB2	1:B:236:THR:HG22	1.97	0.46
1:C:114:PHE:HZ	2:C:504:C8E:H162	1.81	0.46
2:B:502:C8E:H12	2:B:503:C8E:H13	1.97	0.46
1:B:374:VAL:HG11	1:C:226:GLU:HG3	1.98	0.45
1:B:223:LEU:HD12	1:B:223:LEU:HA	1.82	0.45
1:B:225:LYS:HB3	1:B:225:LYS:HE3	1.88	0.45
1:B:179:ALA:O	1:B:418:ARG:NH2	2.47	0.44
1:B:54:LEU:HD21	1:B:156:ILE:HD11	1.98	0.44
1:A:157:SER:HB3	1:A:444:LYS:HE2	2.00	0.44
1:A:471:PHE:CE1	1:A:472:ARG:HG2	2.53	0.44
1:B:177:LYS:O	1:B:181:GLU:HG2	2.18	0.44
1:A:246:LYS:HE2	1:A:246:LYS:HB3	1.79	0.43
1:C:170:TYR:CZ	1:C:225:LYS:HD3	2.53	0.43
1:A:225:LYS:HB3	1:A:225:LYS:HE3	1.89	0.43
1:C:332:LEU:HD22	1:C:333:PRO:HD2	2.00	0.43
1:A:269:LEU:HD11	1:A:362:LEU:HD21	2.01	0.43
1:B:188:ARG:NH1	1:B:192:GLU:OE2	2.51	0.43
1:A:177:LYS:O	1:A:181:GLU:HG2	2.19	0.43
1:C:242:ASP:HA	1:C:246:LYS:HD3	2.01	0.43
1:A:471:PHE:CD1	1:A:471:PHE:C	2.92	0.43
1:C:68:GLU:OE1	1:C:472:ARG:NH2	2.47	0.43
2:A:1005:C8E:H102	2:A:1005:C8E:H132	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:502:C8E:H201	2:B:502:C8E:H171	1.70	0.42
1:C:359:GLN:O	1:C:363:ILE:HG12	2.19	0.42
1:C:100:ALA:HA	1:C:101:PRO:HD3	1.93	0.42
1:A:152:ARG:NH2	5:A:1215:HOH:O	2.53	0.42
1:C:21:GLY:N	1:C:262:THR:O	2.49	0.42
1:C:397:TYR:CE1	1:C:418:ARG:HG2	2.55	0.42
1:A:379:ILE:HA	1:A:382:GLN:HE21	1.84	0.41
1:C:163:TYR:O	1:C:167:VAL:HG23	2.20	0.41
1:C:272:ARG:HA	1:C:273:PRO:HD3	1.90	0.41
1:A:414:TYR:O	1:A:418:ARG:HG3	2.21	0.41
1:A:318:LYS:HD2	2:A:1007:C8E:H172	2.03	0.41
1:C:223:LEU:HA	1:C:223:LEU:HD12	1.86	0.41
1:C:225:LYS:HB3	1:C:225:LYS:HE2	1.87	0.41
1:A:100:ALA:HA	1:A:101:PRO:HD3	1.92	0.41
1:B:163:TYR:O	1:B:167:VAL:HG23	2.21	0.41
1:B:359:GLN:O	1:B:363:ILE:HG12	2.20	0.40
1:A:68:GLU:CD	1:A:472:ARG:HH22	2.24	0.40
1:B:30:ASN:ND2	5:B:711:HOH:O	2.46	0.40
1:A:185:GLU:O	1:A:189:ILE:HG12	2.21	0.40
1:C:53:ALA:HB2	1:C:236:THR:HG22	2.02	0.40
1:C:290:GLY:O	1:C:294:THR:HG23	2.21	0.40
2:A:1005:C8E:H161	2:A:1005:C8E:H191	1.78	0.40
1:C:117:GLY:HA2	2:C:502:C8E:H102	2.03	0.40
1:A:383:TYR:HE2	1:A:432:LYS:HG3	1.87	0.40
1:B:100:ALA:HA	1:B:101:PRO:HD3	1.91	0.40
1:B:271:GLN:O	1:B:447:GLY:HA3	2.22	0.40
1:C:33:ILE:HD13	1:C:443:ILE:HG23	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	470/479 (98%)	463 (98%)	7 (2%)	0	100	100
1	B	471/479 (98%)	465 (99%)	6 (1%)	0	100	100
1	C	471/479 (98%)	465 (99%)	6 (1%)	0	100	100
All	All	1412/1437 (98%)	1393 (99%)	19 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	403/410 (98%)	394 (98%)	9 (2%)	52	69
1	B	404/410 (98%)	394 (98%)	10 (2%)	47	65
1	C	404/410 (98%)	397 (98%)	7 (2%)	60	76
All	All	1211/1230 (98%)	1185 (98%)	26 (2%)	53	70

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLU
1	A	49	VAL
1	A	118	LEU
1	A	123	GLU
1	A	168	ASN
1	A	211	LEU
1	A	229	LEU
1	A	283	THR
1	A	472	ARG
1	B	28	GLU
1	B	34	THR
1	B	104	ARG
1	B	168	ASN
1	B	208	ARG
1	B	211	LEU

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Mol	Chain	Res	Type
1	B	225	LYS
1	B	229	LEU
1	B	283	THR
1	B	332	LEU
1	C	49	VAL
1	C	168	ASN
1	C	174	ASN
1	C	229	LEU
1	C	283	THR
1	C	418	ARG
1	C	472	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	382	GLN
1	B	382	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](#)

23 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	B	504	-	20,20,20	0.60	0	19,19,19	1.33	0
2	C8E	B	503	-	20,20,20	0.61	0	19,19,19	1.30	0
2	C8E	A	1004	-	20,20,20	0.62	0	19,19,19	1.31	0
2	C8E	C	501	-	20,20,20	0.59	0	19,19,19	1.34	0
2	C8E	C	505	-	20,20,20	0.60	0	19,19,19	1.30	0
2	C8E	C	502	-	20,20,20	0.61	0	19,19,19	1.28	0
2	C8E	A	1002	-	20,20,20	0.62	0	19,19,19	1.27	0
2	C8E	B	506	-	20,20,20	0.61	0	19,19,19	1.30	0
2	C8E	A	1001	-	20,20,20	0.62	0	19,19,19	1.36	0
2	C8E	C	504	-	20,20,20	0.61	0	19,19,19	1.26	0
2	C8E	A	1005	-	20,20,20	0.61	0	19,19,19	1.32	0
4	3PK	B	507	1	13,13,17	2.43	2 (15%)	15,15,19	2.64	5 (33%)
4	3PK	A	1008	1	16,16,17	2.03	3 (18%)	18,18,19	2.00	8 (44%)
2	C8E	A	1007	-	20,20,20	0.60	0	19,19,19	1.32	0
3	SO4	B	501	-	4,4,4	0.15	0	6,6,6	0.10	0
2	C8E	A	1009	-	20,20,20	0.60	0	19,19,19	1.32	0
4	3PK	C	507	1	14,14,17	2.04	2 (14%)	16,16,19	1.97	5 (31%)
3	SO4	A	1003	-	4,4,4	0.14	0	6,6,6	0.08	0
2	C8E	C	506	-	20,20,20	0.61	0	19,19,19	1.35	0
2	C8E	A	1006	-	20,20,20	1.14	1 (5%)	19,19,19	1.54	4 (21%)
2	C8E	C	503	-	20,20,20	0.60	0	19,19,19	1.31	0
2	C8E	B	505	-	20,20,20	0.60	0	19,19,19	1.34	0
2	C8E	B	502	-	20,20,20	0.62	0	19,19,19	1.26	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	C	502	-	-	8/18/18/18	-
2	C8E	A	1007	-	-	5/18/18/18	-
2	C8E	C	506	-	-	8/18/18/18	-
2	C8E	B	504	-	-	8/18/18/18	-
2	C8E	B	503	-	-	5/18/18/18	-
2	C8E	A	1002	-	-	14/18/18/18	-
2	C8E	C	501	-	-	9/18/18/18	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	C8E	A	1006	-	-	10/18/18/18	-
2	C8E	B	506	-	-	3/18/18/18	-
2	C8E	A	1001	-	-	8/18/18/18	-
2	C8E	C	504	-	-	6/18/18/18	-
2	C8E	C	503	-	-	7/18/18/18	-
2	C8E	A	1005	-	-	7/18/18/18	-
4	3PK	B	507	1	-	7/13/13/18	-
2	C8E	A	1004	-	-	8/18/18/18	-
2	C8E	A	1009	-	-	9/18/18/18	-
4	3PK	A	1008	1	-	7/17/17/18	-
2	C8E	B	505	-	-	14/18/18/18	-
2	C8E	B	502	-	-	10/18/18/18	-
4	3PK	C	507	1	-	6/15/15/18	-
2	C8E	C	505	-	-	6/18/18/18	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	507	3PK	OG2-CG2	-7.46	1.34	1.47
4	A	1008	3PK	OG2-CG2	-6.47	1.36	1.47
4	C	507	3PK	OG2-CG2	-6.09	1.36	1.47
4	C	507	3PK	OG1-CG1	-3.82	1.36	1.45
4	B	507	3PK	OG1-CG1	-3.73	1.36	1.45
4	A	1008	3PK	OG1-CG1	-3.51	1.37	1.45
2	A	1006	C8E	O18-C19	-2.51	1.31	1.42
4	A	1008	3PK	CB5-CB4	-2.17	1.36	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	507	3PK	CG2-OG2-CB1	-6.34	107.37	118.31
4	B	507	3PK	OG2-CB1-OB1	-5.39	112.25	122.96
4	C	507	3PK	OG1-CA1-OA1	-4.38	112.54	123.59
4	A	1008	3PK	OG2-CB1-CB2	4.31	120.80	111.50
4	B	507	3PK	OG2-CG2-CG1	3.09	113.29	106.13
2	A	1006	C8E	O18-C17-C16	3.02	124.01	110.39
4	C	507	3PK	OG2-CB1-CB2	2.84	118.73	110.80
4	A	1008	3PK	OG1-CG1-CG2	2.79	116.42	108.38
2	A	1006	C8E	C6-C7-C8	-2.78	101.17	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	507	3PK	OG2-CB1-OB1	-2.63	117.36	123.70
4	C	507	3PK	OG1-CA1-CA2	2.62	120.13	111.91
2	A	1006	C8E	O21-C20-C19	2.56	126.68	111.81
2	A	1006	C8E	C16-O15-C14	2.53	124.23	113.29
4	A	1008	3PK	CG2-OG2-CB1	2.49	121.08	117.88
4	A	1008	3PK	OG1-CA1-OA1	-2.49	117.31	123.59
4	A	1008	3PK	OG2-CG2-CG3	2.48	113.61	107.93
4	B	507	3PK	OG1-CA1-OA1	-2.34	117.69	123.59
4	A	1008	3PK	OG1-CA1-CA2	2.30	119.13	111.91
4	C	507	3PK	OG2-CG2-CG1	2.20	111.22	106.13
4	B	507	3PK	OB1-CB1-CB2	-2.07	117.28	124.81
4	A	1008	3PK	OA1-CA1-CA2	-2.04	115.79	123.73
4	A	1008	3PK	CG1-OG1-CA1	2.03	124.64	117.12

There are no chirality outliers.

