



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 2, 2024 – 02:43 pm GMT

PDB ID : 5DL7  
Title : Crystal structure of Acinetobacter baumannii OccAB3  
Authors : Zahn, M.; Basle, A.; van den Berg, B.  
Deposited on : 2015-09-04  
Resolution : 1.75 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.

The types of validation reports are described at

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

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

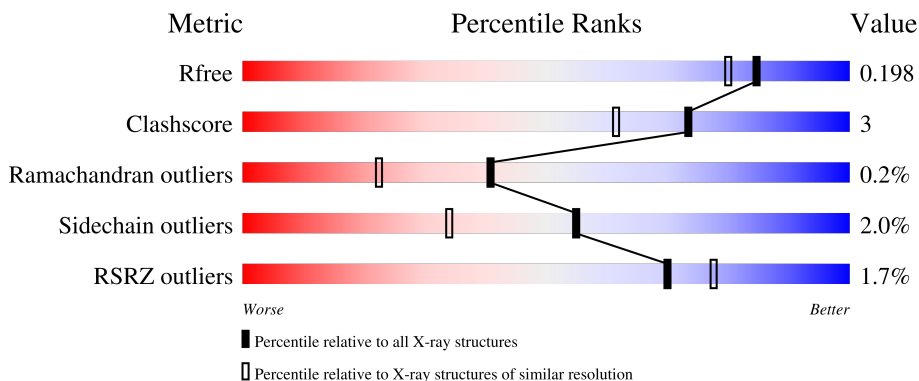
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	419	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3586 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 Porin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	402	3260	2070	559	623	8	0	0	0

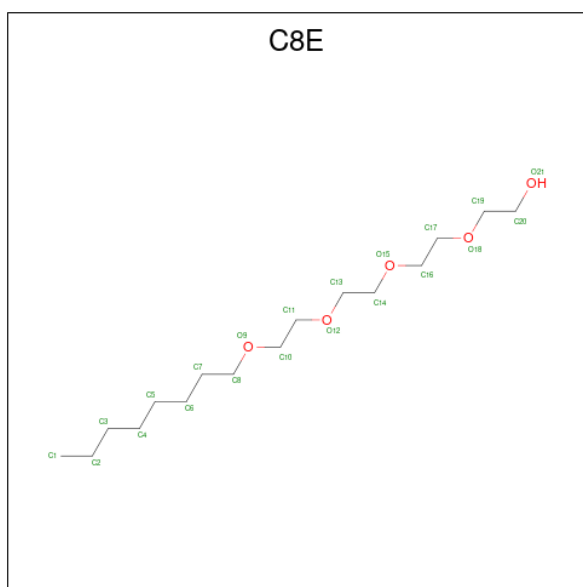
There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	ALA	-	expression tag	UNP A0A0D5YKR4
A	-13	ASN	-	expression tag	UNP A0A0D5YKR4
A	-12	VAL	-	expression tag	UNP A0A0D5YKR4
A	-11	ARG	-	expression tag	UNP A0A0D5YKR4
A	-10	LEU	-	expression tag	UNP A0A0D5YKR4
A	-9	GLN	-	expression tag	UNP A0A0D5YKR4
A	-8	HIS	-	expression tag	UNP A0A0D5YKR4
A	-7	HIS	-	expression tag	UNP A0A0D5YKR4
A	-6	HIS	-	expression tag	UNP A0A0D5YKR4
A	-5	HIS	-	expression tag	UNP A0A0D5YKR4
A	-4	HIS	-	expression tag	UNP A0A0D5YKR4
A	-3	HIS	-	expression tag	UNP A0A0D5YKR4
A	-2	HIS	-	expression tag	UNP A0A0D5YKR4
A	-1	LEU	-	expression tag	UNP A0A0D5YKR4
A	0	GLU	-	expression tag	UNP A0A0D5YKR4

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Ca	0	0
			4	4		

- Molecule 3 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
3	A	1	Total	C	O	0	0
			21	16	5		
3	A	1	Total	C	O	0	0
			21	16	5		
3	A	1	Total	C	O	0	0
			16	13	3		
3	A	1	Total	C	O	0	0
			15	12	3		
3	A	1	Total	C	O	0	0
			12	8	4		
3	A	1	Total	C	O	0	0
			10	6	4		
3	A	1	Total	C	O	0	0
			11	7	4		

