



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 03:10 pm BST

PDB ID : 4GF4
Title : Low pH structure of Pseudomonas putida OprB
Authors : van den Berg, B.
Deposited on : 2012-08-02
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

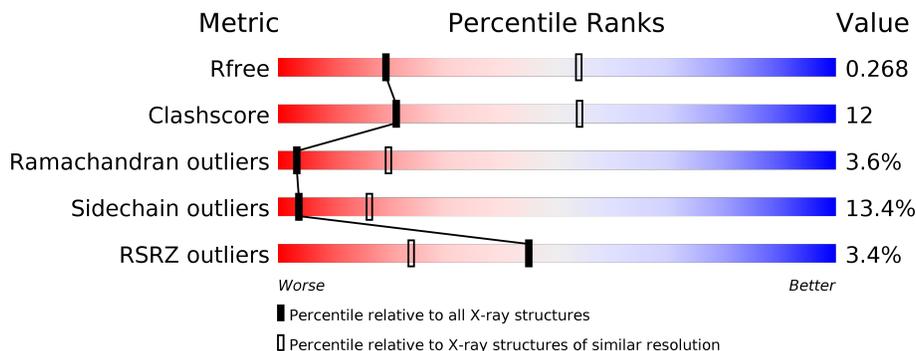
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	436	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	C8E	A	503	-	-	-	X
2	C8E	A	504	-	-	-	X

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2398 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.

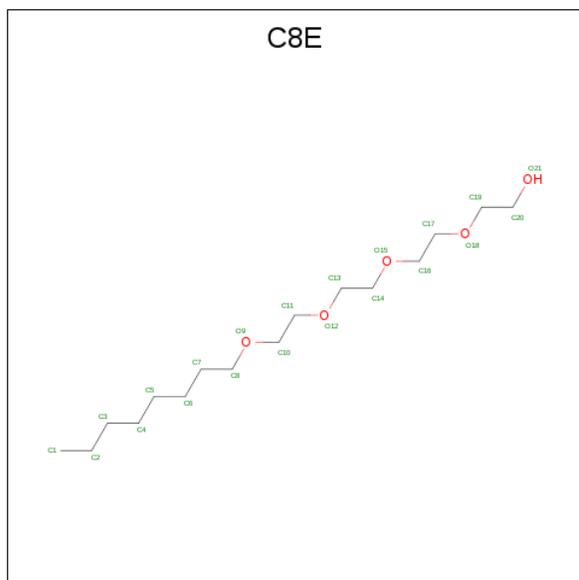
- Molecule 1 is a protein called Porin B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	299	2330	1501	390	433	6	0	0	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	ALA	-	EXPRESSION TAG	UNP E4R6F8
A	-13	ASN	-	EXPRESSION TAG	UNP E4R6F8
A	-12	VAL	-	EXPRESSION TAG	UNP E4R6F8
A	-11	ARG	-	EXPRESSION TAG	UNP E4R6F8
A	-10	LEU	-	EXPRESSION TAG	UNP E4R6F8
A	-9	GLN	-	EXPRESSION TAG	UNP E4R6F8
A	-8	HIS	-	EXPRESSION TAG	UNP E4R6F8
A	-7	HIS	-	EXPRESSION TAG	UNP E4R6F8
A	-6	HIS	-	EXPRESSION TAG	UNP E4R6F8
A	-5	HIS	-	EXPRESSION TAG	UNP E4R6F8
A	-4	HIS	-	EXPRESSION TAG	UNP E4R6F8
A	-3	HIS	-	EXPRESSION TAG	UNP E4R6F8
A	-2	HIS	-	EXPRESSION TAG	UNP E4R6F8
A	-1	LEU	-	EXPRESSION TAG	UNP E4R6F8
A	0	GLU	-	EXPRESSION TAG	UNP E4R6F8
A	220	MSE	LEU	ENGINEERED MUTATION	UNP E4R6F8
A	222	MSE	VAL	ENGINEERED MUTATION	UNP E4R6F8
A	415	MSE	LEU	ENGINEERED MUTATION	UNP E4R6F8
A	417	MSE	ILE	ENGINEERED MUTATION	UNP E4R6F8