All (165) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	507	3PK	OB1-CB1-OG2-CG2
4	B	507	3PK	CB2-CB1-OG2-CG2
4	A	1008	3PK	OG1-CG1-CG2-OG2
4	A	1008	3PK	OG1-CG1-CG2-CG3
4	C	507	3PK	OG1-CG1-CG2-OG2
4	C	507	3PK	OG1-CG1-CG2-CG3
4	B	507	3PK	OA1-CA1-OG1-CG1
4	A	1008	3PK	OA1-CA1-OG1-CG1
2	A	1001	C8E	C13-C14-O15-C16
2	C	506	C8E	C10-C11-O12-C13
4	A	1008	3PK	CB2-CB1-OG2-CG2
2	A	1005	C8E	C10-C11-O12-C13
2	A	1005	C8E	C16-C17-O18-C19
2	B	505	C8E	C16-C17-O18-C19
4	B	507	3PK	CA2-CA1-OG1-CG1
4	A	1008	3PK	CA2-CA1-OG1-CG1
2	C	501	C8E	O18-C19-C20-O21
2	B	502	C8E	C20-C19-O18-C17
2	C	501	C8E	O9-C10-C11-O12
2	C	501	C8E	O15-C16-C17-O18
2	B	506	C8E	O12-C13-C14-O15
2	B	505	C8E	O12-C13-C14-O15
2	B	504	C8E	C14-C13-O12-C11
2	A	1004	C8E	O9-C10-C11-O12

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Mol	Chain	Res	Type	Atoms
2	C	501	C8E	C14-C13-O12-C11
2	A	1004	C8E	C14-C13-O12-C11
2	C	505	C8E	O15-C16-C17-O18
2	C	505	C8E	C20-C19-O18-C17
2	A	1001	C8E	C16-C17-O18-C19
2	B	504	C8E	O9-C10-C11-O12
2	C	502	C8E	O15-C16-C17-O18
4	C	507	3PK	CB2-CB1-OG2-CG2
2	C	502	C8E	C16-C17-O18-C19
2	A	1005	C8E	O15-C16-C17-O18
2	A	1002	C8E	O12-C13-C14-O15
2	A	1009	C8E	O12-C13-C14-O15
2	C	506	C8E	C6-C7-C8-O9
4	C	507	3PK	CA1-CA2-CA3-CA4
2	B	503	C8E	O15-C16-C17-O18
2	B	506	C8E	C6-C7-C8-O9
2	A	1001	C8E	C6-C7-C8-O9
2	C	504	C8E	C6-C7-C8-O9
2	C	501	C8E	O12-C13-C14-O15
2	A	1007	C8E	C6-C7-C8-O9
2	A	1009	C8E	C6-C7-C8-O9
2	C	503	C8E	C6-C7-C8-O9
2	B	502	C8E	C6-C7-C8-O9
2	A	1002	C8E	C16-C17-O18-C19
2	A	1005	C8E	C17-C16-O15-C14
2	C	506	C8E	C16-C17-O18-C19
2	A	1002	C8E	C6-C7-C8-O9
2	A	1002	C8E	O15-C16-C17-O18
2	A	1006	C8E	O15-C16-C17-O18
2	C	504	C8E	O15-C16-C17-O18
2	A	1002	C8E	O18-C19-C20-O21
2	A	1001	C8E	O18-C19-C20-O21
2	B	502	C8E	O18-C19-C20-O21
2	B	503	C8E	C6-C7-C8-O9
2	A	1004	C8E	C16-C17-O18-C19
2	B	504	C8E	C6-C7-C8-O9
2	C	506	C8E	C4-C5-C6-C7
2	C	505	C8E	C2-C3-C4-C5
2	C	506	C8E	C17-C16-O15-C14
2	C	506	C8E	O15-C16-C17-O18
2	C	502	C8E	C2-C3-C4-C5
2	C	502	C8E	O12-C13-C14-O15

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Mol	Chain	Res	Type	Atoms
2	B	502	C8E	O15-C16-C17-O18
2	A	1006	C8E	C3-C4-C5-C6
4	A	1008	3PK	OB1-CB1-OG2-CG2
2	B	502	C8E	C5-C6-C7-C8
2	C	504	C8E	C20-C19-O18-C17
2	C	504	C8E	C13-C14-O15-C16
2	B	503	C8E	C5-C6-C7-C8
2	C	501	C8E	C6-C7-C8-O9
2	A	1002	C8E	C5-C6-C7-C8
2	B	503	C8E	C4-C5-C6-C7
2	A	1005	C8E	C6-C7-C8-O9
2	B	505	C8E	C1-C2-C3-C4
2	C	505	C8E	O9-C10-C11-O12
4	C	507	3PK	CA2-CA3-CA4-CA5
2	A	1006	C8E	O18-C19-C20-O21
2	A	1001	C8E	C5-C6-C7-C8
2	A	1006	C8E	C1-C2-C3-C4
2	B	503	C8E	O9-C10-C11-O12
4	B	507	3PK	CA2-CA3-CA4-CA5
2	A	1009	C8E	C3-C4-C5-C6
4	B	507	3PK	OG1-CG1-CG2-CG3
2	B	502	C8E	C3-C4-C5-C6
2	A	1004	C8E	O12-C13-C14-O15
4	B	507	3PK	OG1-CG1-CG2-OG2
2	B	504	C8E	O12-C13-C14-O15
2	B	505	C8E	C2-C3-C4-C5
4	A	1008	3PK	CB1-CB2-CB3-CB4
2	B	502	C8E	C13-C14-O15-C16
2	B	504	C8E	C11-C10-O9-C8
2	A	1004	C8E	C17-C16-O15-C14
2	C	501	C8E	C11-C10-O9-C8
2	C	505	C8E	C17-C16-O15-C14
2	C	503	C8E	C20-C19-O18-C17
2	B	504	C8E	C13-C14-O15-C16
2	B	504	C8E	C10-C11-O12-C13
2	C	502	C8E	C17-C16-O15-C14
2	A	1002	C8E	C11-C10-O9-C8
2	A	1006	C8E	C5-C6-C7-C8
2	A	1004	C8E	C10-C11-O12-C13
2	A	1005	C8E	C14-C13-O12-C11
2	B	502	C8E	C10-C11-O12-C13
2	B	505	C8E	C13-C14-O15-C16

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Mol	Chain	Res	Type	Atoms
2	B	505	C8E	C4-C5-C6-C7
2	A	1004	C8E	O18-C19-C20-O21
2	A	1009	C8E	O18-C19-C20-O21
2	A	1007	C8E	C11-C10-O9-C8
2	C	501	C8E	C10-C11-O12-C13
2	A	1002	C8E	C13-C14-O15-C16
2	A	1002	C8E	C7-C8-O9-C10
2	C	501	C8E	C13-C14-O15-C16
2	B	505	C8E	C20-C19-O18-C17
2	A	1009	C8E	C14-C13-O12-C11
4	C	507	3PK	CA2-CA1-OG1-CG1
2	A	1006	C8E	O9-C10-C11-O12
2	B	505	C8E	C11-C10-O9-C8
2	C	502	C8E	O18-C19-C20-O21
2	A	1009	C8E	C16-C17-O18-C19
2	A	1002	C8E	C10-C11-O12-C13
2	B	505	C8E	C6-C7-C8-O9
2	B	504	C8E	C20-C19-O18-C17
2	A	1004	C8E	O15-C16-C17-O18
2	B	505	C8E	O18-C19-C20-O21
2	C	505	C8E	C10-C11-O12-C13
2	A	1009	C8E	C2-C3-C4-C5
2	B	505	C8E	C14-C13-O12-C11
2	A	1001	C8E	O12-C13-C14-O15
2	C	506	C8E	O9-C10-C11-O12
2	C	506	C8E	C14-C13-O12-C11
2	A	1002	C8E	C17-C16-O15-C14
2	B	505	C8E	O15-C16-C17-O18
2	C	502	C8E	C11-C10-O9-C8
2	A	1006	C8E	C2-C3-C4-C5
2	C	503	C8E	C10-C11-O12-C13
2	A	1001	C8E	C2-C3-C4-C5
2	C	503	C8E	O9-C10-C11-O12
2	C	504	C8E	C5-C6-C7-C8
2	A	1002	C8E	C14-C13-O12-C11
2	B	502	C8E	C2-C3-C4-C5
2	C	504	C8E	O12-C13-C14-O15
2	A	1002	C8E	C20-C19-O18-C17
2	A	1009	C8E	O15-C16-C17-O18
2	A	1006	C8E	C17-C16-O15-C14
2	C	503	C8E	C13-C14-O15-C16
2	B	506	C8E	O9-C10-C11-O12

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Mol	Chain	Res	Type	Atoms
2	B	505	C8E	O9-C10-C11-O12
2	A	1006	C8E	C14-C13-O12-C11
2	C	503	C8E	O12-C13-C14-O15
2	B	505	C8E	C10-C11-O12-C13
2	A	1009	C8E	O9-C10-C11-O12
2	A	1005	C8E	O9-C10-C11-O12
2	A	1006	C8E	O12-C13-C14-O15
2	A	1001	C8E	O9-C10-C11-O12
2	C	503	C8E	O15-C16-C17-O18
2	C	502	C8E	O9-C10-C11-O12
2	A	1002	C8E	O9-C10-C11-O12
2	A	1007	C8E	C14-C13-O12-C11
2	B	502	C8E	O12-C13-C14-O15
2	A	1007	C8E	O9-C10-C11-O12
2	A	1007	C8E	O15-C16-C17-O18

