



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 25, 2024 – 07:09 PM EST

PDB ID : 5O65  
Title : Crystal Structure of the Pseudomonas functional amyloid secretion protein FapF  
Authors : Rouse, S.L.; Hare, S.; Lambert, S.; Morgan, R.M.L.; Hawthorne, W.J.; Berry, J.; Matthews, S.J.  
Deposited on : 2017-06-05  
Resolution : 2.50 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>.

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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 : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.21  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.004 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.40

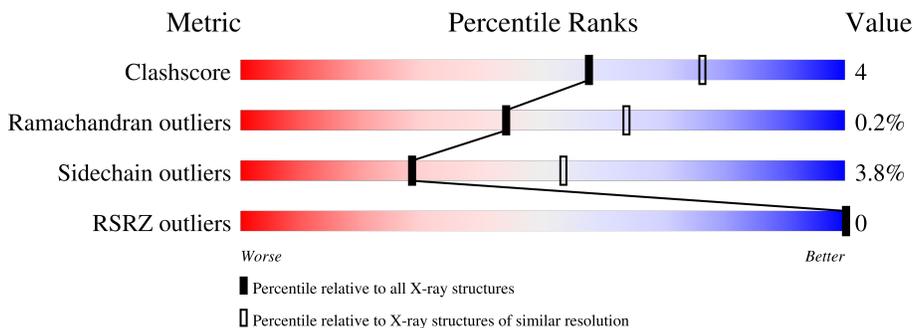
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	334	72% (green), 9% (yellow), 17% (grey)
1	B	334	78% (green), 8% (yellow), 11% (grey)
1	C	334	75% (green), 8% (yellow), 17% (grey)

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7008 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 FapF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	276	2144	1369	348	421	6	0	0	0
1	B	296	2278	1444	375	453	6	0	0	0
1	C	278	2158	1377	353	422	6	0	0	0

There are 33 discrepancies between the modelled and reference sequences:

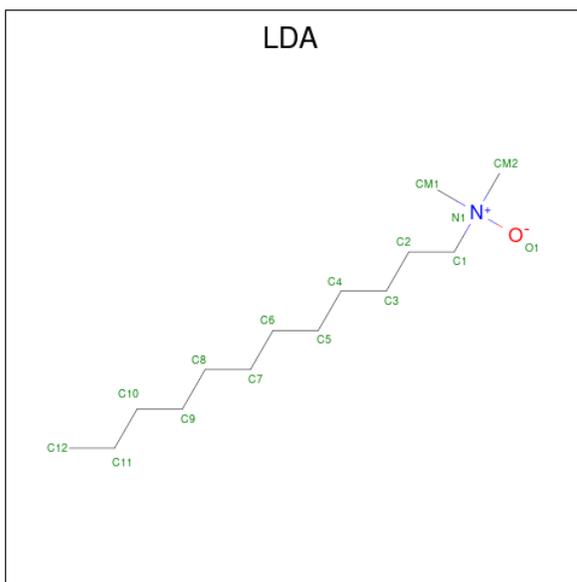
Chain	Residue	Modelled	Actual	Comment	Reference
A	73	THR	-	expression tag	UNP C4IN73
A	74	SER	-	expression tag	UNP C4IN73
A	75	HIS	-	expression tag	UNP C4IN73
A	76	HIS	-	expression tag	UNP C4IN73
A	77	HIS	-	expression tag	UNP C4IN73
A	78	HIS	-	expression tag	UNP C4IN73
A	79	HIS	-	expression tag	UNP C4IN73
A	80	HIS	-	expression tag	UNP C4IN73
A	81	GLY	-	expression tag	UNP C4IN73
A	82	THR	-	expression tag	UNP C4IN73
A	273	MSE	LEU	engineered mutation	UNP C4IN73
B	73	THR	-	expression tag	UNP C4IN73
B	74	SER	-	expression tag	UNP C4IN73
B	75	HIS	-	expression tag	UNP C4IN73
B	76	HIS	-	expression tag	UNP C4IN73
B	77	HIS	-	expression tag	UNP C4IN73
B	78	HIS	-	expression tag	UNP C4IN73
B	79	HIS	-	expression tag	UNP C4IN73
B	80	HIS	-	expression tag	UNP C4IN73
B	81	GLY	-	expression tag	UNP C4IN73
B	82	THR	-	expression tag	UNP C4IN73
B	273	MSE	LEU	engineered mutation	UNP C4IN73
C	73	THR	-	expression tag	UNP C4IN73

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Chain	Residue	Modelled	Actual	Comment	Reference
C	74	SER	-	expression tag	UNP C4IN73
C	75	HIS	-	expression tag	UNP C4IN73
C	76	HIS	-	expression tag	UNP C4IN73
C	77	HIS	-	expression tag	UNP C4IN73
C	78	HIS	-	expression tag	UNP C4IN73
C	79	HIS	-	expression tag	UNP C4IN73
C	80	HIS	-	expression tag	UNP C4IN73
C	81	GLY	-	expression tag	UNP C4IN73
C	82	THR	-	expression tag	UNP C4IN73
C	273	MSE	LEU	engineered mutation	UNP C4IN73

- Molecule 2 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:  $C_{14}H_{31}NO$ ).