- Molecule 2 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C₁₆H₃₄O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			18	14	4		
2	A	1	Total	C	O	0	0
			18	14	4		
2	A	1	Total	C	O	0	0
			20	15	5		
2	A	1	Total	C	O	0	0
			12	8	4		

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	79.04Å 122.59Å 135.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.77 – 3.10 33.90 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.77-3.10) 92.8 (33.90-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 3.12Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.214 , 0.271 0.217 , 0.268	Depositor DCC
R_{free} test set	1218 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	66.2	Xtrriage
Anisotropy	0.552	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	2398	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.48	0/2383	0.68	1/3218 (0.0%)

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 (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	71	TRP	CA-CB-CG	5.01	123.22	113.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	171	TRP	Peptide

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	2330	0	2126	56	0
2	A	68	0	98	10	0
All	All	2398	0	2224	56	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 12.

All (56) 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:125:TYR:O	1:A:127:ASP:N	2.16	0.78
1:A:238:ARG:HB2	1:A:279:VAL:HB	1.74	0.70
1:A:65:LEU:HD22	1:A:69:LEU:HD22	1.75	0.67
1:A:277:TRP:HB3	1:A:302:THR:HG23	1.78	0.66
1:A:223:GLU:OE2	1:A:238:ARG:NH1	2.30	0.65
1:A:393:PRO:HB3	1:A:415:MSE:HE3	1.78	0.64
1:A:233:LEU:HB3	1:A:283:GLN:HG2	1.79	0.64
1:A:282:GLN:HG2	2:A:501:C8E:H31	1.80	0.64
1:A:389:LEU:HD21	1:A:417:MSE:HE2	1.82	0.62
1:A:286:ALA:O	1:A:288:GLY:N	2.32	0.61
1:A:131:ASP:HB3	1:A:181:LYS:HB3	1.86	0.57
1:A:116:LEU:HD21	1:A:119:MSE:HE2	1.86	0.57
1:A:385:VAL:HB	1:A:389:LEU:HB3	1.87	0.56
1:A:225:VAL:HG22	1:A:238:ARG:HG2	1.88	0.56
1:A:69:LEU:HD23	1:A:71:TRP:HD1	1.71	0.56
1:A:314:TYR:HD1	1:A:340:ILE:HG12	1.70	0.55
1:A:79:ALA:HB3	1:A:118:GLN:HB2	1.88	0.55
1:A:37:VAL:HG22	2:A:504:C8E:H192	1.88	0.54
1:A:282:GLN:HB3	2:A:501:C8E:H72	1.90	0.54
1:A:399:LYS:HG3	1:A:400:SER:N	2.21	0.54
1:A:142:ASP:O	1:A:191:GLN:NE2	2.35	0.52
1:A:386:THR:HG23	1:A:389:LEU:H	1.73	0.52
1:A:143:PHE:O	1:A:144:ASN:HB2	2.10	0.51
1:A:305:ASP:HA	1:A:311:VAL:HA	1.92	0.51
1:A:219:ILE:O	1:A:221:PRO:HD3	2.11	0.51
1:A:314:TYR:OH	1:A:316:GLN:OE1	2.26	0.50
1:A:68:ILE:HG22	1:A:69:LEU:HD13	1.93	0.49
1:A:117:THR:HG22	1:A:118:GLN:HG3	1.95	0.48
1:A:284:VAL:HG23	1:A:285:THR:HG23	1.96	0.48
1:A:314:TYR:CD1	1:A:340:ILE:HG12	2.48	0.48
1:A:15:TRP:CZ3	1:A:19:ARG:HG3	2.48	0.48
1:A:23:LEU:HD12	1:A:27:TYR:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:VAL:HG12	2:A:501:C8E:H171	1.97	0.47
1:A:192:VAL:CG2	2:A:503:C8E:H202	2.45	0.46
1:A:8:SER:C	1:A:10:TRP:H	2.18	0.46
1:A:244:SER:HB2	1:A:273:LYS:HB2	1.98	0.46
1:A:388:TRP:O	1:A:419:SER:HA	2.15	0.46
1:A:283:GLN:HA	1:A:296:SER:OG	2.17	0.45
1:A:240:GLY:HA3	1:A:277:TRP:CE2	2.51	0.45
1:A:381:TYR:O	1:A:393:PRO:HD2	2.17	0.44
1:A:21:GLU:O	1:A:24:ASP:HB2	2.17	0.44
1:A:118:GLN:HE21	1:A:141:GLU:CD	2.20	0.44
1:A:171:TRP:CD1	1:A:172:PRO:HD2	2.53	0.43
1:A:317:VAL:CG1	2:A:501:C8E:H171	2.48	0.43
1:A:61:ALA:O	1:A:77:LYS:HD2	2.18	0.43
1:A:33:TYR:CE2	2:A:504:C8E:H101	2.54	0.43
1:A:192:VAL:HG11	2:A:503:C8E:H161	2.01	0.43
1:A:4:PHE:CD2	1:A:4:PHE:N	2.87	0.43
1:A:41:LEU:HD22	1:A:411:LEU:HD12	2.00	0.42
1:A:170:ASN:O	1:A:171:TRP:HB3	2.19	0.42
1:A:4:PHE:HA	1:A:11:MSE:O	2.20	0.42
1:A:241:TYR:HD1	1:A:275:GLY:O	2.02	0.42
1:A:4:PHE:HD2	1:A:4:PHE:N	2.18	0.41
1:A:385:VAL:HG21	1:A:389:LEU:HD13	2.03	0.40
1:A:226:TRP:CZ3	2:A:502:C8E:H32	2.55	0.40
1:A:192:VAL:HG21	2:A:503:C8E:H202	2.04	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	281/436 (64%)	258 (92%)	13 (5%)	10 (4%)	3 20