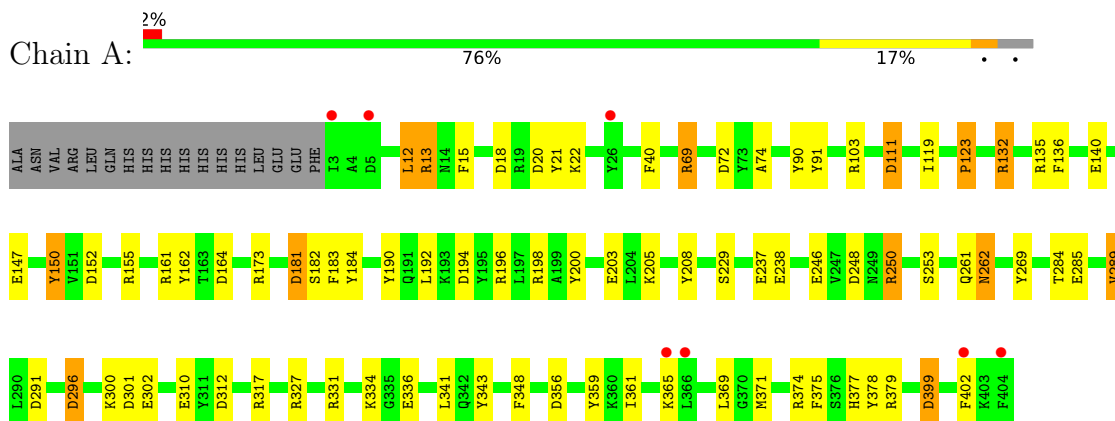
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	216	Total	O	0	0
			216	216		

### 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: Porin



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.56Å 125.72Å 137.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.14 – 1.75 70.14 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (70.14-1.75) 99.9 (70.14-1.75)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.88 (at 1.75Å)	Xtrriage
Refinement program	REFMAC 5.8.0131	Depositor
R, $R_{free}$	0.168 , 0.191 0.178 , 0.198	Depositor DCC
$R_{free}$ test set	1831 reflections (2.57%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.4	Xtrriage
Anisotropy	0.375	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 53.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3586	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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: C8E, CA

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	1.73	48/3337 (1.4%)	1.72	54/4498 (1.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111	ASP	CB-CG	12.83	1.78	1.51
1	A	150	TYR	CE1-CZ	12.56	1.54	1.38
1	A	336	GLU	CB-CG	-8.66	1.35	1.52
1	A	310	GLU	CB-CG	-8.16	1.36	1.52
1	A	269	TYR	CG-CD2	-7.83	1.28	1.39
1	A	147	GLU	CD-OE1	7.79	1.34	1.25
1	A	359	TYR	CE1-CZ	-7.76	1.28	1.38
1	A	90	TYR	CB-CG	-7.30	1.40	1.51
1	A	310	GLU	CG-CD	7.28	1.62	1.51
1	A	162	TYR	CG-CD2	-7.27	1.29	1.39
1	A	237	GLU	CG-CD	7.07	1.62	1.51
1	A	291	ASP	CG-OD1	6.98	1.41	1.25
1	A	162	TYR	CD1-CE1	-6.86	1.29	1.39
1	A	173	ARG	CZ-NH2	-6.81	1.24	1.33
1	A	111	ASP	CG-OD1	6.68	1.40	1.25
1	A	237	GLU	CD-OE2	-6.67	1.18	1.25
1	A	13	ARG	CD-NE	-6.30	1.35	1.46
1	A	123	PRO	N-CA	-6.27	1.36	1.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	91	TYR	CE2-CZ	6.21	1.46	1.38
1	A	140	GLU	CD-OE1	-6.12	1.19	1.25
1	A	375	PHE	CG-CD1	6.11	1.48	1.38
1	A	135	ARG	CZ-NH1	-6.06	1.25	1.33
1	A	181	ASP	CA-CB	-6.03	1.40	1.53
1	A	21	TYR	CE2-CZ	5.93	1.46	1.38
1	A	317	ARG	CD-NE	-5.92	1.36	1.46
1	A	181	ASP	CB-CG	-5.87	1.39	1.51
1	A	184	TYR	CB-CG	-5.87	1.42	1.51
1	A	147	GLU	CB-CG	-5.86	1.41	1.52
1	A	150	TYR	CG-CD2	5.69	1.46	1.39
1	A	237	GLU	CB-CG	-5.68	1.41	1.52
1	A	208	TYR	CE1-CZ	5.67	1.46	1.38
1	A	40	PHE	CG-CD2	-5.64	1.30	1.38
1	A	229	SER	CA-CB	5.63	1.61	1.52
1	A	203	GLU	CD-OE1	-5.58	1.19	1.25
1	A	285	GLU	CG-CD	5.41	1.60	1.51
1	A	246	GLU	CD-OE2	5.33	1.31	1.25
1	A	262	ASN	CG-ND2	-5.33	1.19	1.32
1	A	90	TYR	CE1-CZ	5.17	1.45	1.38
1	A	378	TYR	CZ-OH	5.13	1.46	1.37
1	A	136	PHE	CG-CD1	-5.12	1.31	1.38
1	A	284	THR	CB-OG1	5.12	1.53	1.43
1	A	18	ASP	CB-CG	5.09	1.62	1.51
1	A	21	TYR	CG-CD2	5.09	1.45	1.39
1	A	302	GLU	CD-OE2	5.06	1.31	1.25
1	A	402	PHE	CG-CD1	5.05	1.46	1.38
1	A	91	TYR	CB-CG	5.04	1.59	1.51
1	A	21	TYR	CB-CG	-5.03	1.44	1.51
1	A	162	TYR	CB-CG	-5.02	1.44	1.51