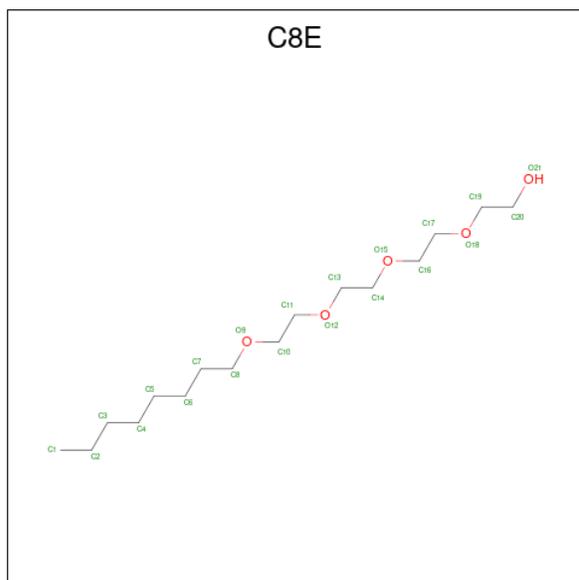
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	A	1	Total	C	N	O	0	0
			16	14	1	1		
2	B	1	Total	C			0	0
			12	12				
2	B	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		
2	C	1	Total	C	N	O	0	0
			16	14	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			16	14	1	1		

- 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
			14	12	2		
3	C	1	Total	C	O	0	0
			14	12	2		
3	C	1	Total	C	O	0	0
			11	10	1		
3	C	1	Total	C		0	0
			7	7			
3	C	1	Total	C	O	0	0
			21	16	5		
3	C	1	Total	C	O	0	0
			21	16	5		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 5 is water.

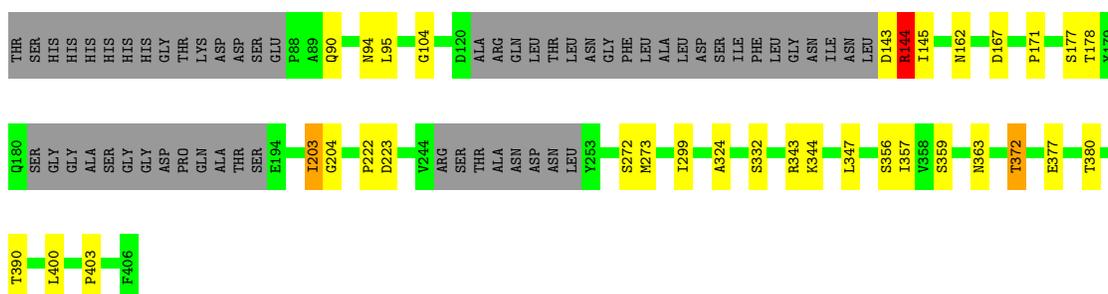
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	A	73	Total 73	O 73	0	0
5	B	71	Total 71	O 71	0	0
5	C	85	Total 85	O 85	0	0

### 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. 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. 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: FapF

Chain A: 



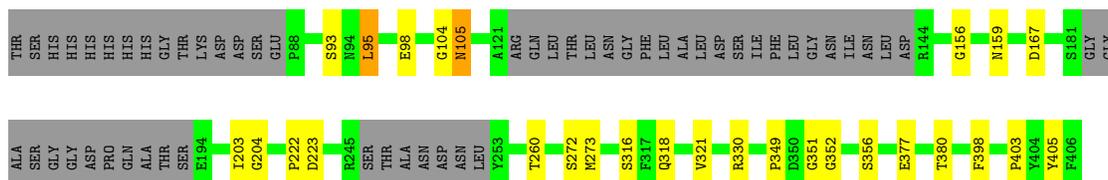
- Molecule 1: FapF

Chain B: 



- Molecule 1: FapF

Chain C: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.26Å 124.73Å 80.36Å 90.00° 96.29° 90.00°	Depositor
Resolution (Å)	2.64 – 2.50 2.64 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (2.64-2.50) 15.1 (2.64-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.8.0107	Depositor
R, $R_{free}$	0.222 , 0.259 0.234 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.8	Xtrriage
Anisotropy	0.155	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.00 , 0.0	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	0.61	EDS
Total number of atoms	7008	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.48% 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, NA, LDA

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	0.68	0/2189	0.85	6/2959 (0.2%)
1	B	0.70	0/2325	0.87	4/3145 (0.1%)
1	C	0.70	0/2203	0.85	2/2977 (0.1%)
All	All	0.69	0/6717	0.86	12/9081 (0.1%)