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	71	TRP
1	A	126	PHE
1	A	196	GLU
1	A	287	HIS
1	A	144	ASN
1	A	288	GLY
1	A	324	ALA
1	A	102	SER
1	A	171	TRP

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	224/350 (64%)	194 (87%)	30 (13%)	4 16

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	PHE
1	A	18	THR
1	A	31	LEU
1	A	37	VAL
1	A	41	LEU
1	A	48	ASP
1	A	56	GLN
1	A	59	LEU
1	A	69	LEU
1	A	71	TRP
1	A	82	GLU
1	A	115	ARG
1	A	130	LEU
1	A	185	THR
1	A	215	THR

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Mol	Chain	Res	Type
1	A	222	MSE
1	A	236	GLU
1	A	281	GLN
1	A	283	GLN
1	A	297	LEU
1	A	305	ASP
1	A	311	VAL
1	A	317	VAL
1	A	326	ASP
1	A	332	ASP
1	A	374	GLU
1	A	389	LEU
1	A	399	LYS
1	A	411	LEU
1	A	417	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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	A	503	-	19,19,20	0.45	0	18,18,19	0.55	0
2	C8E	A	501	-	17,17,20	0.46	0	16,16,19	0.44	0
2	C8E	A	504	-	10,10,20	0.50	0	8,8,19	0.17	0
2	C8E	A	502	-	17,17,20	0.43	0	16,16,19	0.42	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	A	503	-	-	8/17/17/18	-
2	C8E	A	501	-	-	8/15/15/18	-
2	C8E	A	504	-	-	3/6/6/18	-
2	C8E	A	502	-	-	8/15/15/18	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	502	C8E	C2-C3-C4-C5
2	A	503	C8E	O15-C16-C17-O18
2	A	502	C8E	O12-C13-C14-O15
2	A	503	C8E	O12-C13-C14-O15
2	A	503	C8E	O18-C19-C20-O21
2	A	501	C8E	O12-C13-C14-O15
2	A	503	C8E	C6-C7-C8-O9
2	A	501	C8E	C2-C3-C4-C5
2	A	501	C8E	C3-C4-C5-C6
2	A	503	C8E	O9-C10-C11-O12
2	A	504	C8E	O18-C19-C20-O21
2	A	503	C8E	C2-C3-C4-C5
2	A	502	C8E	C5-C6-C7-C8
2	A	504	C8E	C7-C8-O9-C10
2	A	504	C8E	O9-C10-C11-O12