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	ARG	NE-CZ-NH2	30.14	135.37	120.30
1	A	13	ARG	NE-CZ-NH1	-24.75	107.92	120.30
1	A	13	ARG	CD-NE-CZ	12.01	140.41	123.60
1	A	162	TYR	CB-CG-CD1	-11.86	113.89	121.00
1	A	312	ASP	CB-CG-OD1	11.38	128.55	118.30
1	A	301	ASP	CB-CG-OD2	-11.38	108.06	118.30
1	A	173	ARG	NE-CZ-NH2	11.28	125.94	120.30
1	A	248	ASP	CB-CG-OD2	10.02	127.31	118.30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	312	ASP	CB-CG-OD2	-9.19	110.03	118.30
1	A	301	ASP	CB-CG-OD1	9.18	126.56	118.30
1	A	20	ASP	CB-CG-OD2	-8.85	110.34	118.30
1	A	399	ASP	CB-CG-OD1	8.40	125.86	118.30
1	A	285	GLU	OE1-CD-OE2	8.31	133.27	123.30
1	A	200	TYR	CB-CG-CD2	-8.23	116.06	121.00
1	A	181	ASP	CB-CG-OD2	-8.00	111.10	118.30
1	A	198	ARG	NE-CZ-NH2	7.93	124.26	120.30
1	A	296	ASP	CB-CG-OD1	7.69	125.22	118.30
1	A	150	TYR	CB-CG-CD2	-7.69	116.39	121.00
1	A	208	TYR	CB-CG-CD2	7.68	125.61	121.00
1	A	152	ASP	CB-CG-OD1	7.39	124.95	118.30
1	A	289	VAL	CG1-CB-CG2	-7.21	99.36	110.90
1	A	327	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	A	343	TYR	CB-CG-CD1	-7.11	116.74	121.00
1	A	161	ARG	NE-CZ-NH1	7.05	123.82	120.30
1	A	250	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	A	291	ASP	CB-CG-OD1	6.84	124.45	118.30
1	A	238	GLU	OE1-CD-OE2	-6.67	115.29	123.30
1	A	331	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	A	331	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	A	196	ARG	NE-CZ-NH1	-6.46	117.07	120.30
1	A	379	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	356	ASP	CB-CG-OD1	6.35	124.02	118.30
1	A	378	TYR	CB-CG-CD2	-6.25	117.25	121.00
1	A	183	PHE	CB-CG-CD2	6.13	125.09	120.80
1	A	162	TYR	CE1-CZ-OH	-6.12	103.58	120.10
1	A	194	ASP	CB-CG-OD1	5.93	123.63	118.30
1	A	194	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	A	334	LYS	CD-CE-NZ	5.85	125.15	111.70
1	A	371	MET	CA-CB-CG	5.78	123.13	113.30
1	A	348	PHE	CD1-CE1-CZ	-5.71	113.25	120.10
1	A	205	LYS	CD-CE-NZ	-5.63	98.75	111.70
1	A	152	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	A	248	ASP	CB-CG-OD1	-5.60	113.26	118.30
1	A	103	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	164	ASP	CB-CG-OD1	5.54	123.29	118.30
1	A	379	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	150	TYR	CG-CD2-CE2	5.40	125.62	121.30
1	A	155	ARG	NE-CZ-NH1	-5.39	117.60	120.30
1	A	374	ARG	NE-CZ-NH1	-5.37	117.61	120.30
1	A	147	GLU	OE1-CD-OE2	5.36	129.73	123.30

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	ASP	CB-CG-OD1	5.30	123.07	118.30
1	A	132	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	A	402	PHE	CB-CA-C	-5.19	100.02	110.40
1	A	91	TYR	CZ-CE2-CD2	-5.04	115.27	119.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	150	TYR	Sidechain
1	A	296	ASP	Sidechain
1	A	74	ALA	Mainchain

## 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	3260	0	3123	15	0
2	A	4	0	0	0	0
3	A	106	0	159	7	0
4	A	216	0	0	1	0
All	All	3586	0	3282	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 3.

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:111:ASP:CB	1:A:111:ASP:CG	1.78	1.48
3:A:505:C8E:H201	3:A:505:C8E:H161	1.53	0.88
3:A:505:C8E:H161	3:A:505:C8E:C20	2.23	0.68
1:A:13:ARG:HD2	1:A:399:ASP:CG	2.14	0.68
1:A:13:ARG:HD2	1:A:399:ASP:OD2	1.95	0.65
1:A:253:SER:HB2	1:A:289:VAL:HG12	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ARG:HD2	1:A:399:ASP:OD1	2.05	0.56
1:A:261:GLN:O	1:A:262:ASN:HB2	2.05	0.55
1:A:111:ASP:CG	1:A:111:ASP:CA	2.71	0.55
1:A:69:ARG:NH1	1:A:72:ASP:OD2	2.39	0.55
1:A:13:ARG:CD	1:A:399:ASP:OD2	2.55	0.54
1:A:361:ILE:HD12	1:A:369:LEU:HB3	1.90	0.53
3:A:505:C8E:H112	3:A:506:C8E:H102	1.95	0.48
3:A:506:C8E:H72	3:A:508:C8E:C10	2.44	0.48
3:A:505:C8E:C20	3:A:505:C8E:C16	2.91	0.47
1:A:190:TYR:CE2	1:A:192:LEU:HD21	2.51	0.44
1:A:181:ASP:O	1:A:182:SER:HB3	2.17	0.44
3:A:506:C8E:H72	3:A:508:C8E:H102	2.00	0.43
3:A:506:C8E:H191	4:A:777:HOH:O	2.18	0.43
1:A:22:LYS:NZ	1:A:377:HIS:HE1	2.16	0.43
1:A:12:LEU:CD1	1:A:12:LEU:N	2.83	0.42
1:A:300:LYS:HD2	1:A:341:LEU:HD21	2.03	0.41