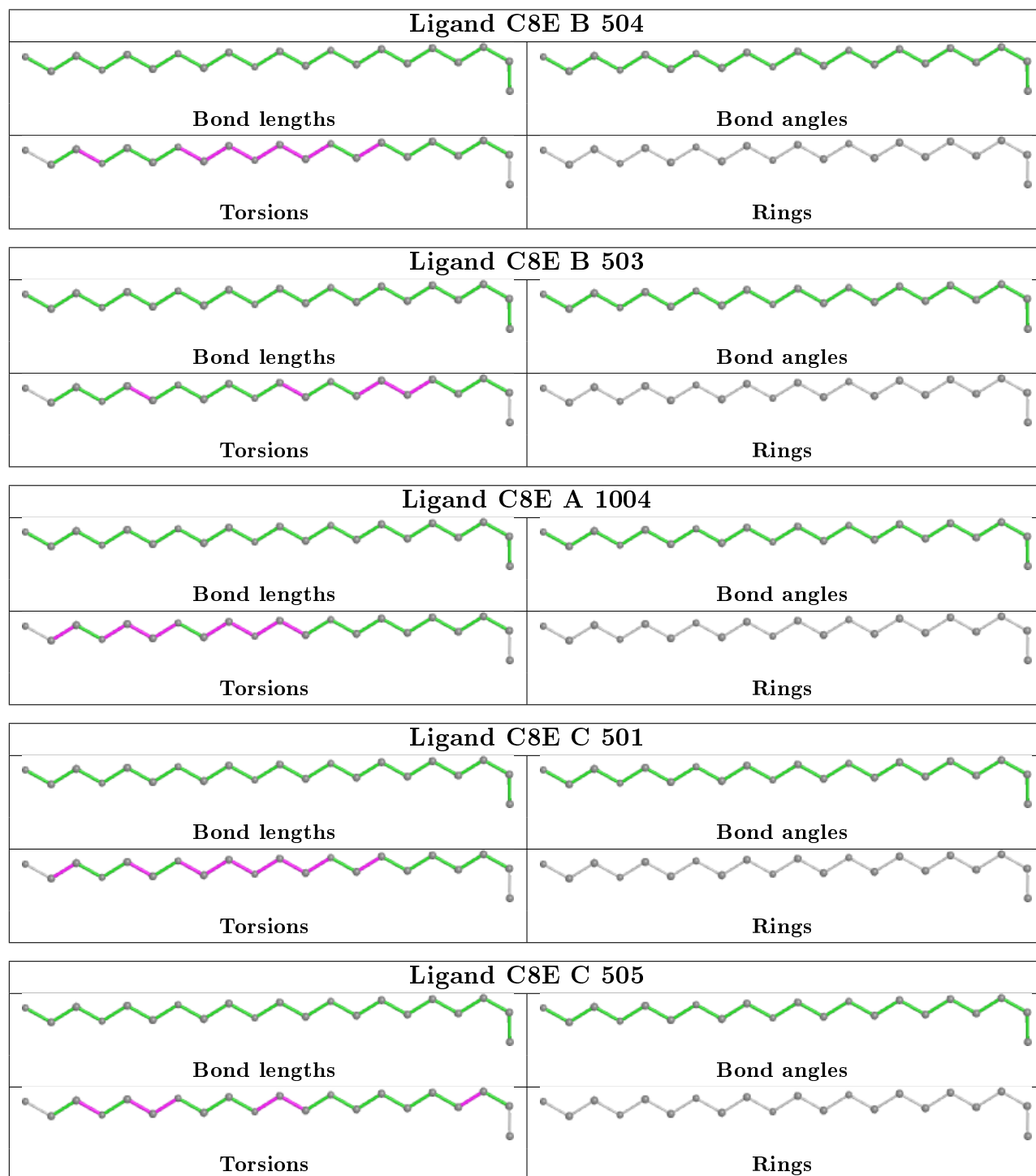
There are no ring outliers.

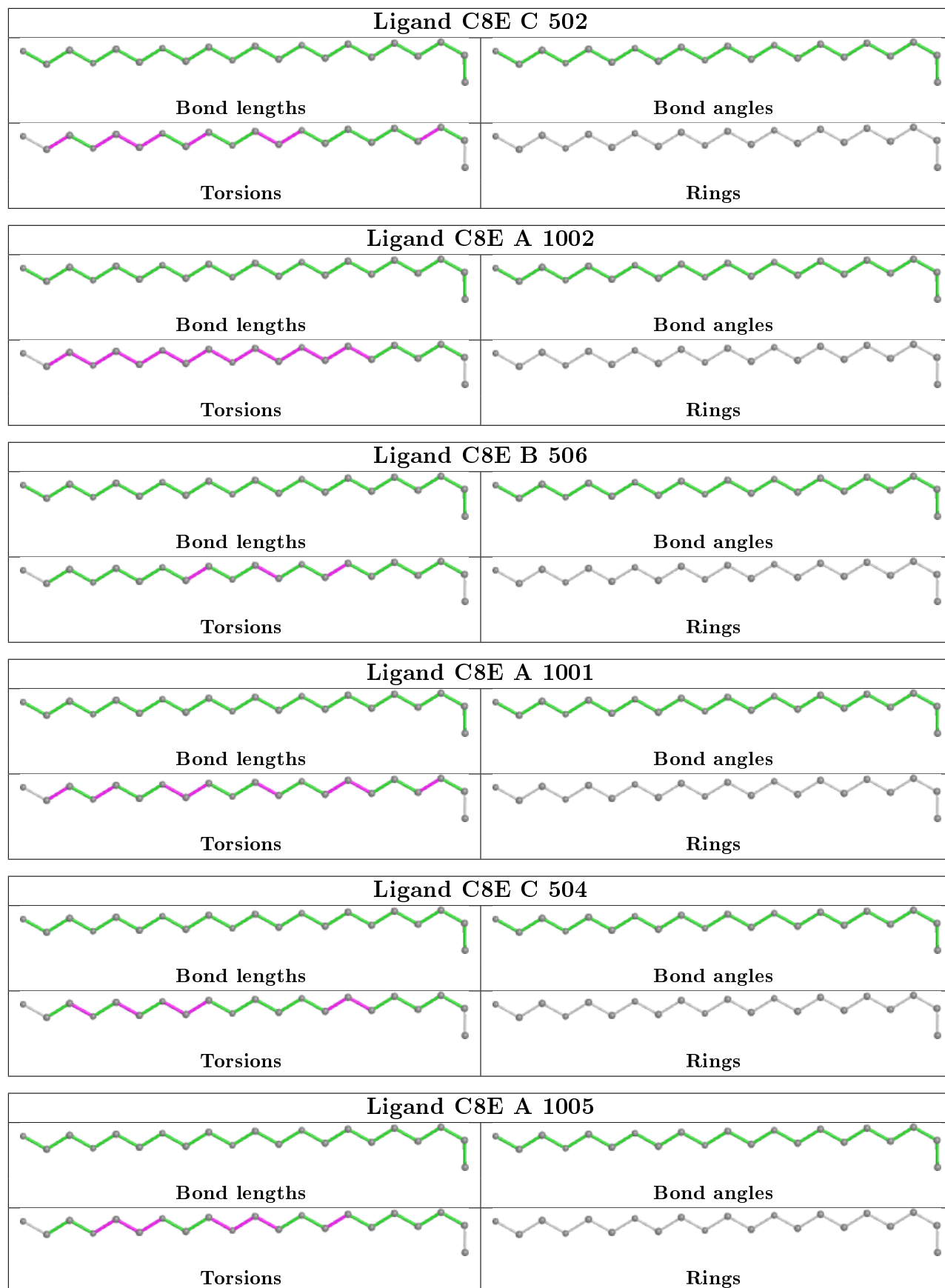
13 monomers are involved in 24 short contacts:

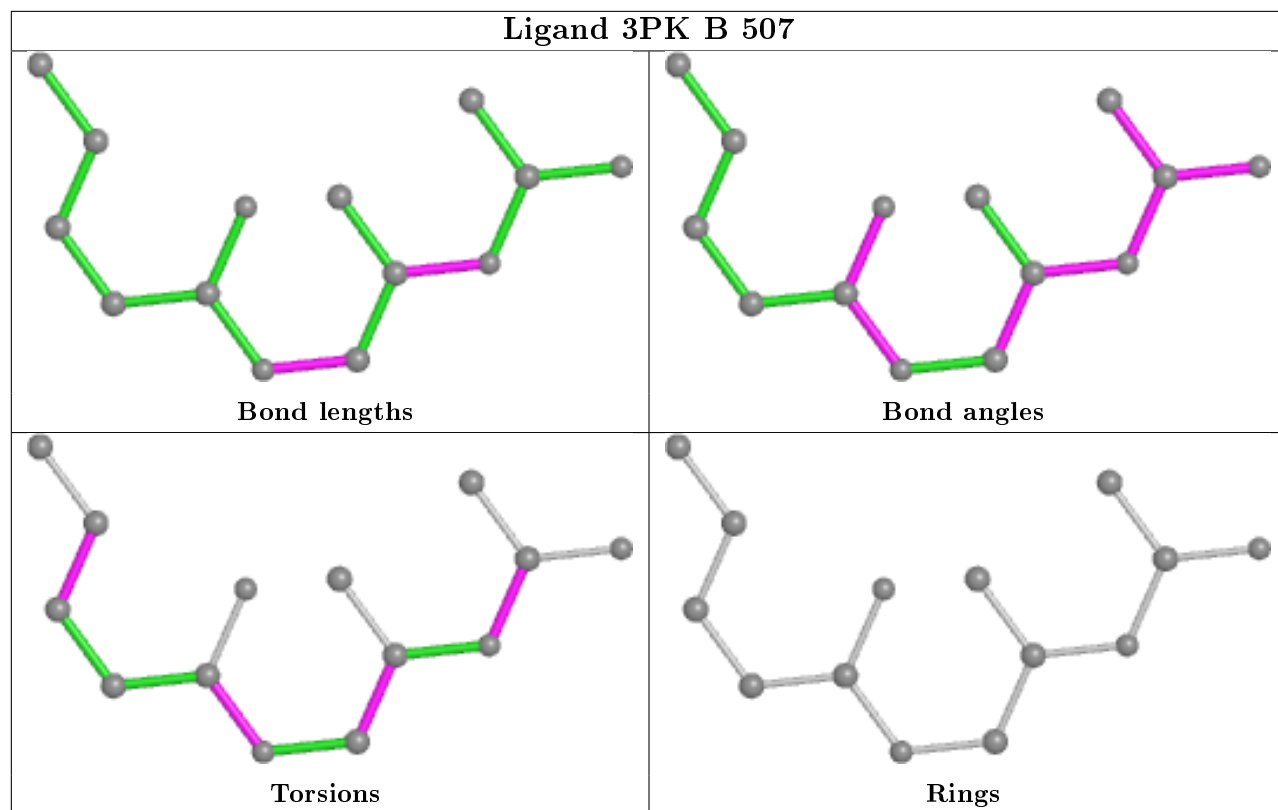
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	503	C8E	2	0
2	A	1004	C8E	1	0
2	C	501	C8E	1	0
2	C	502	C8E	2	0
2	A	1002	C8E	1	0
2	B	506	C8E	1	0
2	C	504	C8E	2	0
2	A	1005	C8E	3	0
4	B	507	3PK	6	0
2	A	1007	C8E	2	0
2	A	1009	C8E	1	0
2	A	1006	C8E	2	0
2	B	502	C8E	4	0