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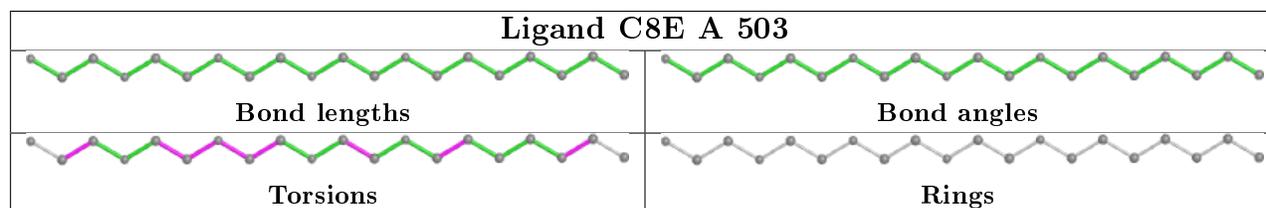
Mol	Chain	Res	Type	Atoms
2	A	501	C8E	C13-C14-O15-C16
2	A	501	C8E	C11-C10-O9-C8
2	A	502	C8E	C10-C11-O12-C13
2	A	503	C8E	C17-C16-O15-C14
2	A	503	C8E	C13-C14-O15-C16
2	A	501	C8E	C7-C8-O9-C10
2	A	501	C8E	C17-C16-O15-C14
2	A	501	C8E	C14-C13-O12-C11
2	A	502	C8E	C17-C16-O15-C14
2	A	502	C8E	C14-C13-O12-C11
2	A	502	C8E	C11-C10-O9-C8
2	A	502	C8E	O9-C10-C11-O12

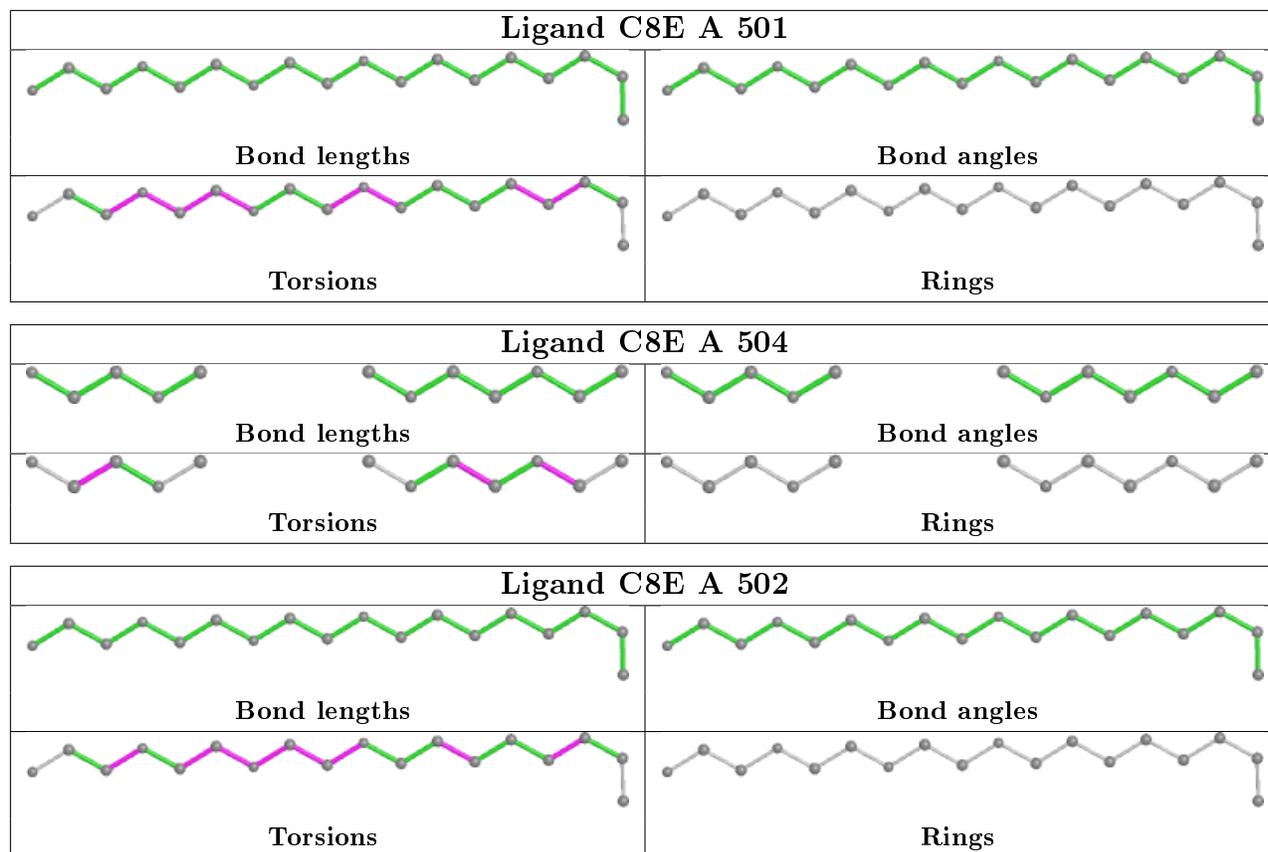
There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	503	C8E	3	0
2	A	501	C8E	4	0
2	A	504	C8E	2	0
2	A	502	C8E	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](#)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	293/436 (67%)	0.14	10 (3%) 45 24	15, 35, 67, 98	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	41	LEU	3.9
1	A	85	GLY	3.4
1	A	90	ASN	2.9
1	A	89	SER	2.8
1	A	50	THR	2.7
1	A	327	ALA	2.6
1	A	104	VAL	2.6
1	A	6	SER	2.3
1	A	51	ALA	2.2
1	A	171	TRP	2.1