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	400/419 (96%)	386 (96%)	13 (3%)	1 (0%)	41 22

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	ILE

### 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	347/363 (96%)	340 (98%)	7 (2%)	55 34

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	15	PHE
1	A	69	ARG
1	A	123	PRO
1	A	132	ARG
1	A	250	ARG
1	A	365	LYS

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

Mol	Chain	Res	Type
1	A	315	ASN
1	A	377	HIS

### 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

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	A	508	-	14,14,20	0.89	1 (7%)	13,13,19	1.57	2 (15%)
3	C8E	A	505	-	20,20,20	0.88	0	19,19,19	2.19	6 (31%)
3	C8E	A	509	-	11,11,20	0.94	0	10,10,19	1.97	5 (50%)
3	C8E	A	511	-	10,10,20	0.92	0	9,9,19	0.80	0
3	C8E	A	510	-	9,9,20	0.64	0	8,8,19	0.80	0
3	C8E	A	506	-	20,20,20	0.72	0	19,19,19	1.34	3 (15%)
3	C8E	A	507	-	15,15,20	0.73	0	14,14,19	0.97	1 (7%)

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	A	508	-	-	5/12/12/18	-
3	C8E	A	505	-	-	8/18/18/18	-
3	C8E	A	509	-	-	1/9/9/18	-
3	C8E	A	511	-	-	0/8/8/18	-
3	C8E	A	510	-	-	4/7/7/18	-
3	C8E	A	506	-	-	4/18/18/18	-
3	C8E	A	507	-	-	5/13/13/18	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	508	C8E	O12-C13	2.03	1.50	1.42

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	505	C8E	C10-O9-C8	5.59	137.51	113.29
3	A	505	C8E	O9-C8-C7	-5.08	83.54	110.26
3	A	508	C8E	C13-O12-C11	-3.45	98.33	113.29
3	A	508	C8E	O12-C13-C14	3.43	125.12	110.07
3	A	509	C8E	C16-O15-C14	3.22	127.26	113.29
3	A	506	C8E	O18-C17-C16	3.15	124.60	110.39
3	A	509	C8E	O18-C17-C16	-3.06	96.58	110.39
3	A	505	C8E	O18-C17-C16	2.96	123.73	110.39
3	A	506	C8E	C13-O12-C11	2.84	125.60	113.29
3	A	505	C8E	O9-C10-C11	-2.67	98.34	110.39
3	A	507	C8E	C10-O9-C8	2.42	123.77	113.29
3	A	509	C8E	O18-C19-C20	-2.40	99.53	110.07
3	A	505	C8E	O12-C11-C10	2.31	120.80	110.39
3	A	509	C8E	O12-C13-C14	2.23	120.44	110.39
3	A	505	C8E	O21-C20-C19	2.10	123.98	111.81
3	A	509	C8E	C11-O12-C13	2.05	120.24	112.90
3	A	506	C8E	O18-C19-C20	2.03	118.99	110.07

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	505	C8E	O12-C13-C14-O15
3	A	505	C8E	C20-C19-O18-C17
3	A	505	C8E	O15-C16-C17-O18
3	A	508	C8E	C2-C3-C4-C5
3	A	508	C8E	C6-C7-C8-O9
3	A	506	C8E	O15-C16-C17-O18
3	A	508	C8E	C4-C5-C6-C7
3	A	505	C8E	O18-C19-C20-O21
3	A	508	C8E	O12-C13-C14-O15
3	A	510	C8E	O18-C19-C20-O21
3	A	507	C8E	C13-C14-O15-C16
3	A	505	C8E	C16-C17-O18-C19
3	A	507	C8E	C3-C4-C5-C6
3	A	506	C8E	C1-C2-C3-C4
3	A	507	C8E	O9-C10-C11-O12
3	A	505	C8E	C11-C10-O9-C8
3	A	507	C8E	C4-C5-C6-C7
3	A	505	C8E	C10-C11-O12-C13
3	A	510	C8E	C17-C16-O15-C14
3	A	506	C8E	O9-C10-C11-O12
3	A	506	C8E	O12-C13-C14-O15

*Continued on next page...*

Continued from previous page...

