



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2024 – 02:31 PM EST

PDB ID : 3SZD  
Title : Crystal structure of Pseudomonas aeruginosa OccK2 (OpdF)  
Authors : van den Berg, B.; Eren, E.  
Deposited on : 2011-07-18  
Resolution : 2.31 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 : 1.8.5 (274361), 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

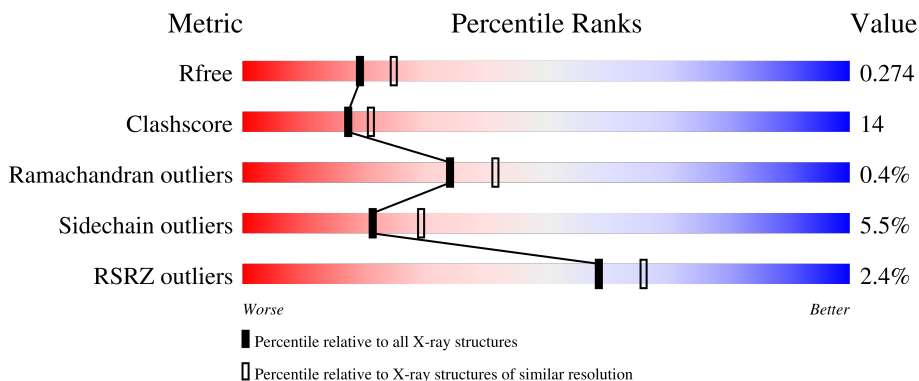
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.31 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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	405	 3% 66% 23% 9%
1	B	405	 % 67% 21% 8%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6126 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.

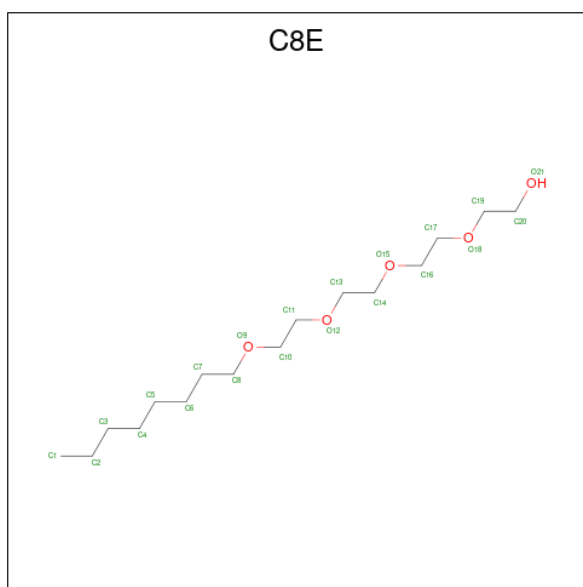
- Molecule 1 is a protein called porin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	371	2896	1813	531	547	5	0	1	0
1	A	368	2869	1799	530	535	5	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	398	GLY	-	expression tag	UNP Q9I6P8
B	399	GLY	-	expression tag	UNP Q9I6P8
B	400	HIS	-	expression tag	UNP Q9I6P8
B	401	HIS	-	expression tag	UNP Q9I6P8
B	402	HIS	-	expression tag	UNP Q9I6P8
B	403	HIS	-	expression tag	UNP Q9I6P8
B	404	HIS	-	expression tag	UNP Q9I6P8
B	405	HIS	-	expression tag	UNP Q9I6P8
A	398	GLY	-	expression tag	UNP Q9I6P8
A	399	GLY	-	expression tag	UNP Q9I6P8
A	400	HIS	-	expression tag	UNP Q9I6P8
A	401	HIS	-	expression tag	UNP Q9I6P8
A	402	HIS	-	expression tag	UNP Q9I6P8
A	403	HIS	-	expression tag	UNP Q9I6P8
A	404	HIS	-	expression tag	UNP Q9I6P8
A	405	HIS	-	expression tag	UNP Q9I6P8

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



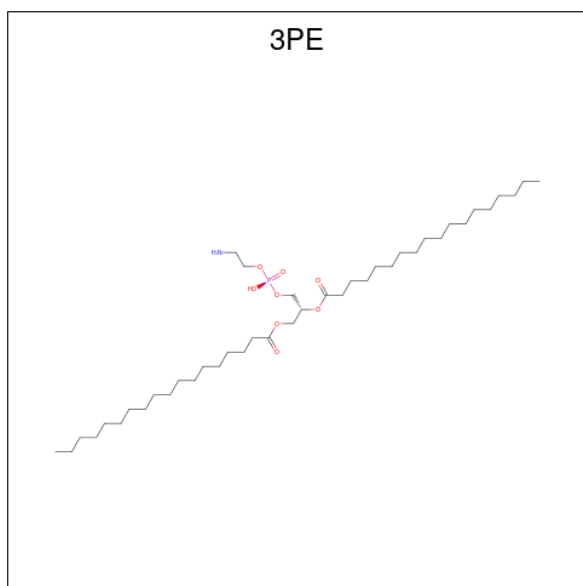
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 7 6 1	0	0
2	B	1	Total C O 8 5 3	0	0
2	B	1	Total C O 19 15 4	0	0
2	A	1	Total C O 14 9 5	0	0
2	A	1	Total C O 16 11 5	0	0