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

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

6.3 Carbohydrates [i](#)

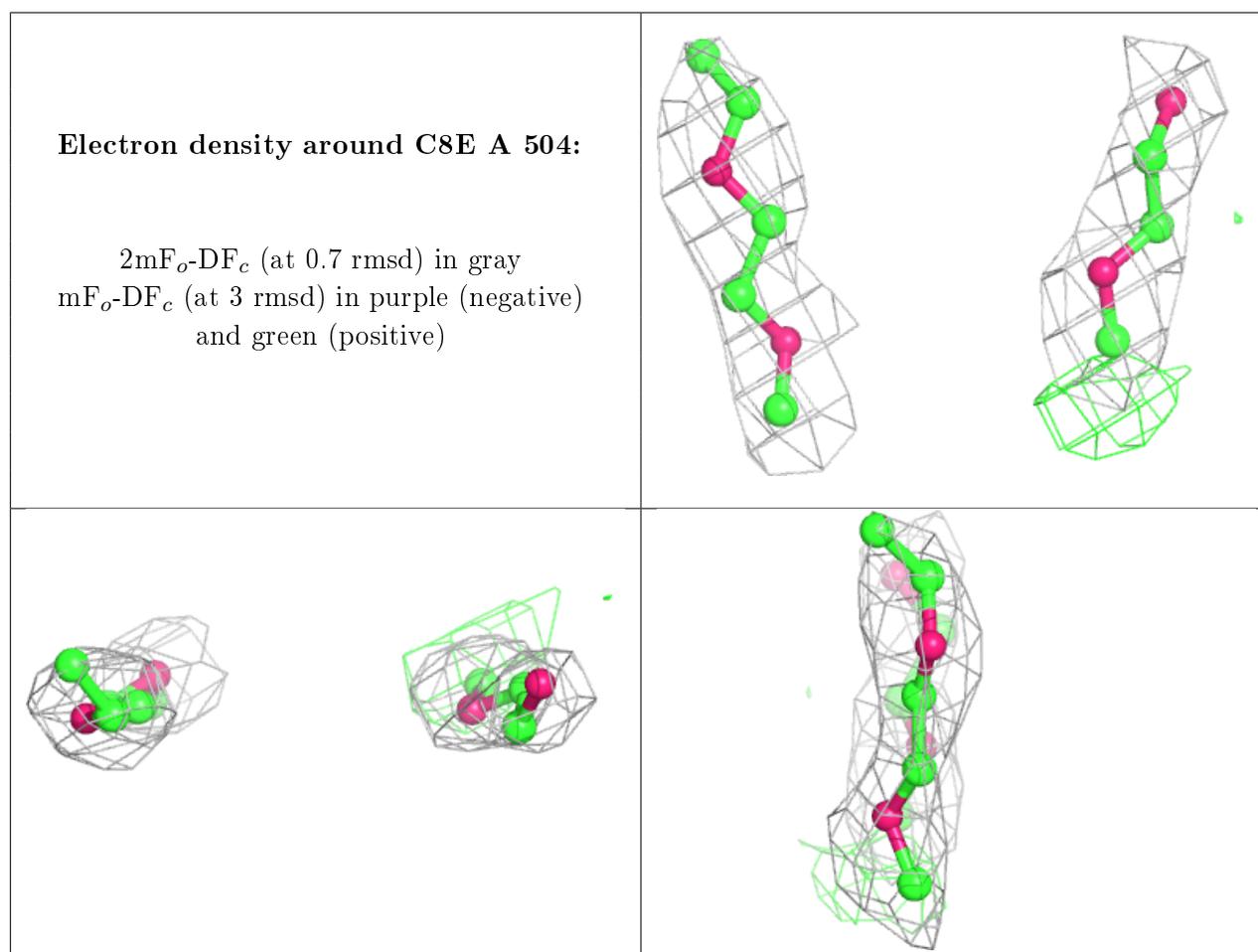
There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