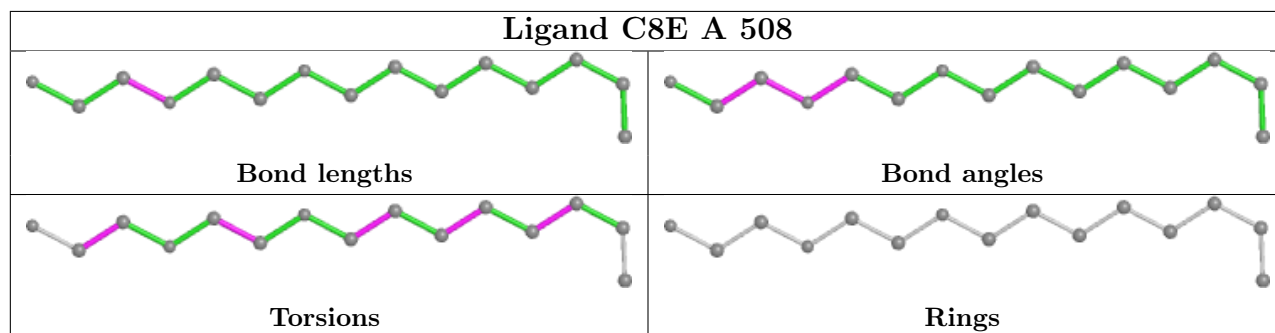
Mol	Chain	Res	Type	Atoms
3	A	510	C8E	C16-C17-O18-C19
3	A	507	C8E	O12-C13-C14-O15
3	A	510	C8E	O15-C16-C17-O18
3	A	505	C8E	O9-C10-C11-O12
3	A	508	C8E	O9-C10-C11-O12
3	A	509	C8E	C10-C11-O12-C13

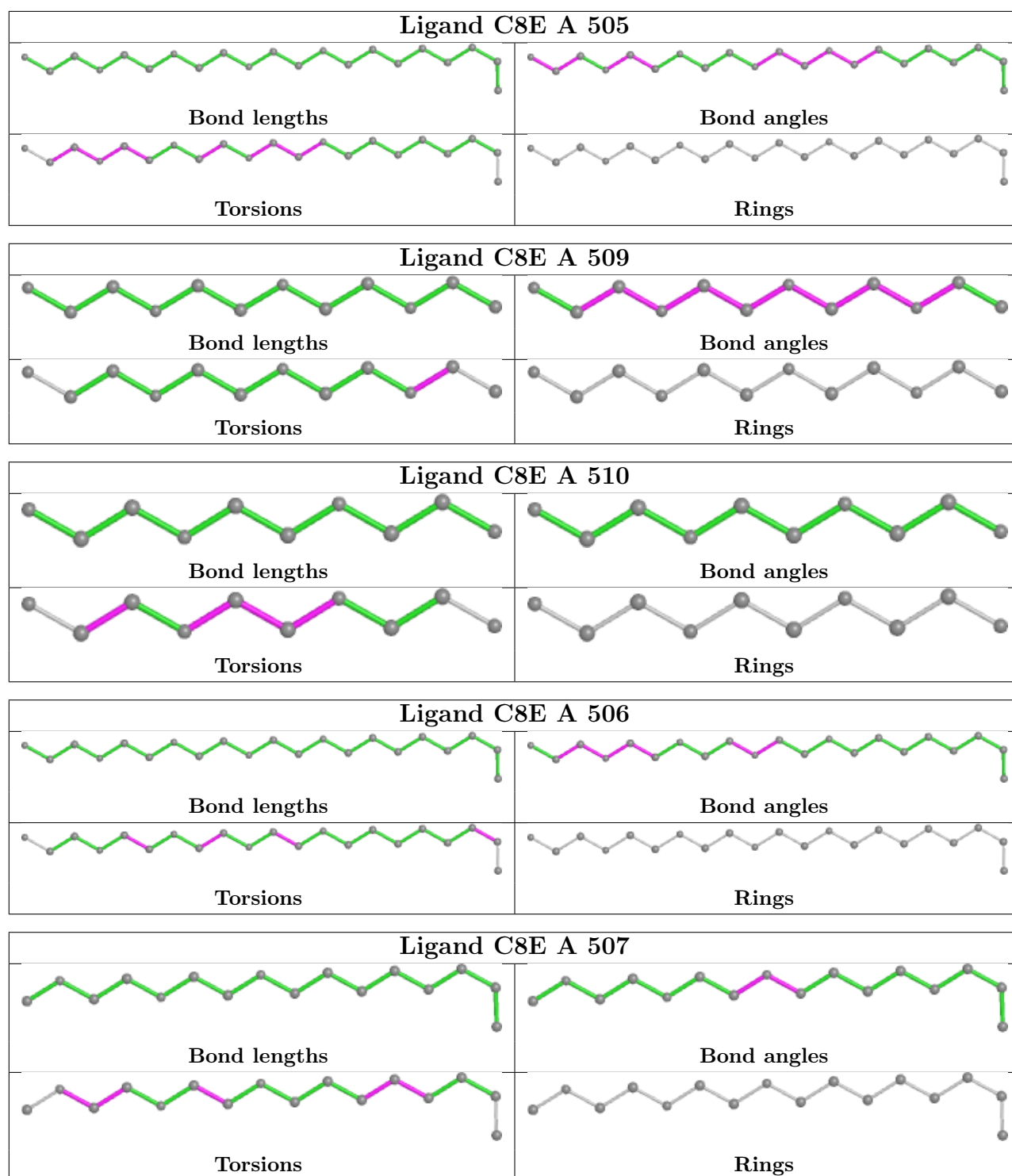
There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	508	C8E	2	0
3	A	505	C8E	4	0
3	A	506	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