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	1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	351	GLY	N-CA-C	8.17	133.53	113.10
1	B	323	VAL	CB-CA-C	-7.58	97.00	111.40
1	B	229	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	B	229	ARG	CG-CD-NE	-6.16	98.87	111.80
1	B	405	TYR	N-CA-C	5.91	126.96	111.00
1	A	144	ARG	CG-CD-NE	5.81	124.00	111.80
1	A	203	ILE	CA-C-N	5.80	127.80	116.20
1	A	343	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	A	143	ASP	CB-CG-OD1	5.61	123.35	118.30
1	A	144	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	A	203	ILE	O-C-N	-5.28	114.23	123.20
1	C	95	LEU	CA-CB-CG	5.22	127.31	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	203	ILE	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2144	0	2051	20	0
1	B	2278	0	2172	25	0
1	C	2158	0	2070	16	0
2	A	32	0	62	0	0
2	B	28	0	54	2	0
2	C	48	0	93	2	0
3	A	14	0	23	0	0
3	C	74	0	123	2	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
5	A	73	0	0	1	0
5	B	71	0	0	1	0
5	C	85	0	0	1	0
All	All	7008	0	6648	59	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 (59) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ASN:HB3	1:B:405:TYR:HE2	1.28	0.96
1:B:105:ASN:HB3	1:B:405:TYR:CE2	2.02	0.93
1:A:347:LEU:HD13	1:A:357:ILE:HD11	1.59	0.84
1:C:204:GLY:HA2	1:C:260:THR:HG22	1.68	0.76
1:C:98:GLU:OE1	5:C:601:HOH:O	2.09	0.70
1:B:384:ASN:ND2	5:B:601:HOH:O	2.27	0.67
1:C:318:GLN:HB3	2:C:503:LDA:H61	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:SER:OG	1:B:372:THR:HB	1.97	0.64
1:A:332:SER:OG	1:A:372:THR:HB	1.96	0.64
1:C:316:SER:OG	1:C:318:GLN:NE2	2.31	0.63
1:A:95:LEU:HD11	1:A:324:ALA:CB	2.30	0.61
1:A:144:ARG:HD2	1:A:145:ILE:H	1.67	0.58
1:B:183:GLY:N	1:B:184:ALA:HB2	2.20	0.57
1:C:273:MSE:HE2	3:C:507:C8E:H142	1.87	0.56
1:B:180:GLN:HA	1:B:193:SER:O	2.07	0.55
1:A:95:LEU:HD11	1:A:324:ALA:HB1	1.88	0.54
1:A:344:LYS:NZ	1:B:194:GLU:OE1	2.20	0.54
1:C:203:ILE:O	1:C:260:THR:HG21	2.08	0.53
1:C:156:GLY:HA3	2:C:501:LDA:H122	1.90	0.53
1:B:94:ASN:HB2	1:B:372:THR:HG21	1.90	0.52
1:A:145:ILE:HD11	1:A:177:SER:HB3	1.90	0.52
1:B:167:ASP:OD1	1:B:229:ARG:NH2	2.34	0.52
1:B:192:THR:HB	1:B:193:SER:CA	2.40	0.51
1:B:192:THR:HB	1:B:193:SER:HA	1.91	0.51
1:B:296:PHE:HE1	1:B:311:VAL:HG22	1.75	0.51
1:A:95:LEU:HD12	5:A:662:HOH:O	2.11	0.50
1:C:380:THR:HB	1:C:403:PRO:HG2	1.94	0.50
1:B:337:VAL:HG21	1:C:398:PHE:HE1	1.75	0.50
1:A:104:GLY:HA3	1:A:162:ASN:HD22	1.76	0.50
1:A:171:PRO:HG2	1:A:204:GLY:HA2	1.95	0.49
1:A:171:PRO:O	1:A:204:GLY:HA3	2.11	0.49
1:B:110:PHE:HE1	2:B:501:LDA:H111	1.77	0.49
1:A:94:ASN:HB2	1:A:372:THR:HG21	1.93	0.49
1:B:380:THR:HB	1:B:403:PRO:HG2	1.96	0.47
1:B:180:GLN:HG2	1:B:194:GLU:HG3	1.96	0.47
1:B:184:ALA:HB3	1:B:191:ALA:HB3	1.98	0.46
1:A:344:LYS:HD2	1:A:356:SER:HB2	1.99	0.45
1:A:171:PRO:HG2	1:A:204:GLY:CA	2.47	0.44
1:A:363:ASN:O	1:A:390:THR:HG21	2.18	0.44
1:A:380:THR:HB	1:A:403:PRO:HG2	1.98	0.44
1:C:104:GLY:HA2	1:C:159:ASN:ND2	2.33	0.44
1:B:103:PHE:HD2	1:B:405:TYR:OH	2.00	0.44
1:B:222:PRO:HG3	1:B:273:MSE:HE3	2.00	0.43
1:C:93:SER:HB3	1:C:105:ASN:ND2	2.34	0.43
1:B:94:ASN:CB	1:B:372:THR:HG21	2.48	0.43
1:A:145:ILE:HD12	1:A:178:THR:O	2.18	0.43
1:C:204:GLY:HA2	1:C:260:THR:CG2	2.42	0.43
1:A:104:GLY:HA3	1:A:162:ASN:ND2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:LYS:NZ	1:B:262:ASN:OD1	2.49	0.42
1:A:222:PRO:HG3	1:A:273:MSE:HE3	2.01	0.42
1:B:282:LEU:HD23	1:B:323:VAL:HG13	2.01	0.42
1:C:273:MSE:HE2	3:C:507:C8E:C14	2.48	0.42
1:A:94:ASN:CB	1:A:372:THR:HG21	2.50	0.41
1:C:349:PRO:O	1:C:352:GLY:HA3	2.20	0.41
1:C:105:ASN:HB2	1:C:405:TYR:CE1	2.55	0.41
1:C:222:PRO:HG3	1:C:273:MSE:HE3	2.02	0.41
1:B:312:ARG:HG3	1:B:354:TRP:CH2	2.55	0.41
1:B:192:THR:CB	1:B:193:SER:HA	2.51	0.41
1:B:285:SER:HB2	2:B:502:LDA:H12	2.02	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	268/334 (80%)	265 (99%)	3 (1%)	0	100	100
1	B	290/334 (87%)	282 (97%)	6 (2%)	2 (1%)	19	35
1	C	270/334 (81%)	265 (98%)	5 (2%)	0	100	100
All	All	828/1002 (83%)	812 (98%)	14 (2%)	2 (0%)	44	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	183	GLY
1	B	189	PRO

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	235/275 (86%)	225 (96%)	10 (4%)	25	48
1	B	249/275 (90%)	241 (97%)	8 (3%)	34	60
1	C	236/275 (86%)	227 (96%)	9 (4%)	28	53
All	All	720/825 (87%)	693 (96%)	27 (4%)	28	53