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

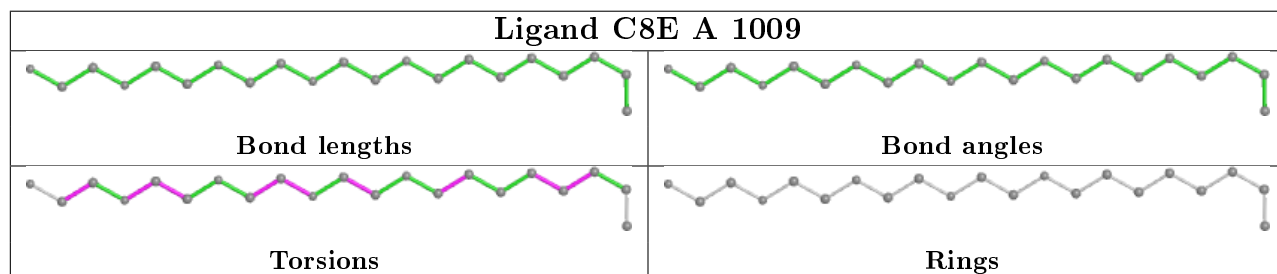
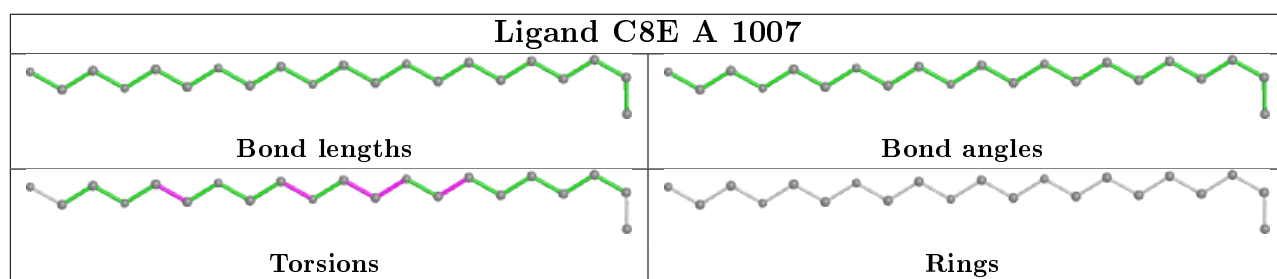
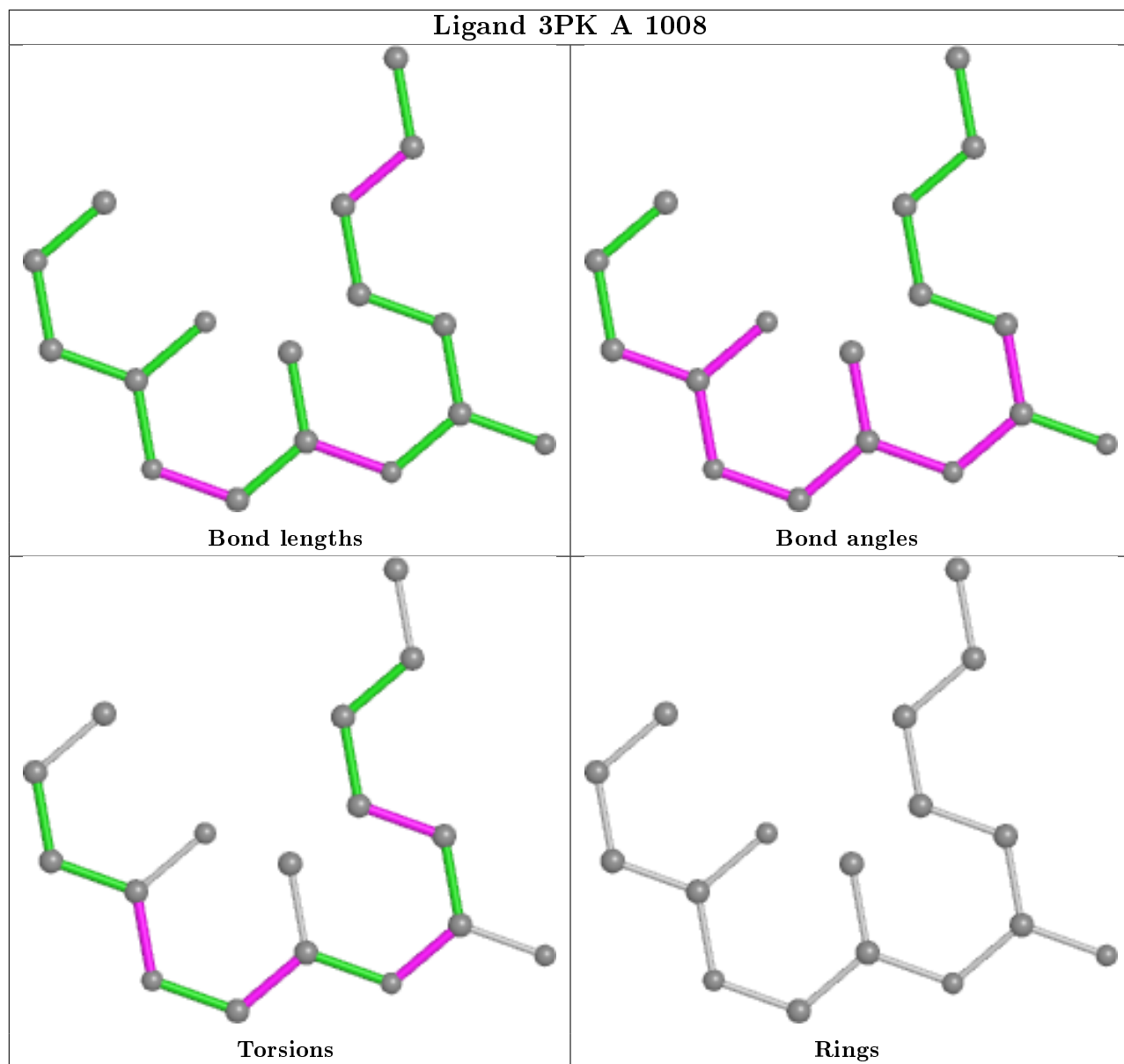
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

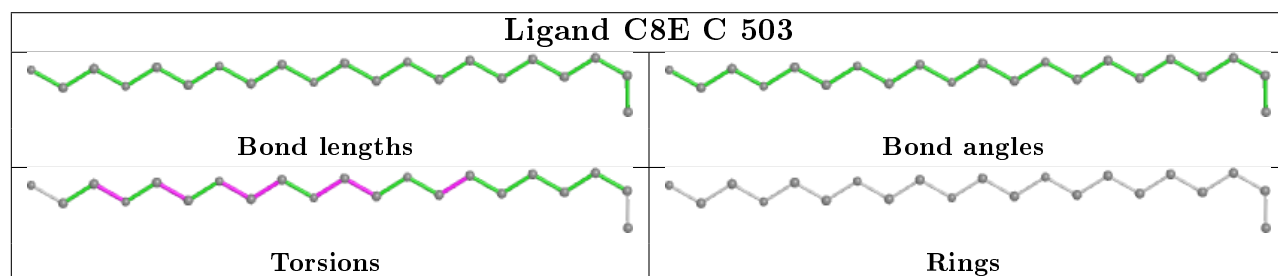
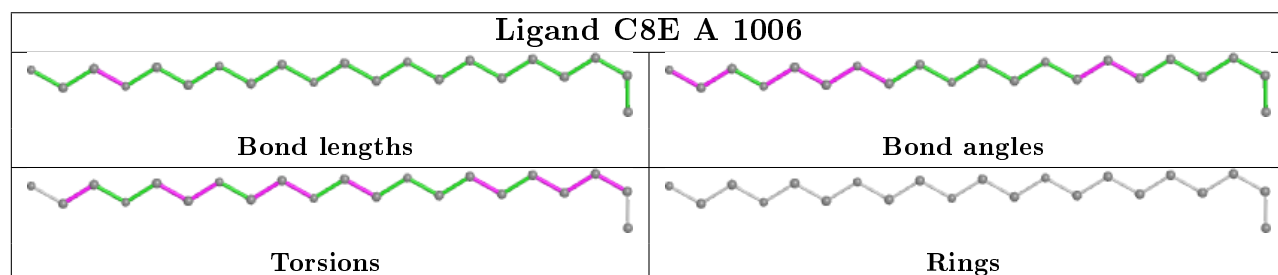
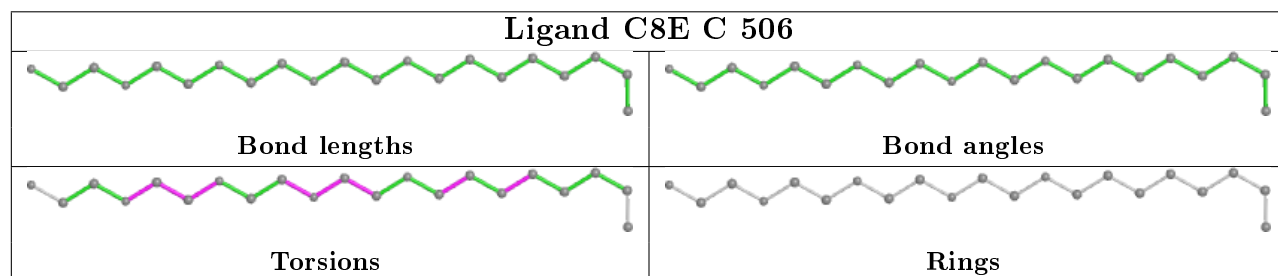
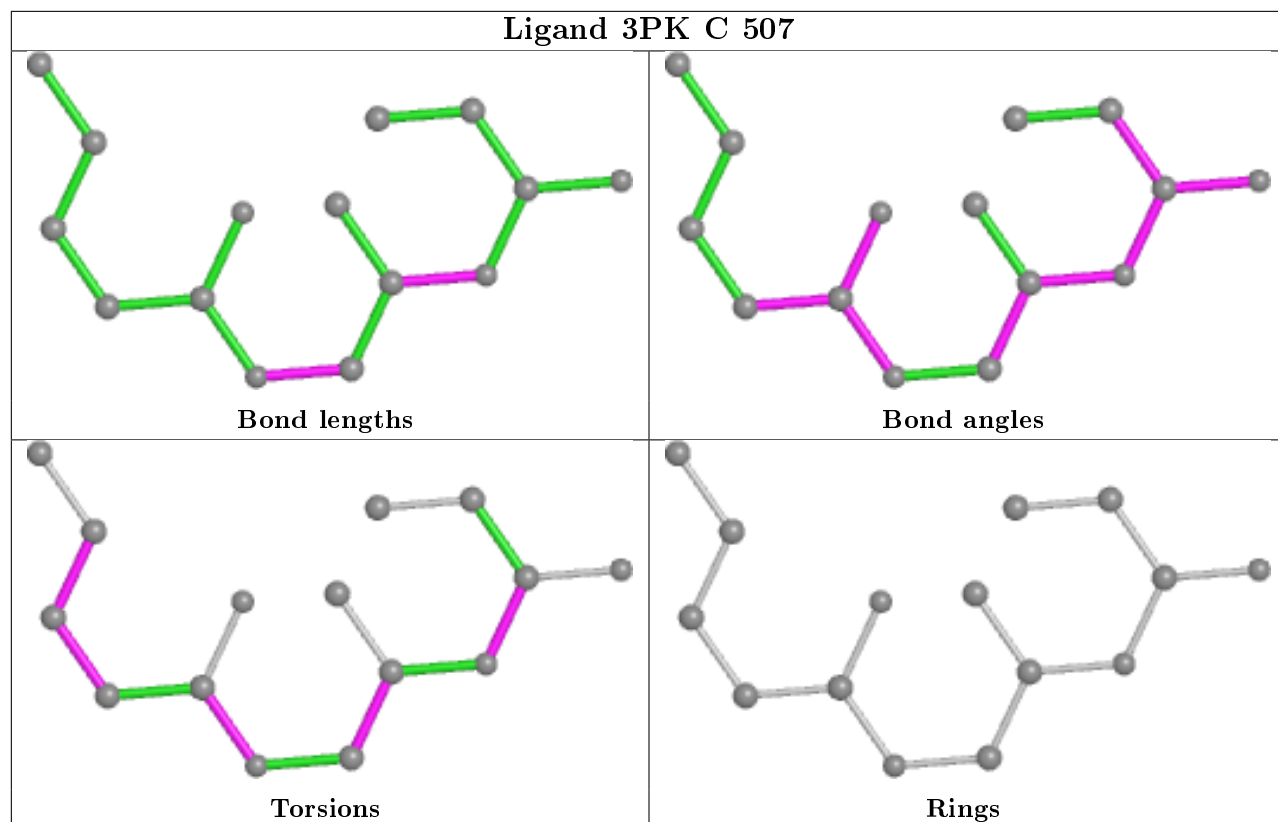