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	402/419 (95%)	-0.07	7 (1%) 70 77	18, 30, 58, 82	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	402	PHE	4.3
1	A	3	ILE	3.7
1	A	404	PHE	3.0
1	A	365	LYS	2.9
1	A	5	ASP	2.7
1	A	26	TYR	2.3
1	A	366	LEU	2.3

### 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.

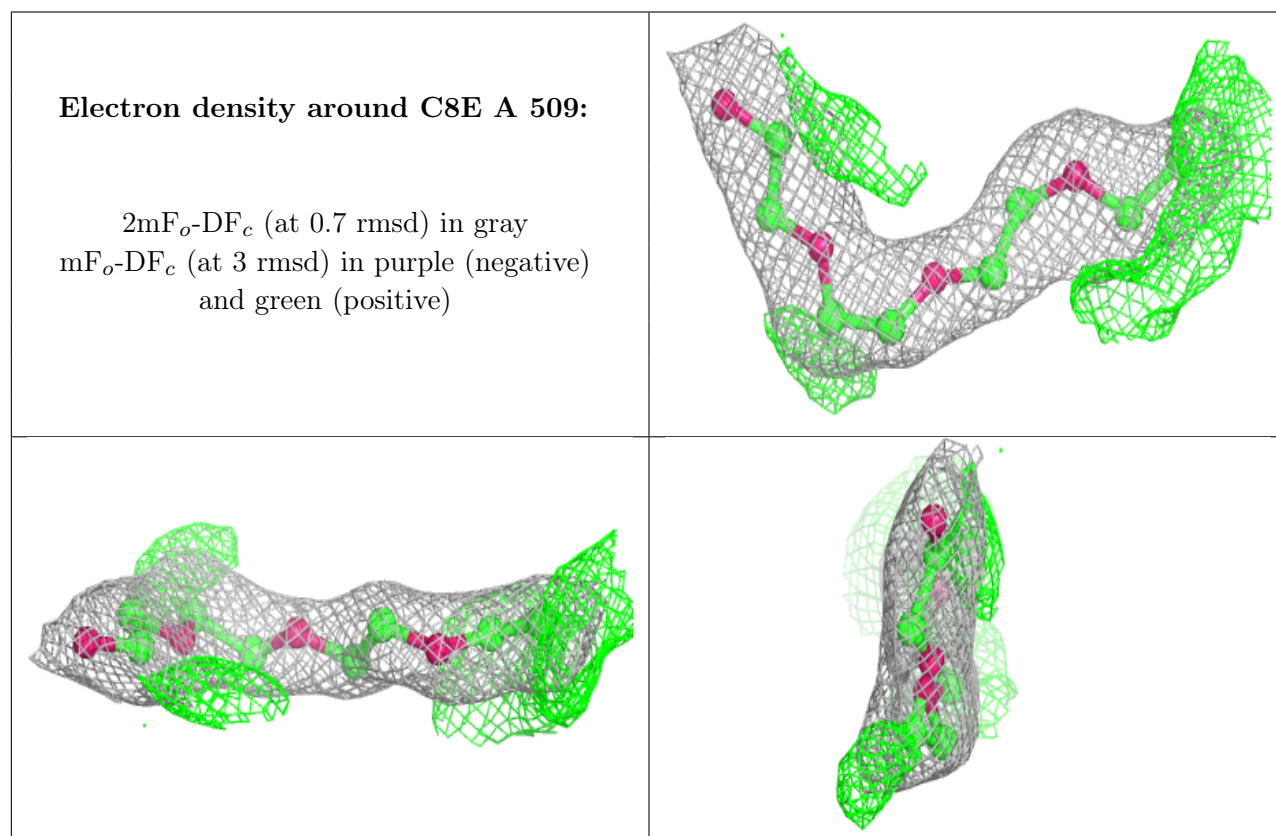
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	C8E	A	509	12/21	0.84	0.11	43,52,64,67	0

*Continued on next page...*

Continued from previous page...