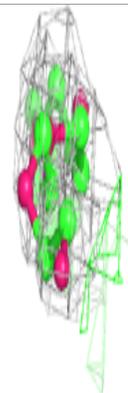
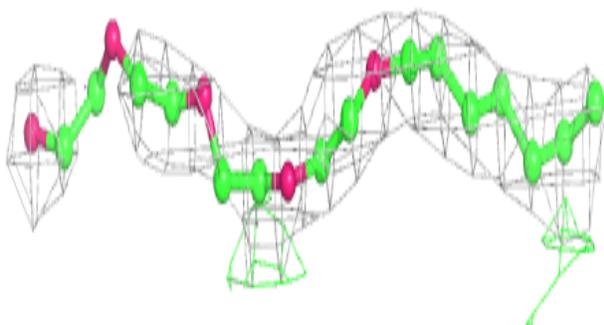
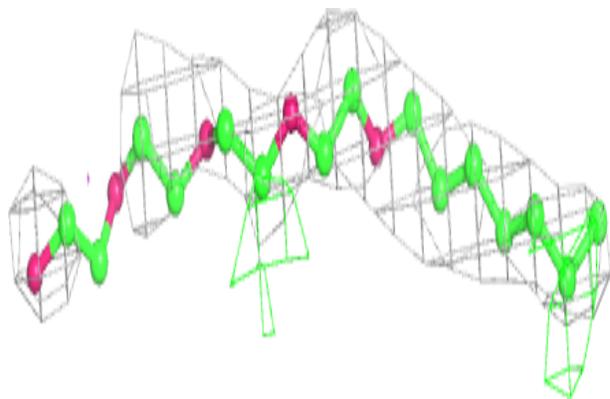
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	C8E	A	504	12/21	0.74	0.42	32,44,49,49	0
2	C8E	A	503	20/21	0.76	0.44	23,45,74,76	0
2	C8E	A	502	18/21	0.87	0.29	29,51,68,68	0
2	C8E	A	501	18/21	0.92	0.35	14,34,44,44	0

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.

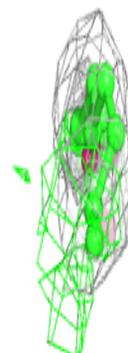
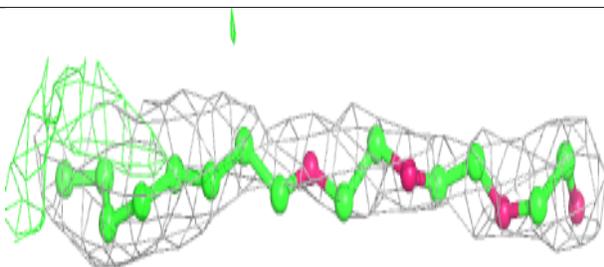
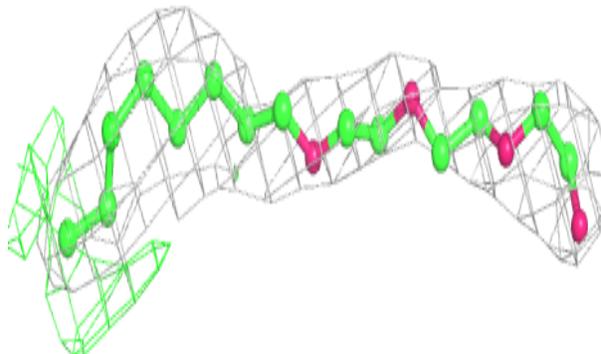