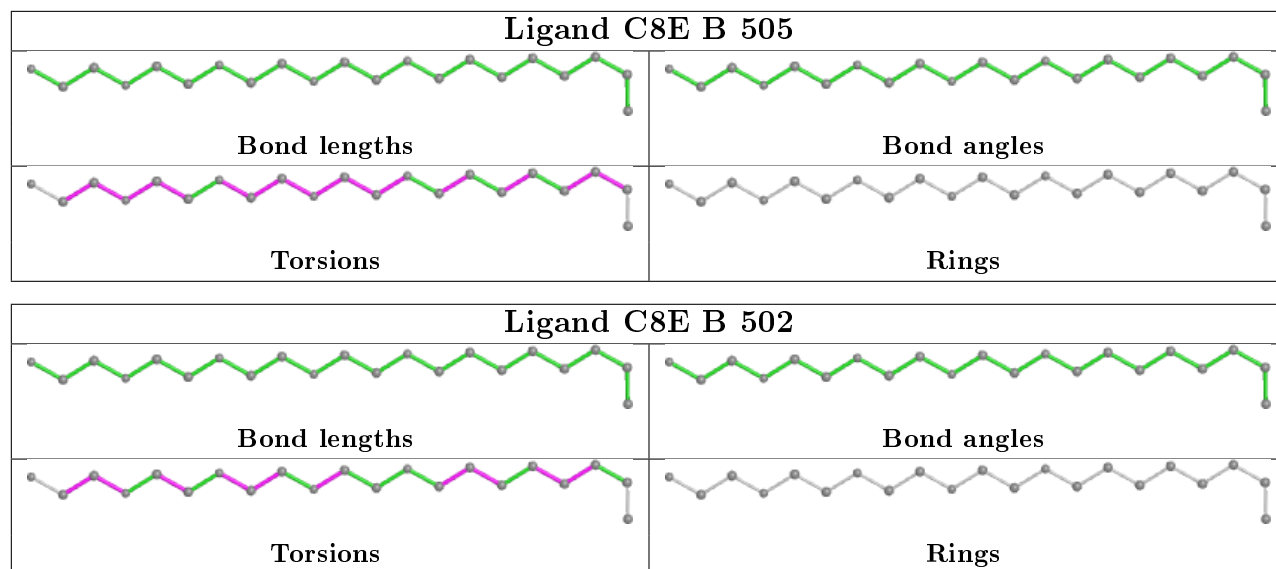












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	472/479 (98%)	0.54	7 (1%) 73 75	36, 52, 77, 101	0
1	B	473/479 (98%)	0.50	5 (1%) 80 81	37, 52, 76, 107	0
1	C	472/479 (98%)	0.55	8 (1%) 70 71	38, 52, 76, 105	0
All	All	1417/1437 (98%)	0.53	20 (1%) 75 77	36, 52, 77, 107	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	104	ARG	6.1
1	A	104	ARG	4.1
1	A	27	LYS	3.8
1	C	409	MET	3.4
1	A	29	THR	3.2
1	C	336[A]	HIS	3.2
1	B	104	ARG	3.1
1	A	11	GLU	3.0
1	C	462	GLU	3.0
1	B	16	ILE	2.6
1	A	25	TRP	2.5
1	B	412	GLN	2.4
1	B	1	CYS	2.3
1	C	1	CYS	2.3
1	C	412	GLN	2.3
1	A	118	LEU	2.2
1	B	19	LYS	2.1
1	A	8	ASN	2.0
1	C	11	GLU	2.0
1	C	465	LYS	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](#)

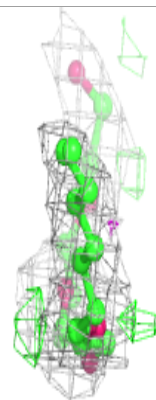
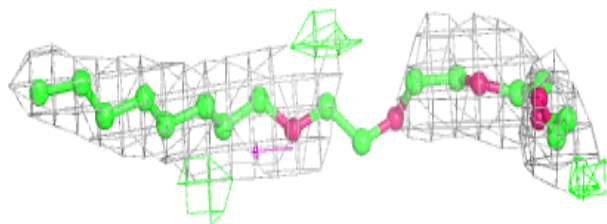
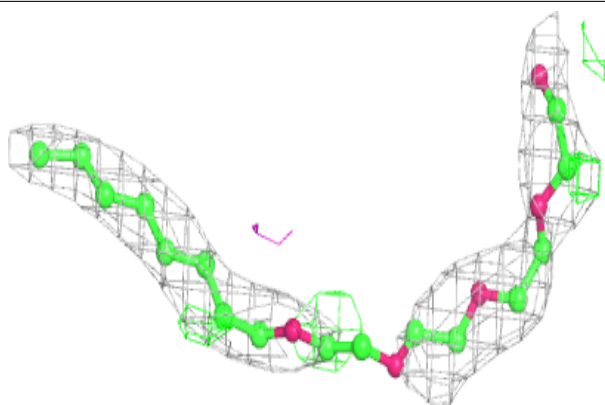
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	C8E	B	506	21/21	0.71	0.23	57,78,95,111	0
2	C8E	A	1006	21/21	0.74	0.22	57,71,87,95	0
2	C8E	C	504	21/21	0.78	0.31	46,69,98,102	0
2	C8E	C	502	21/21	0.78	0.28	51,66,94,108	0
2	C8E	B	505	21/21	0.79	0.24	57,72,93,109	0
2	C8E	A	1007	21/21	0.80	0.15	55,75,91,94	0
2	C8E	C	506	21/21	0.81	0.26	55,74,89,96	0
2	C8E	A	1005	21/21	0.81	0.29	48,68,91,92	0
2	C8E	A	1001	21/21	0.81	0.30	33,76,91,95	0
4	3PK	C	507	15/18	0.83	0.21	68,77,96,96	0
2	C8E	A	1002	21/21	0.83	0.24	44,68,84,87	0
2	C8E	C	503	21/21	0.84	0.18	58,72,84,96	0
2	C8E	A	1004	21/21	0.84	0.24	44,56,71,76	0
2	C8E	A	1009	21/21	0.85	0.23	59,66,95,105	0
2	C8E	C	505	21/21	0.85	0.37	42,80,95,110	0
2	C8E	B	502	21/21	0.85	0.34	50,66,94,100	0
2	C8E	B	503	21/21	0.86	0.34	28,64,97,111	0
4	3PK	B	507	14/18	0.88	0.27	77,85,92,101	0
2	C8E	B	504	21/21	0.89	0.24	40,61,77,78	0
4	3PK	A	1008	17/18	0.89	0.18	63,76,89,91	0
2	C8E	C	501	21/21	0.90	0.23	44,60,69,71	0
3	SO4	B	501	5/5	0.93	0.24	58,61,73,73	0
3	SO4	A	1003	5/5	0.96	0.16	55,63,73,74	0

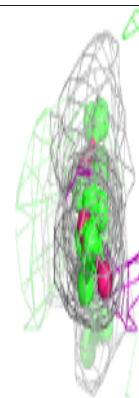
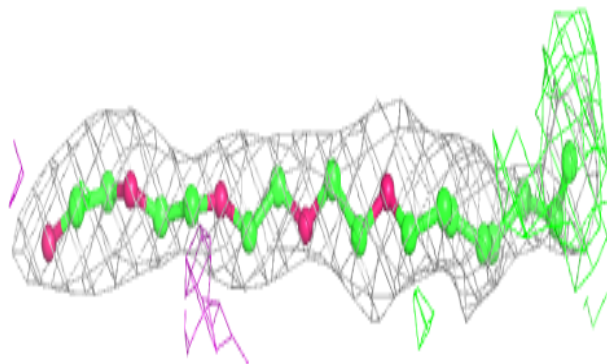
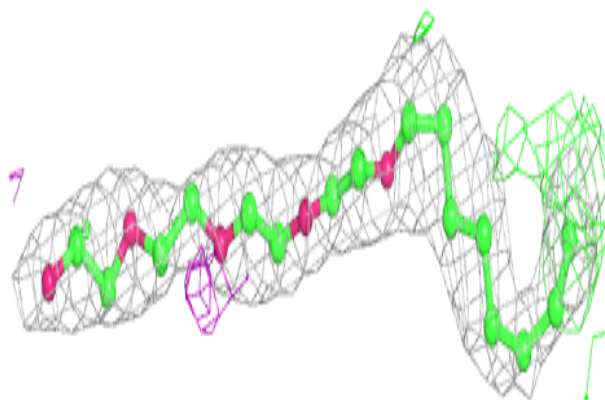
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around C8E B 506:**