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	GLN
1	A	144	ARG
1	A	167	ASP
1	A	223	ASP
1	A	272	SER
1	A	299	ILE
1	A	359	SER
1	A	372	THR
1	A	377	GLU
1	A	400	LEU
1	B	167	ASP
1	B	192	THR
1	B	223	ASP
1	B	228	VAL
1	B	229	ARG
1	B	272	SER
1	B	323	VAL
1	B	372	THR
1	C	95	LEU
1	C	105	ASN
1	C	167	ASP
1	C	223	ASP
1	C	272	SER
1	C	321	VAL
1	C	330	ARG
1	C	356	SER

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Mol	Chain	Res	Type
1	C	377	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	97	ASN
1	C	105	ASN
1	C	318	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 3 are monoatomic - leaving 13 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	$\# Z  > 2$
2	LDA	A	501	-	13,15,15	1.98	1 (7%)	14,17,17	0.92	1 (7%)
3	C8E	C	504	-	13,13,20	0.62	0	12,12,19	0.50	0
2	LDA	C	501	-	13,15,15	2.19	1 (7%)	14,17,17	1.08	2 (14%)
3	C8E	C	505	-	10,10,20	0.62	0	9,9,19	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	C8E	A	503	-	13,13,20	0.62	0	12,12,19	0.55	0
3	C8E	C	507	-	20,20,20	0.49	0	19,19,19	0.75	0
3	C8E	C	508	-	20,20,20	0.66	0	19,19,19	0.49	0
2	LDA	C	502	-	13,15,15	1.88	1 (7%)	14,17,17	0.70	0
2	LDA	B	502	-	13,15,15	1.89	1 (7%)	14,17,17	1.12	1 (7%)
2	LDA	B	501	-	11,11,15	0.70	0	10,10,17	0.69	0
2	LDA	C	503	-	13,15,15	1.93	1 (7%)	14,17,17	0.95	2 (14%)
3	C8E	C	506	-	6,6,20	0.49	0	5,5,19	0.11	0
2	LDA	A	502	-	13,15,15	1.80	2 (15%)	14,17,17	0.89	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
2	LDA	A	501	-	-	6/13/13/13	-
3	C8E	C	504	-	-	3/11/11/18	-
2	LDA	C	501	-	-	9/13/13/13	-
3	C8E	C	505	-	-	3/8/8/18	-
3	C8E	A	503	-	-	5/11/11/18	-
3	C8E	C	507	-	-	8/18/18/18	-
3	C8E	C	508	-	-	14/18/18/18	-
2	LDA	C	502	-	-	2/13/13/13	-
2	LDA	B	502	-	-	4/13/13/13	-
2	LDA	B	501	-	-	3/9/9/13	-
2	LDA	C	503	-	-	5/13/13/13	-
3	C8E	C	506	-	-	1/4/4/18	-
2	LDA	A	502	-	-	3/13/13/13	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	LDA	O1-N1	-7.42	1.24	1.42
2	A	501	LDA	O1-N1	-6.76	1.25	1.42
2	C	503	LDA	O1-N1	-6.48	1.26	1.42
2	C	502	LDA	O1-N1	-6.44	1.26	1.42
2	B	502	LDA	O1-N1	-6.32	1.26	1.42
2	A	502	LDA	O1-N1	-5.87	1.27	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	LDA	C1-N1	-2.41	1.49	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	502	LDA	CM1-N1-C1	3.06	116.67	110.23
2	C	501	LDA	CM2-N1-C1	2.53	115.56	110.23
2	A	501	LDA	CM2-N1-C1	2.46	115.41	110.23
2	C	501	LDA	O1-N1-C1	2.33	114.99	109.27
2	A	502	LDA	CM1-N1-C1	-2.30	105.40	110.23
2	C	503	LDA	CM1-N1-C1	2.21	114.87	110.23
2	C	503	LDA	C1-C2-C3	2.00	119.42	110.81

There are no chirality outliers.

All (66) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	LDA	C2-C1-N1-CM1
2	A	501	LDA	C2-C1-N1-CM2
2	A	501	LDA	N1-C1-C2-C3
2	C	501	LDA	C2-C1-N1-CM1
2	C	501	LDA	C2-C1-N1-CM2
2	C	503	LDA	C2-C3-C4-C5
3	C	507	C8E	O9-C10-C11-O12
3	C	507	C8E	C2-C3-C4-C5
3	C	507	C8E	O12-C13-C14-O15
2	B	502	LDA	C4-C5-C6-C7
3	A	503	C8E	O9-C10-C11-O12
3	C	508	C8E	O12-C13-C14-O15
2	C	503	LDA	C7-C8-C9-C10
3	C	507	C8E	O18-C19-C20-O21
2	A	502	LDA	C7-C8-C9-C10
3	A	503	C8E	C6-C7-C8-O9
3	C	506	C8E	C2-C3-C4-C5
3	C	505	C8E	C3-C4-C5-C6
3	C	507	C8E	O15-C16-C17-O18
2	C	502	LDA	C7-C8-C9-C10
2	B	502	LDA	C7-C8-C9-C10
3	C	508	C8E	C4-C5-C6-C7
2	B	502	LDA	C6-C7-C8-C9
2	C	501	LDA	C4-C5-C6-C7
3	C	508	C8E	C2-C3-C4-C5