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



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

- Molecule 4 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			20	10	1	8	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	119	Total	O	0	0
			119	119		

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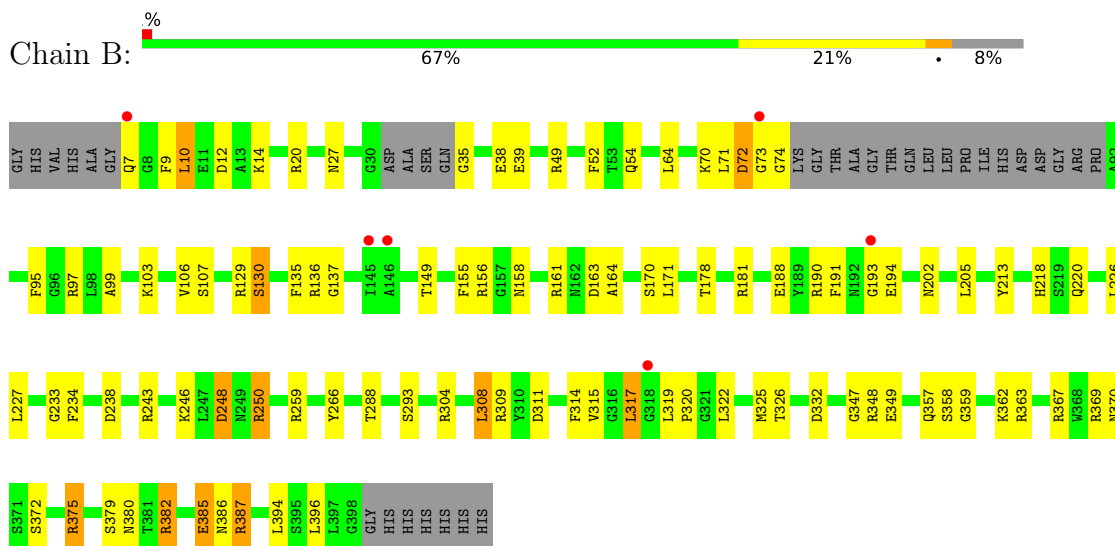
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	A	123	Total 123	O 123	0	0

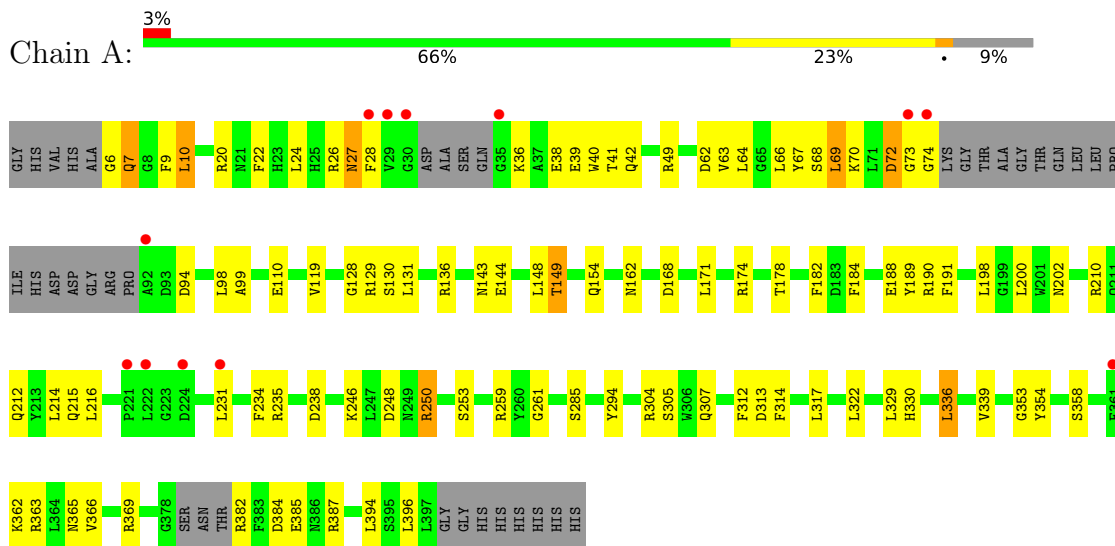
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: porin



- Molecule 1: porin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.32Å 206.90Å 51.58Å 90.00° 99.09° 90.00°	Depositor
Resolution (Å)	14.99 – 2.31 41.83 – 2.31	Depositor EDS
% Data completeness (in resolution range)	92.8 (14.99-2.31) 90.0 (41.83-2.31)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.79 (at 2.32Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.225 , 0.281 0.220 , 0.274	Depositor DCC
$R_{free}$ test set	2249 reflections (5.81%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.2	Xtrriage
Anisotropy	0.533	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 43.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	6126	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.50% 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: SO4, 3PE, 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	0.43	0/2931	0.60	1/3948 (0.0%)
1	B	0.44	0/2962	0.62	0/3993
All	All	0.44	0/5893	0.61	1/7941 (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	73	GLY	N-CA-C	-6.14	97.75	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	72	ASP	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	2869	0	2747	73	0
1	B	2896	0	2756	82	0
2	A	30	0	38	4	0
2	B	34	0	46	9	0
3	A	10	0	0	0	0
3	B	25	0	0	1	0
4	A	20	0	14	0	0
5	A	123	0	0	14	0
5	B	119	0	0	13	0
All	All	6126	0	5601	158	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 14.