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

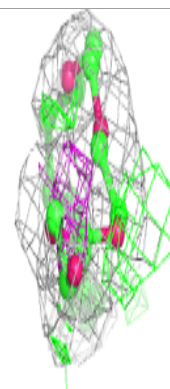
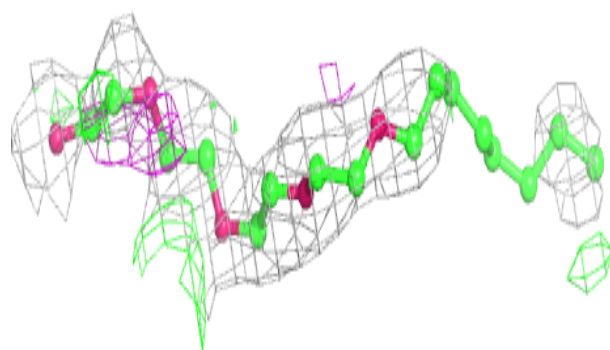
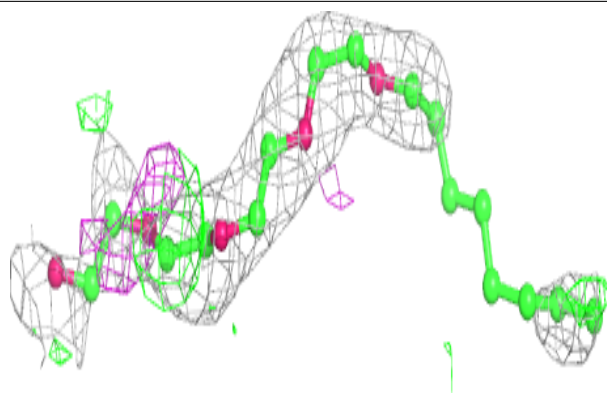
**Electron density around C8E A 1006:**

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

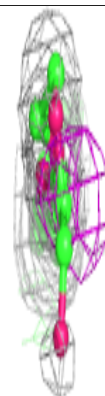
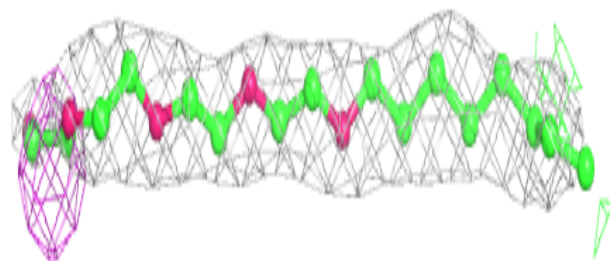
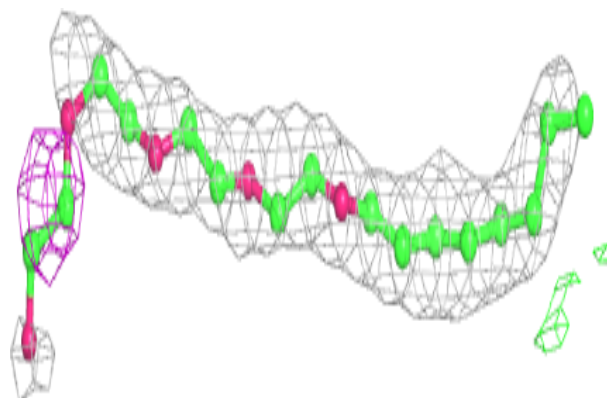


**Electron density around C8E C 504:**

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

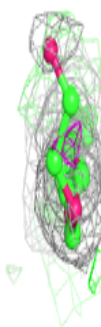
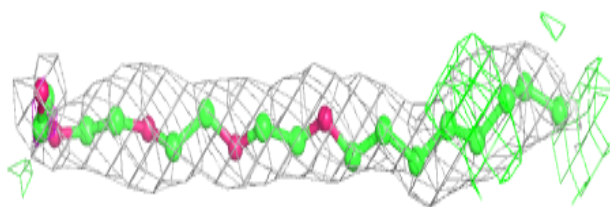
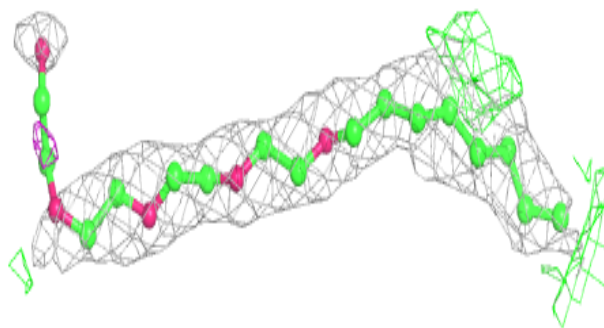
**Electron density around C8E C 502:**

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

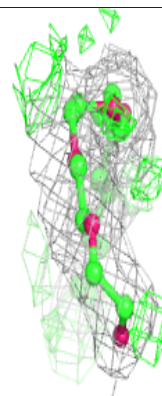
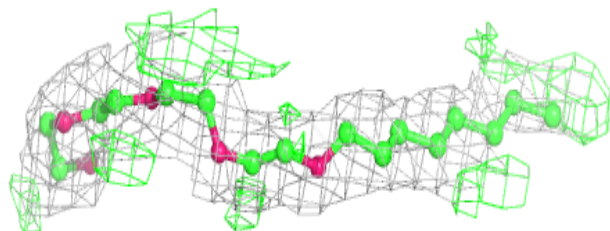
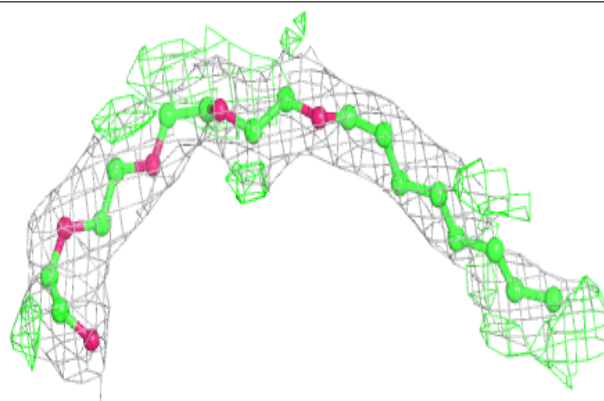


**Electron density around C8E B 505:**

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

**Electron density around C8E A 1007:**

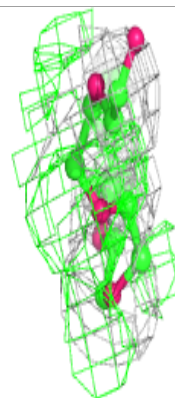
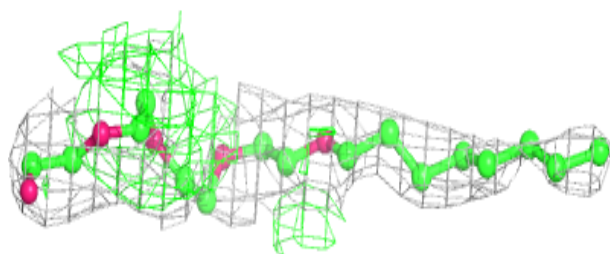
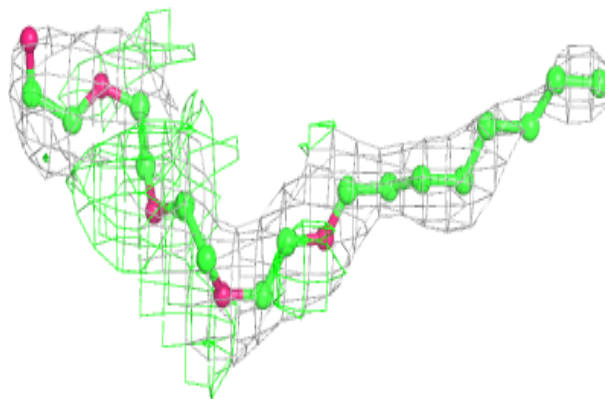
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



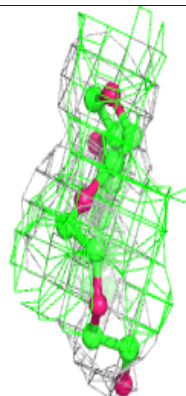
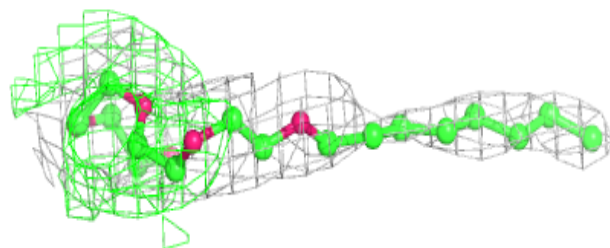
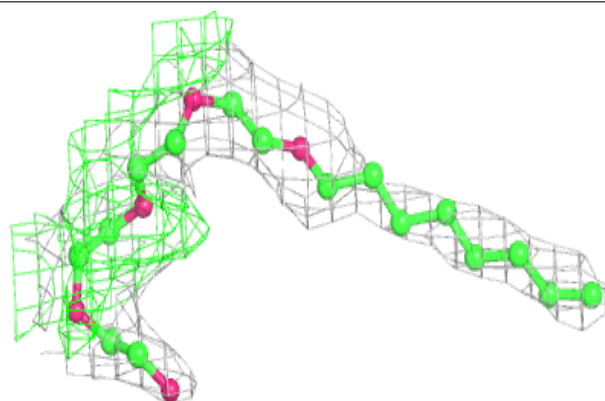


**Electron density around C8E C 506:**

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

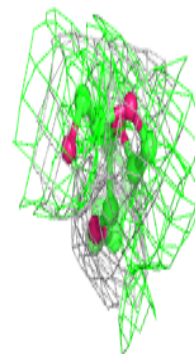
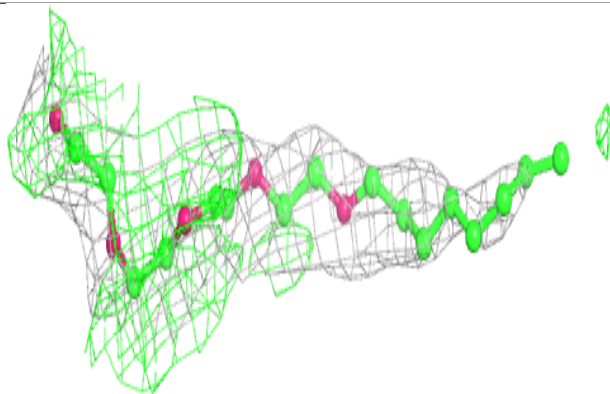
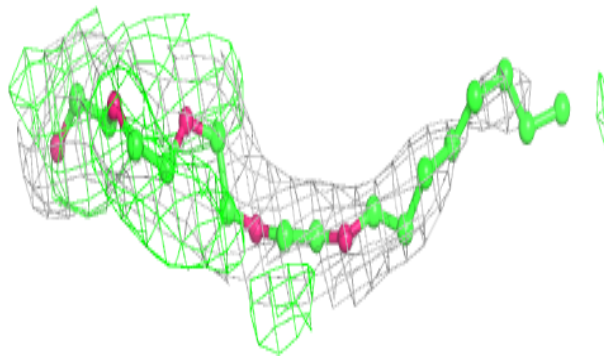
**Electron density around C8E A 1005:**