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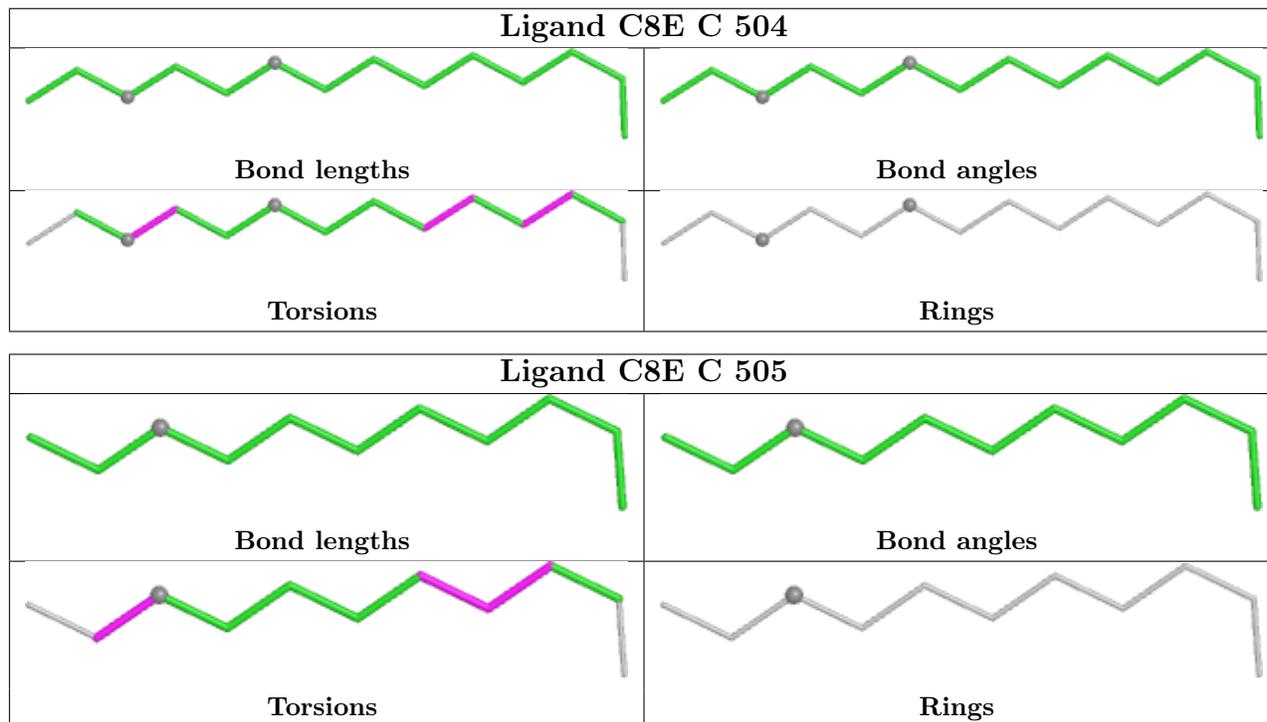
Mol	Chain	Res	Type	Atoms
2	A	501	LDA	C7-C8-C9-C10
2	C	503	LDA	C4-C5-C6-C7
2	C	501	LDA	C2-C3-C4-C5
3	C	505	C8E	C2-C3-C4-C5
2	A	501	LDA	C11-C10-C9-C8
2	C	502	LDA	C4-C5-C6-C7
2	C	501	LDA	C5-C6-C7-C8
3	C	508	C8E	C3-C4-C5-C6
3	C	504	C8E	C2-C3-C4-C5
3	C	507	C8E	C20-C19-O18-C17
3	C	508	C8E	C17-C16-O15-C14
3	C	504	C8E	C4-C5-C6-C7
3	C	505	C8E	C11-C10-O9-C8
3	C	508	C8E	C10-C11-O12-C13
2	C	503	LDA	C1-C2-C3-C4
3	C	507	C8E	C7-C8-O9-C10
3	C	508	C8E	C7-C8-O9-C10
3	C	504	C8E	C10-C11-O12-C13
2	C	501	LDA	C2-C1-N1-O1
2	B	501	LDA	C5-C6-C7-C8
2	A	502	LDA	C6-C7-C8-C9
3	C	508	C8E	C16-C17-O18-C19
3	A	503	C8E	C7-C8-O9-C10
2	B	501	LDA	C4-C5-C6-C7
2	A	502	LDA	C9-C10-C11-C12
2	B	501	LDA	C7-C8-C9-C10
3	C	508	C8E	C6-C7-C8-O9
2	B	502	LDA	C2-C3-C4-C5
3	C	507	C8E	C3-C4-C5-C6
3	C	508	C8E	C1-C2-C3-C4
3	C	508	C8E	C5-C6-C7-C8
2	C	503	LDA	C3-C4-C5-C6
3	A	503	C8E	C14-C13-O12-C11
2	C	501	LDA	C1-C2-C3-C4
3	C	508	C8E	C20-C19-O18-C17
2	C	501	LDA	C6-C7-C8-C9
2	C	501	LDA	C3-C4-C5-C6
3	C	508	C8E	O9-C10-C11-O12
2	A	501	LDA	C2-C1-N1-O1
3	A	503	C8E	C4-C5-C6-C7
3	C	508	C8E	O15-C16-C17-O18