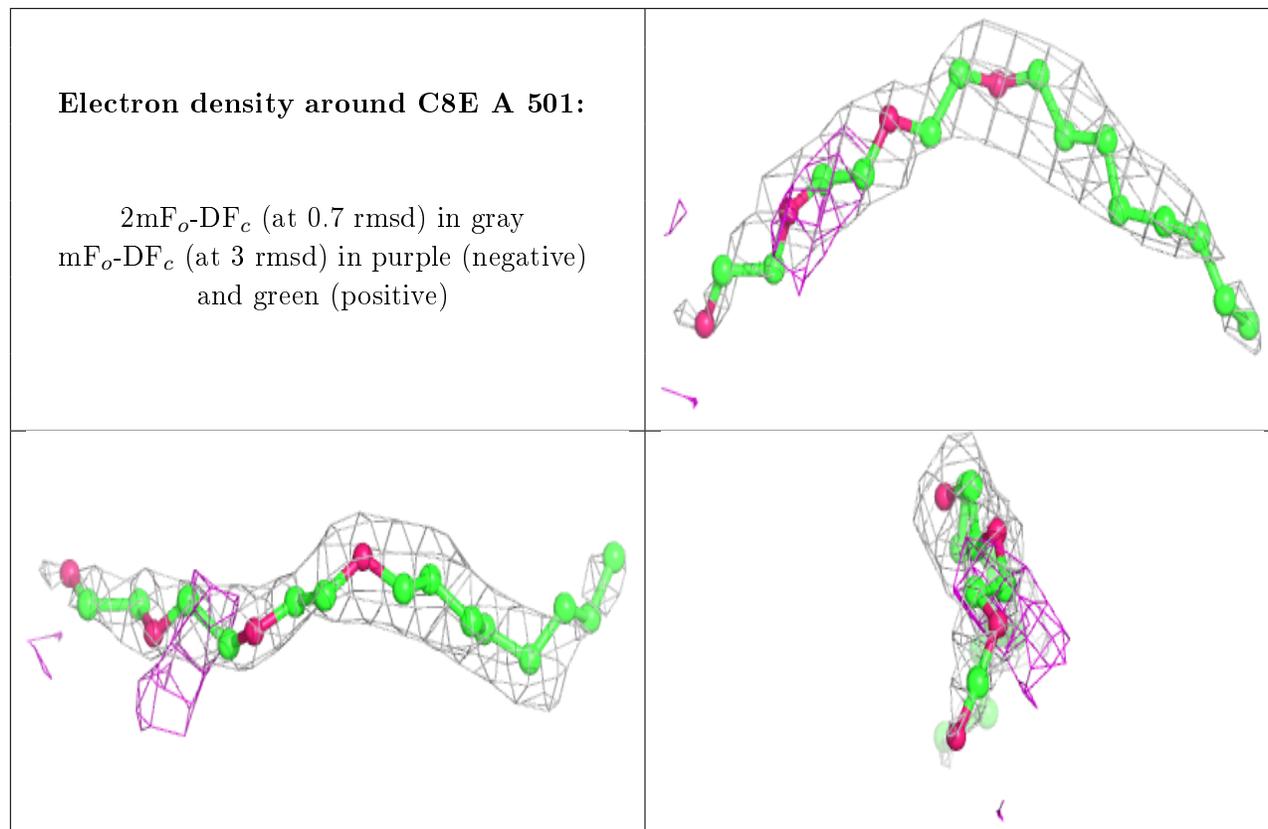
Electron density around C8E A 503:

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

**Electron density around C8E A 502:**

$2mF_o-DF_c$ (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.