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and green (positive)

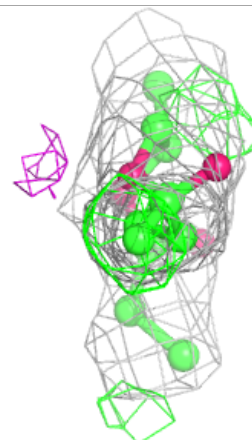
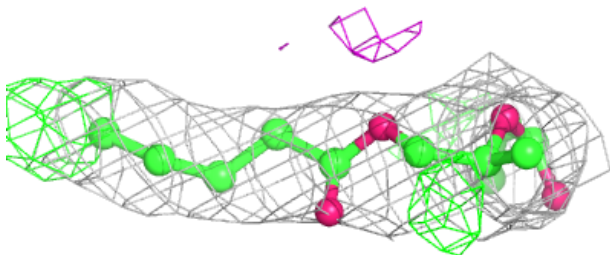
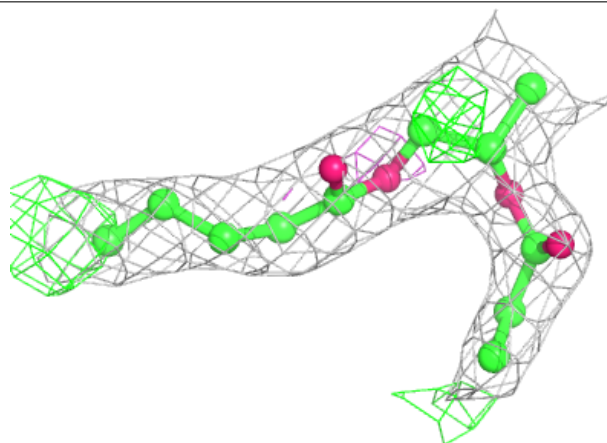


**Electron density around C8E A 1001:**

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

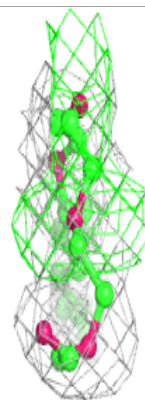
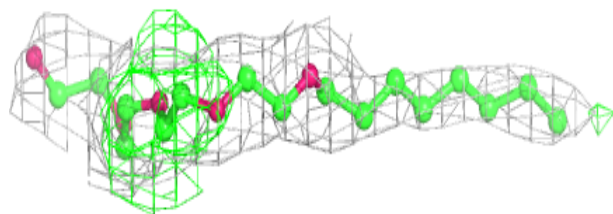
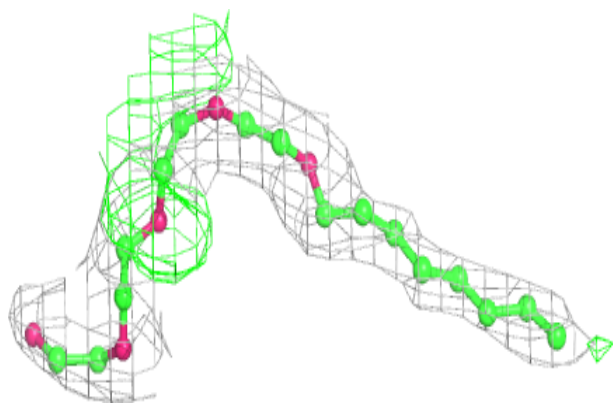
**Electron density around 3PK C 507:**

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

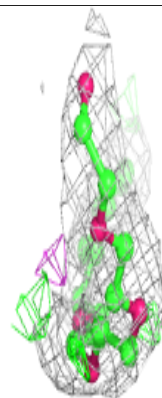
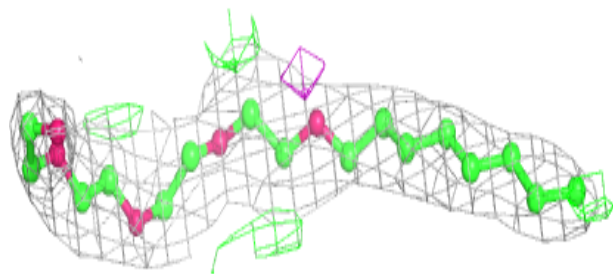
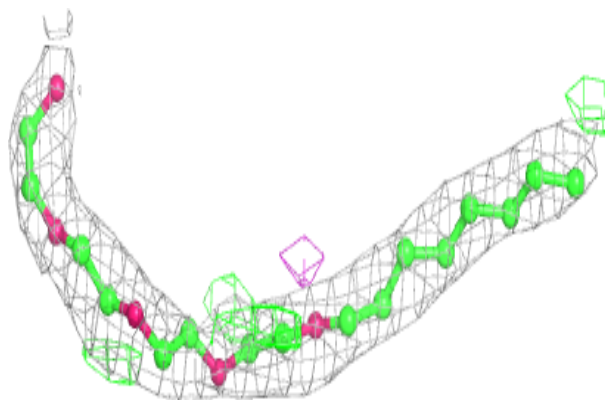


**Electron density around C8E A 1002:**

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

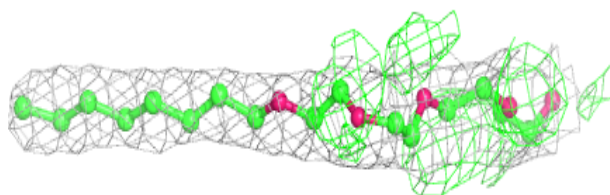
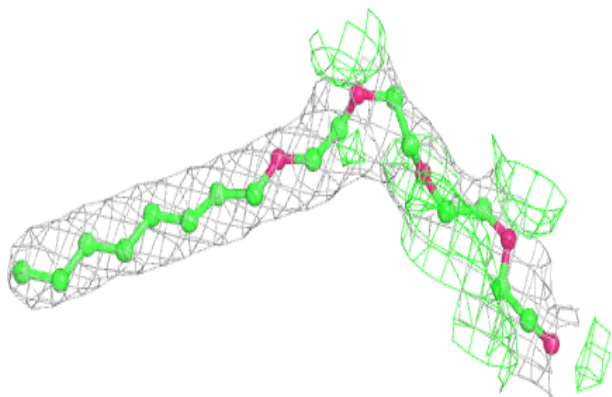
**Electron density around C8E C 503:**

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and green (positive)

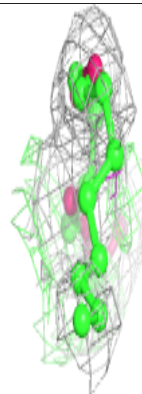
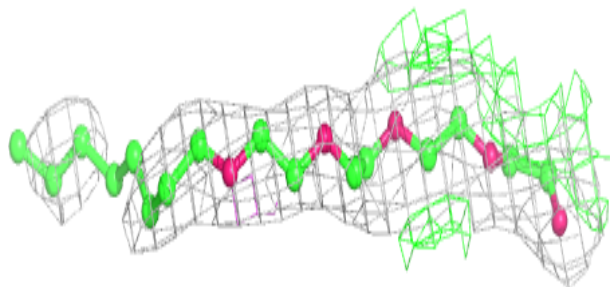
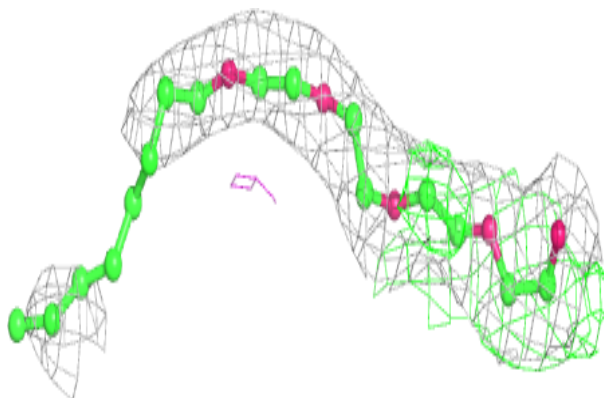


**Electron density around C8E A 1004:**

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and green (positive)

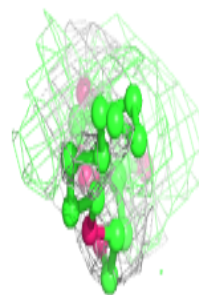
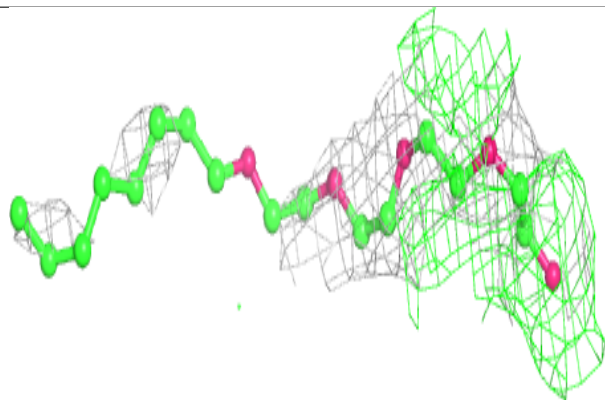
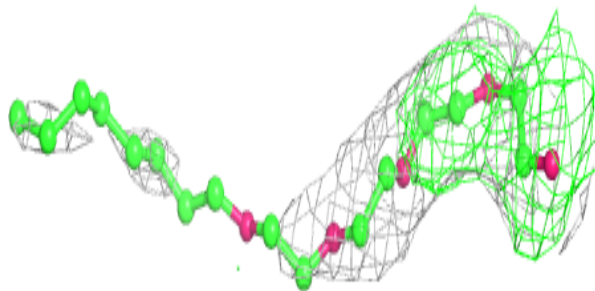
**Electron density around C8E A 1009:**

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and green (positive)

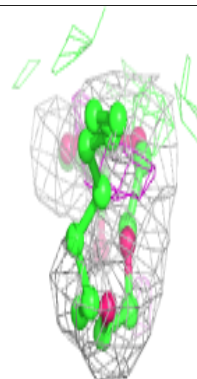
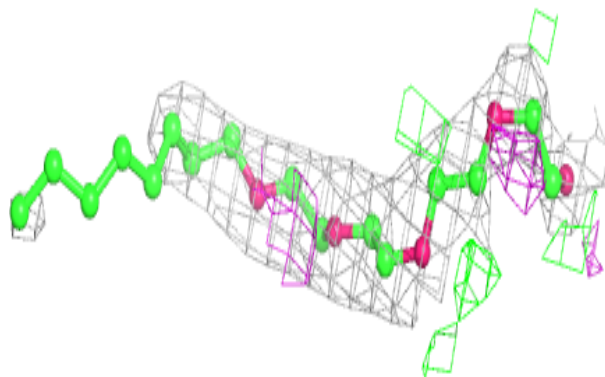
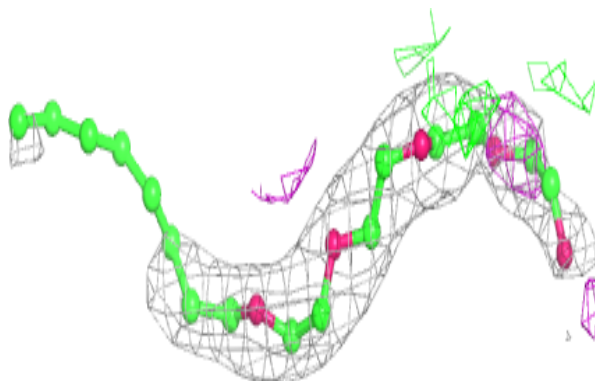