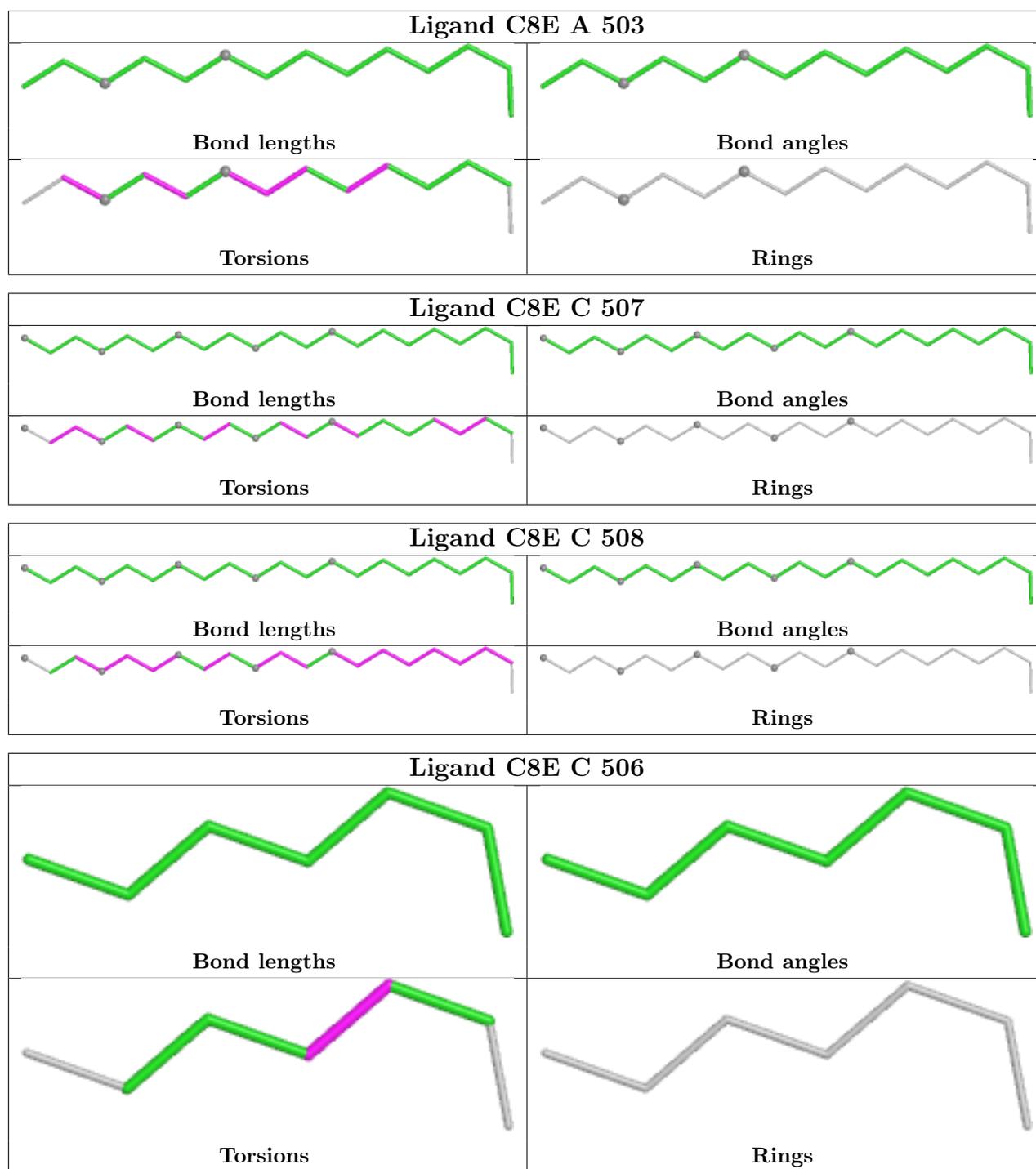
There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	LDA	1	0
3	C	507	C8E	2	0
2	B	502	LDA	1	0
2	B	501	LDA	1	0
2	C	503	LDA	1	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](#)

**Warning:** The R factor obtained from EDS is 0.3258, which does not match the depositor's R factor of 0.22151. Please interpret the results in this section carefully.

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	270/334 (80%)	-0.78	0 100 100	26, 40, 64, 88	0
1	B	290/334 (86%)	-0.77	0 100 100	27, 39, 87, 106	0
1	C	272/334 (81%)	-0.75	0 100 100	27, 40, 74, 95	0
All	All	832/1002 (83%)	-0.77	0 100 100	26, 40, 72, 106	0

There are no RSRZ outliers to report.

### 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.

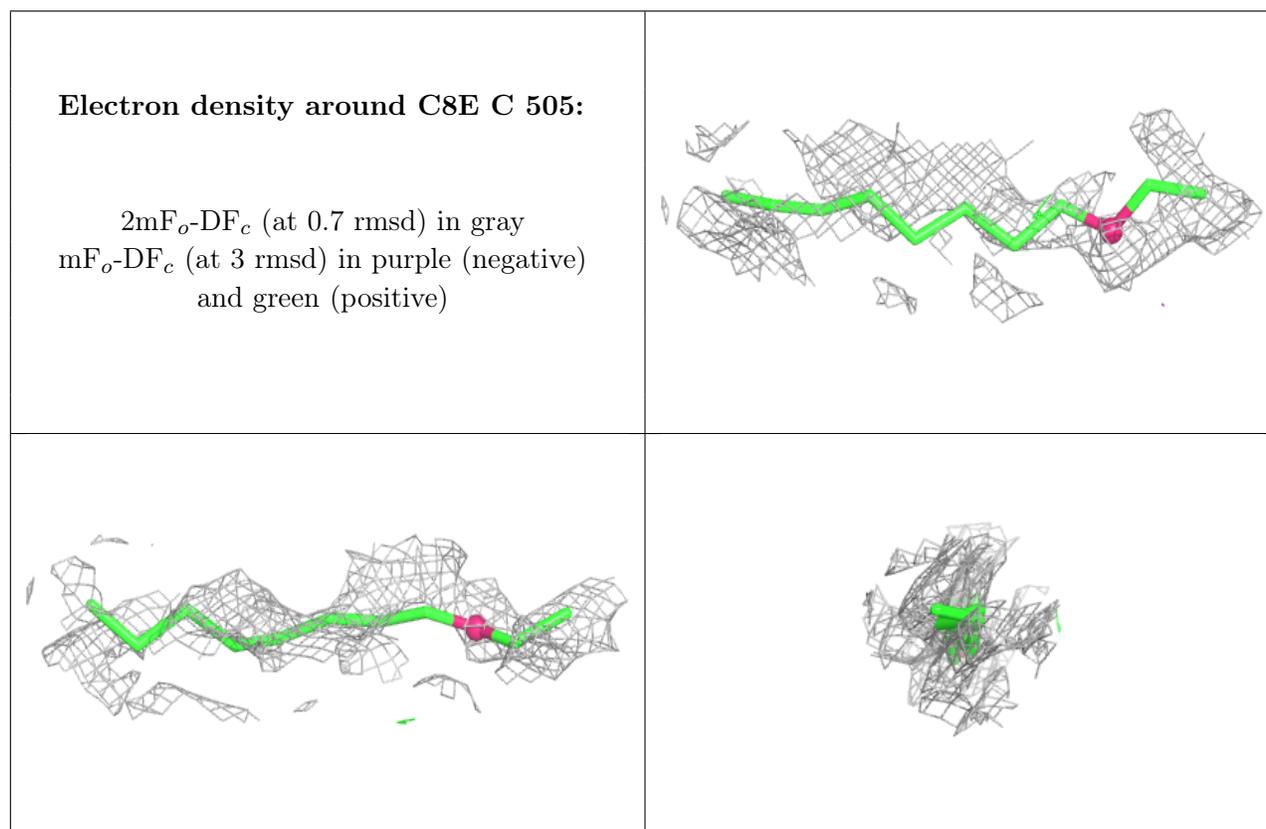
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	NA	B	503	1/1	0.69	0.06	38,38,38,38	0
3	C8E	C	505	11/21	0.74	0.07	45,53,57,59	0
3	C8E	C	504	14/21	0.81	0.07	41,55,68,68	0