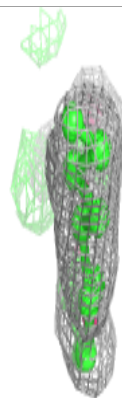
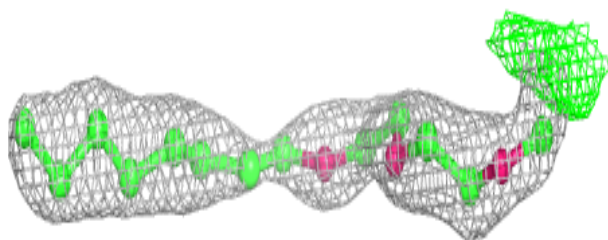
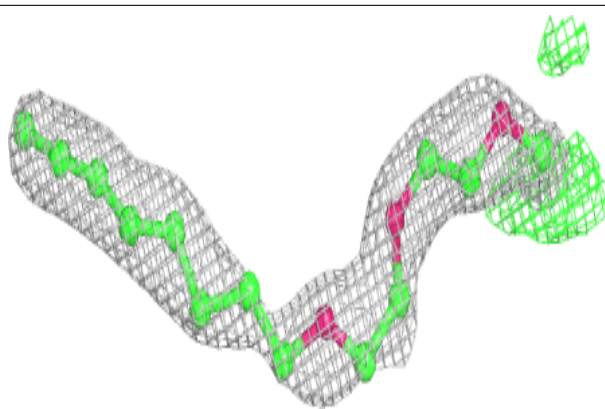
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	C8E	A	507	16/21	0.87	0.22	39,53,63,63	0
3	C8E	A	510	10/21	0.87	0.13	49,56,63,64	0
3	C8E	A	505	21/21	0.89	0.15	29,44,56,63	0
3	C8E	A	508	15/21	0.89	0.24	40,52,66,69	0
3	C8E	A	506	21/21	0.91	0.12	32,40,61,73	0
2	CA	A	504	1/1	0.92	0.08	54,54,54,54	0
3	C8E	A	511	11/21	0.93	0.13	30,42,46,48	0
2	CA	A	502	1/1	0.97	0.09	52,52,52,52	0
2	CA	A	503	1/1	0.98	0.07	35,35,35,35	0
2	CA	A	501	1/1	1.00	0.10	23,23,23,23	0

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

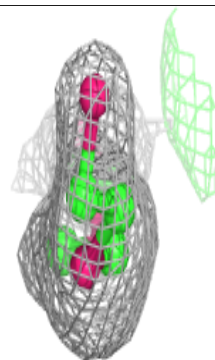
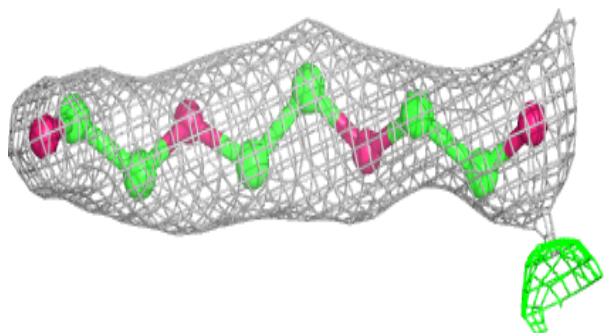
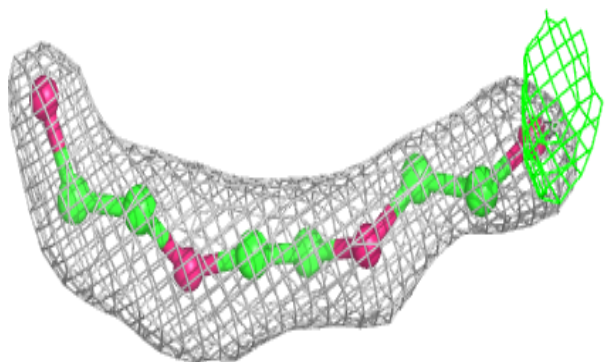


**Electron density around C8E A 507:**

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

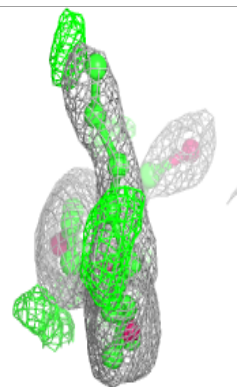
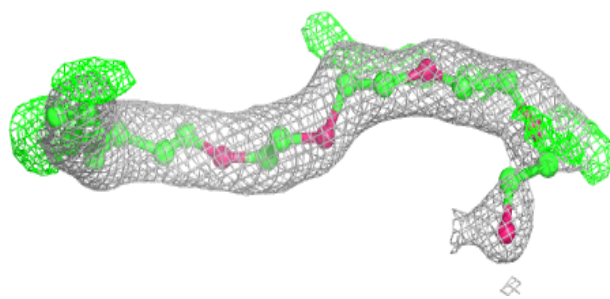
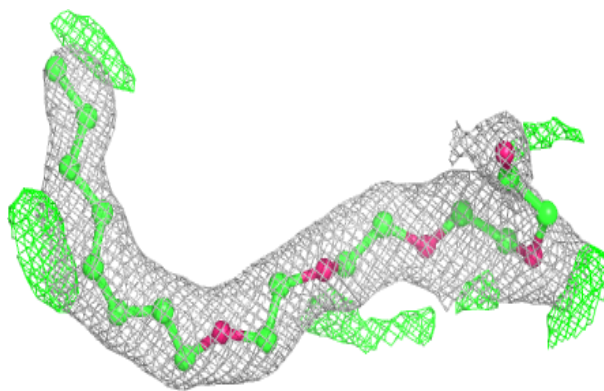
**Electron density around C8E A 510:**