**Electron density around C8E C 505:**

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

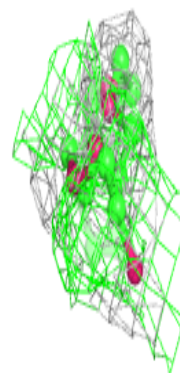
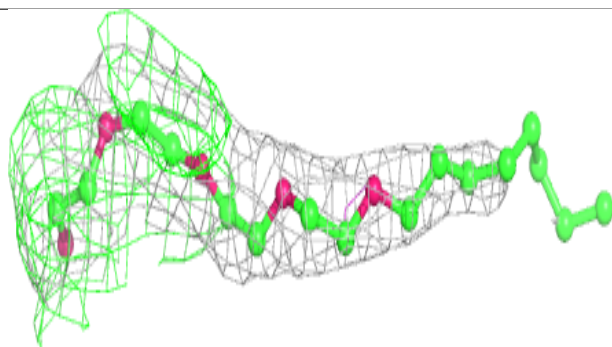
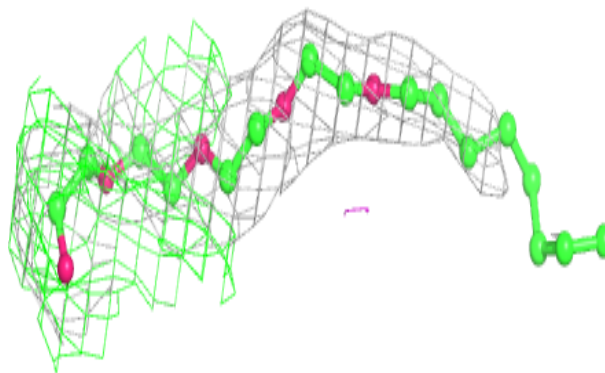
**Electron density around C8E B 502:**

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and green (positive)

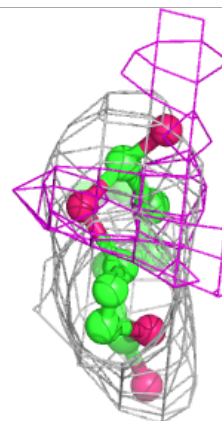
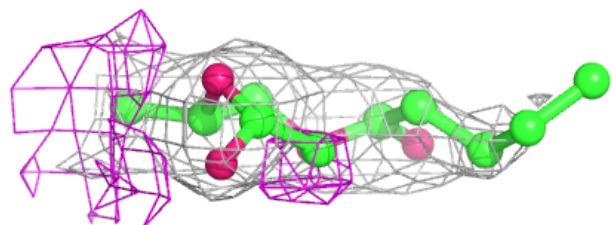
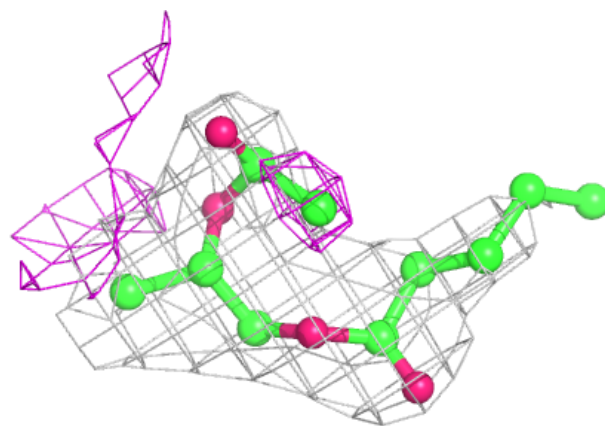


**Electron density around C8E B 503:**

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

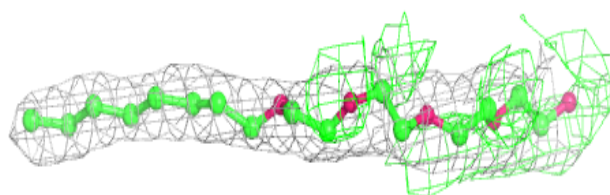
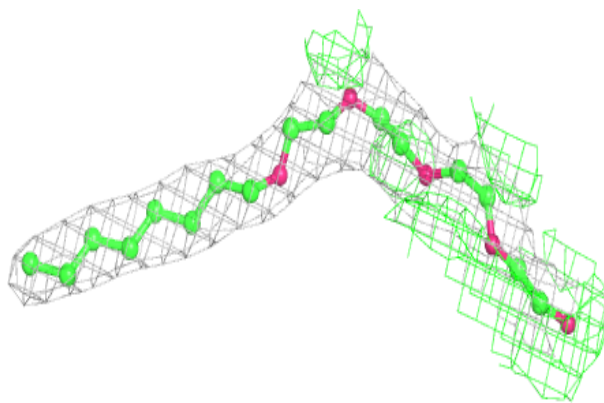
**Electron density around 3PK B 507:**

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



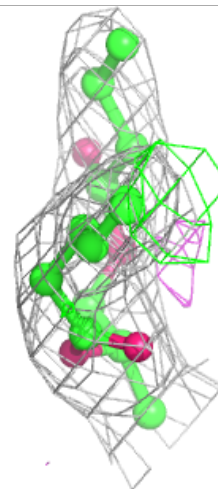
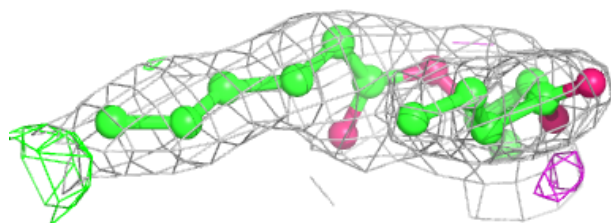
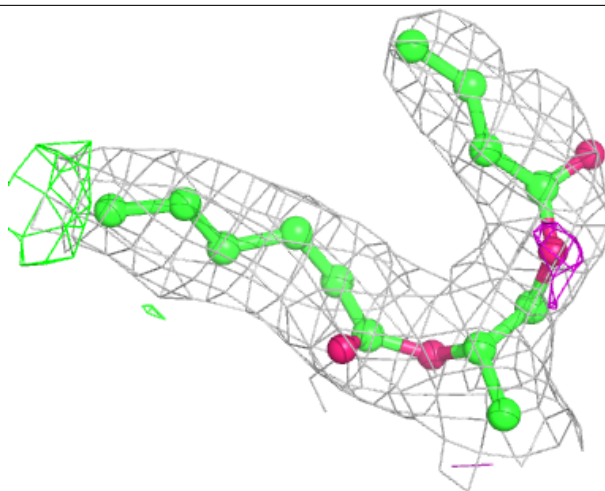
**Electron density around C8E B 504:**

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

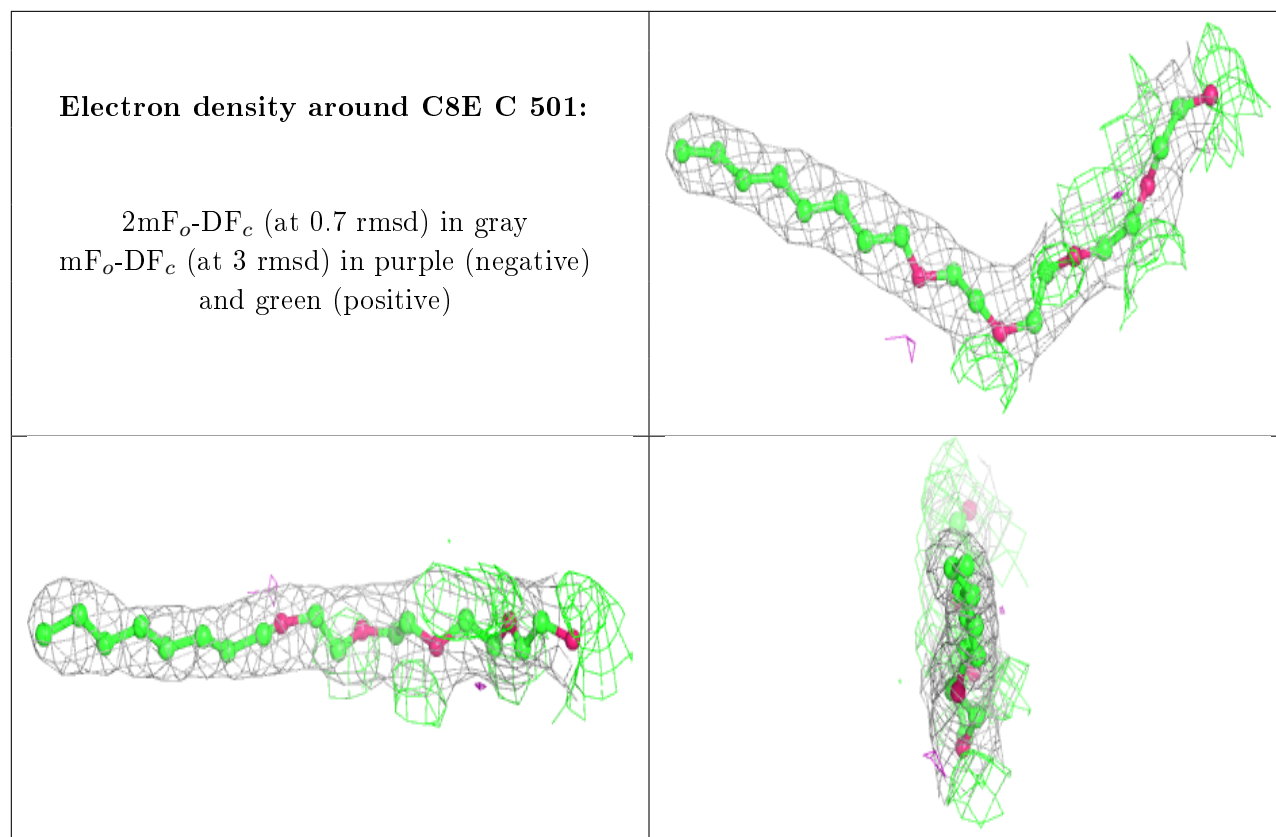


**Electron density around 3PK A 1008:**

$2mF_o-DF_c$  (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.