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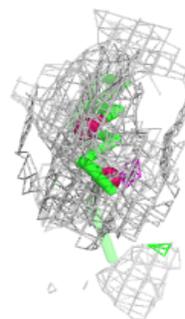
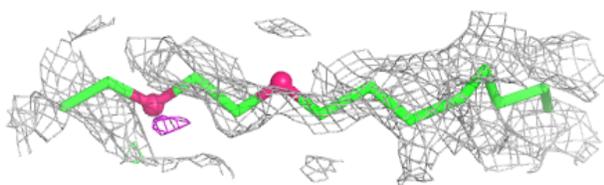
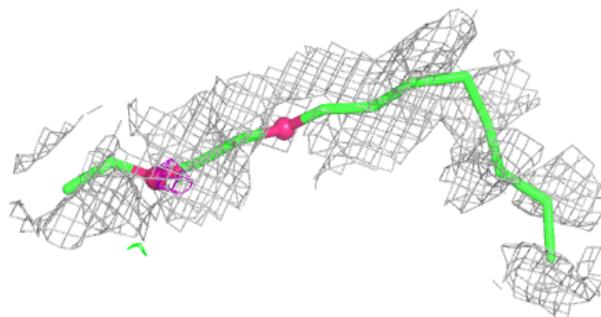
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	C8E	C	506	7/21	0.82	0.09	35,46,56,57	0
2	LDA	C	502	16/16	0.83	0.08	55,66,78,80	0
3	C8E	A	503	14/21	0.83	0.08	37,42,48,50	0
2	LDA	C	501	16/16	0.84	0.06	61,65,71,77	0
3	C8E	C	507	21/21	0.86	0.08	56,63,79,83	0
2	LDA	A	501	16/16	0.87	0.07	45,55,84,91	0
3	C8E	C	508	21/21	0.87	0.09	54,76,85,91	0
2	LDA	C	503	16/16	0.87	0.08	59,66,80,82	0
2	LDA	A	502	16/16	0.90	0.10	60,66,74,74	0
2	LDA	B	501	12/16	0.92	0.06	41,43,46,46	0
2	LDA	B	502	16/16	0.92	0.06	58,67,80,81	0
4	NA	A	504	1/1	1.00	0.09	55,55,55,55	0
4	NA	B	504	1/1	1.00	0.08	56,56,56,56	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.

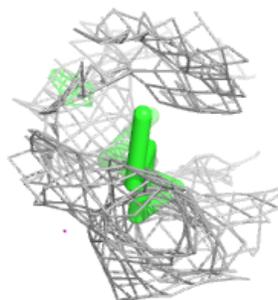
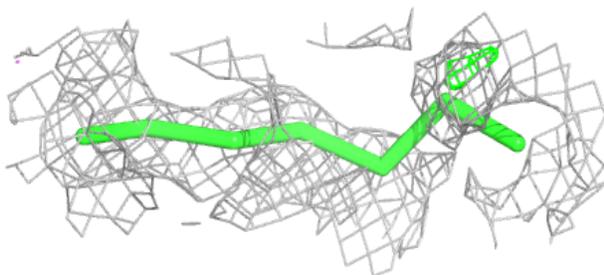
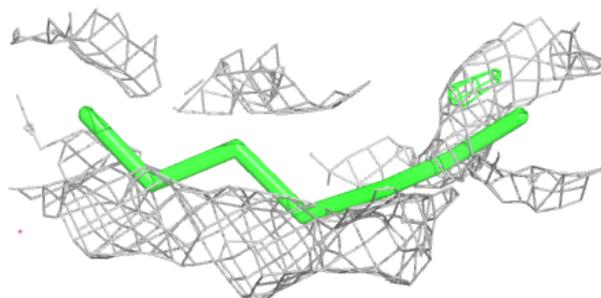