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



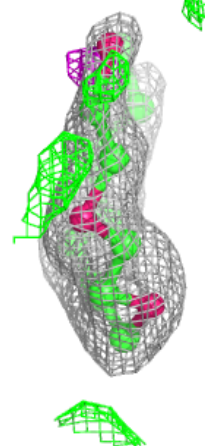
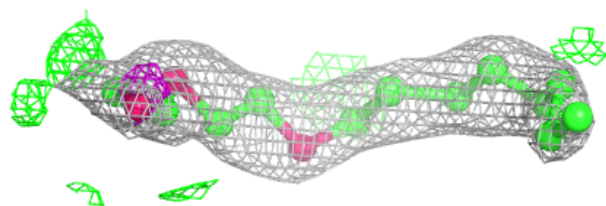
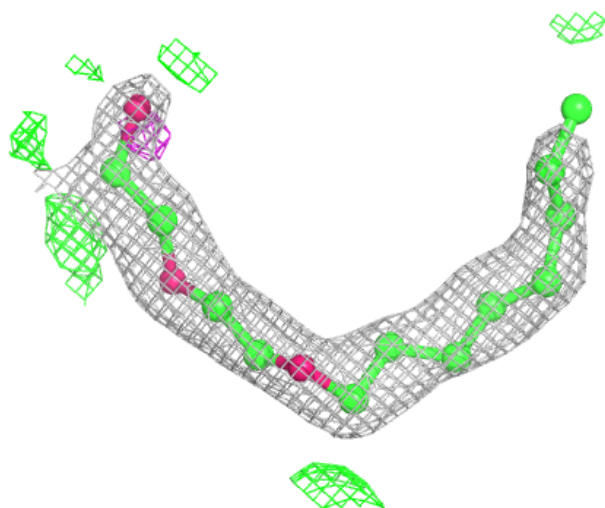
**Electron density around C8E A 505:**

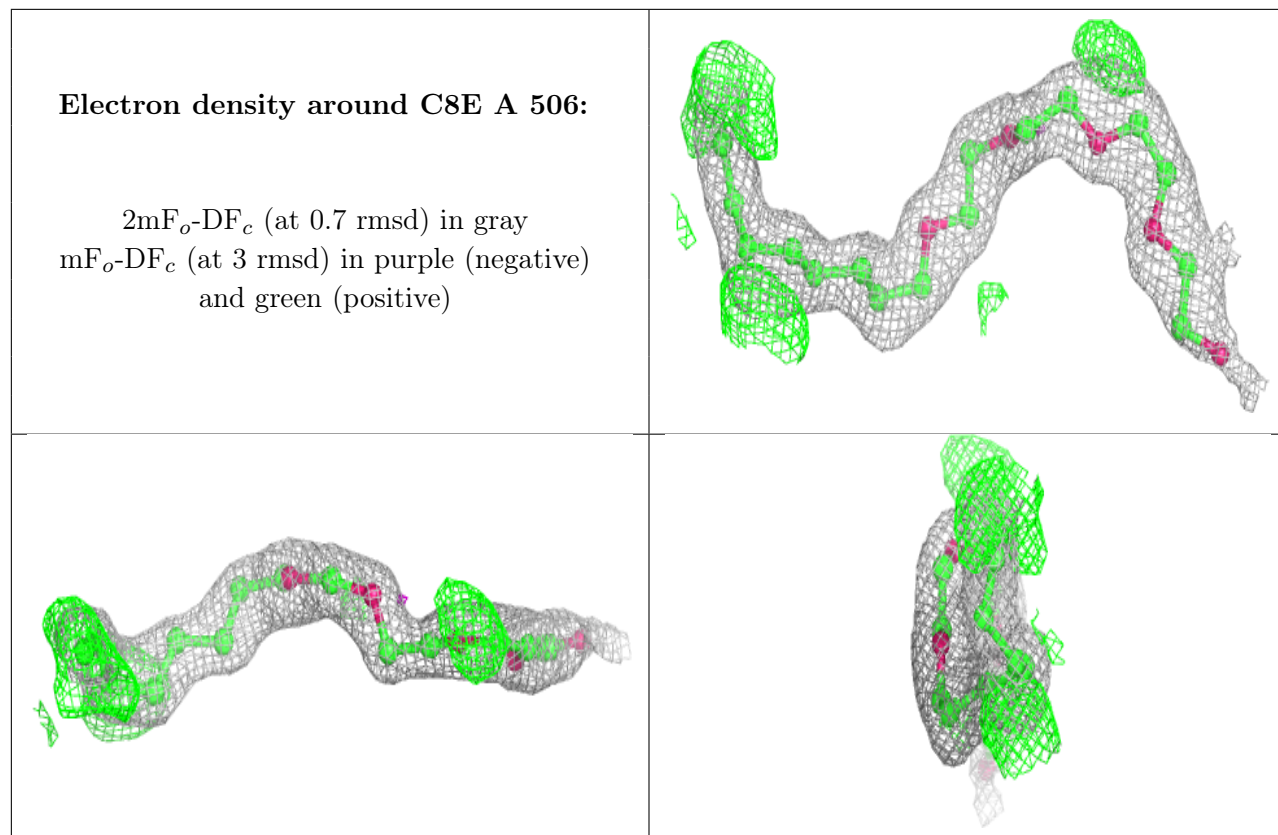
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around C8E A 508:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.