**Electron density around C8E C 504:**

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

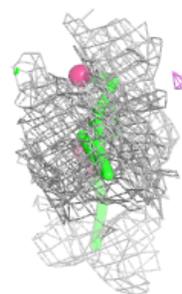
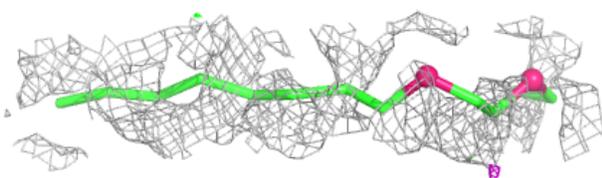
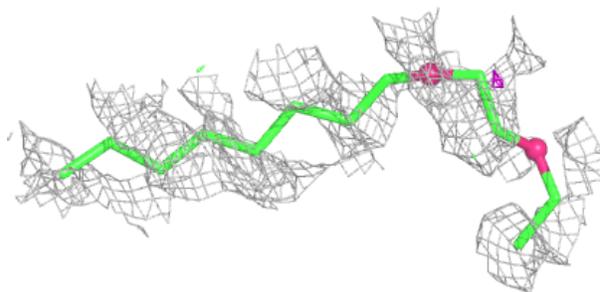
**Electron density around C8E C 506:**

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

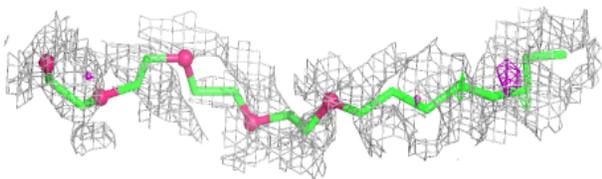
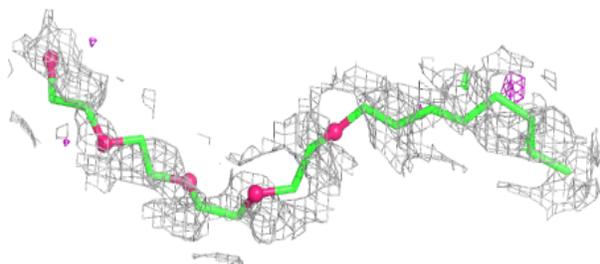


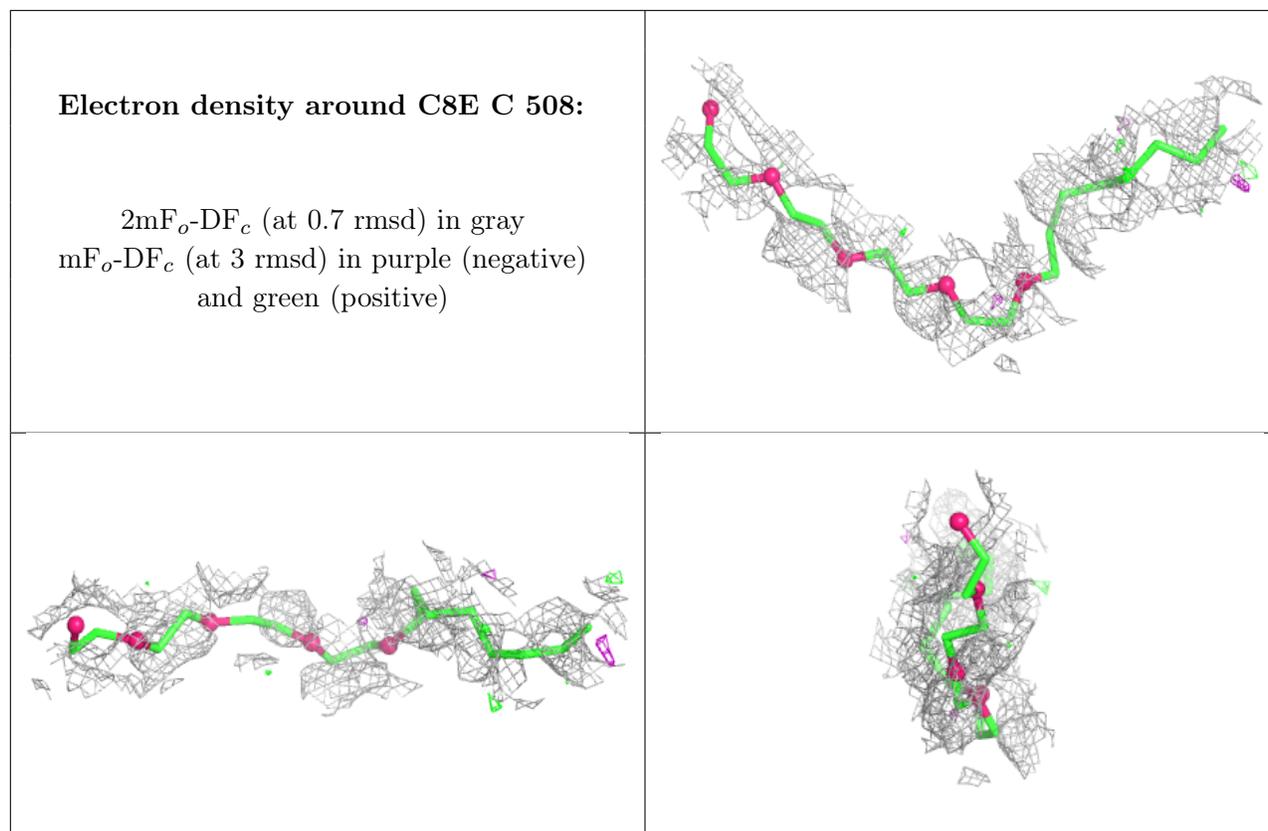
**Electron density around C8E A 503:**

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

**Electron density around C8E 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.