All (158) 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:6:GLY:HA2	1:A:7:GLN:HB2	1.11	1.09
1:B:385:GLU:OE1	1:B:387:ARG:NH1	1.95	1.00
1:B:248:ASP:OD1	1:B:250:ARG:NH2	1.99	0.96
1:A:248:ASP:OD1	1:A:250:ARG:NH2	2.00	0.93
1:A:6:GLY:CA	1:A:7:GLN:HB2	1.97	0.93
1:A:6:GLY:HA2	1:A:7:GLN:CB	1.99	0.93
1:B:35:GLY:N	5:B:479:HOH:O	2.02	0.92
1:B:35:GLY:N	5:B:487:HOH:O	2.01	0.92
1:A:128:GLY:O	5:A:530:HOH:O	1.98	0.81
1:B:326:THR:HG23	2:B:406:C8E:H71	1.63	0.81
1:B:386:ASN:ND2	2:B:408:C8E:H142	1.97	0.80
1:A:70:LYS:HE3	5:A:515:HOH:O	1.80	0.80
1:B:190:ARG:NH2	5:B:523:HOH:O	2.16	0.78
1:B:320:PRO:HB2	1:B:357:GLN:NE2	1.99	0.78
1:A:70:LYS:HD2	1:A:74:GLY:HA2	1.66	0.76
1:A:212:GLN:NE2	5:A:417:HOH:O	2.18	0.75
1:B:27:ASN:ND2	2:B:408:C8E:H132	2.02	0.74
1:B:178:THR:O	1:B:243:ARG:NH1	2.21	0.74
1:B:163:ASP:OD2	5:B:448:HOH:O	2.06	0.74
1:B:39:GLU:HG3	1:B:74:GLY:HA2	1.71	0.73
1:A:190:ARG:NH1	5:A:470:HOH:O	2.23	0.70
1:A:27:ASN:N	1:A:27:ASN:OD1	2.25	0.69
1:B:386:ASN:HD22	2:B:408:C8E:H142	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:VAL:HG23	1:A:119:VAL:O	1.93	0.68
1:B:71:LEU:O	1:B:72:ASP:HB3	1.94	0.67
2:A:408:C8E:H112	2:A:408:C8E:H171	1.77	0.66
1:A:248:ASP:CG	1:A:250:ARG:HH22	1.99	0.65
1:A:110:GLU:OE1	5:A:521:HOH:O	2.15	0.65
1:A:148:LEU:O	5:A:463:HOH:O	2.13	0.65
1:A:144:GLU:OE1	5:A:486:HOH:O	2.14	0.65
1:A:307:GLN:HG3	1:A:329:LEU:HG	1.79	0.65
1:B:379:SER:O	1:B:380:ASN:HB2	1.98	0.64
1:B:348:ARG:HG3	1:A:317:LEU:HD13	1.79	0.63
1:B:238:ASP:OD2	1:B:246:LYS:HG2	1.99	0.62
1:B:27:ASN:HD22	2:B:408:C8E:H132	1.64	0.62
1:B:20:ARG:NH1	1:B:130:SER:O	2.33	0.61
1:B:375:ARG:NH2	5:B:463:HOH:O	2.33	0.60
1:B:266:TYR:HB2	1:B:309:ARG:HB3	1.83	0.60
1:A:41:THR:HG22	1:A:70:LYS:HD3	1.83	0.60
1:B:70:LYS:HG3	1:B:73:GLY:O	2.03	0.59
1:B:9:PHE:HD2	1:B:10:LEU:HD13	1.68	0.59
1:A:238:ASP:OD2	1:A:246:LYS:HD2	2.04	0.58
1:A:143:ASN:OD1	1:A:149:THR:HB	2.05	0.57
1:B:149:THR:CG2	1:B:188:GLU:HB2	2.36	0.56
1:B:38:GLU:HG2	1:B:39:GLU:N	2.21	0.56
1:B:358:SER:OG	1:B:359:GLY:N	2.37	0.56
1:B:362:LYS:O	1:B:363:ARG:HB2	2.06	0.55
1:A:216:LEU:HD12	1:A:231:LEU:HD11	1.87	0.55
1:B:14:LYS:O	1:B:49:ARG:N	2.36	0.55
1:B:38:GLU:HG2	1:B:39:GLU:H	1.72	0.54
1:A:215:GLN:O	1:A:216:LEU:HD23	2.07	0.54
1:B:226:LEU:HD22	1:B:259:ARG:HH21	1.73	0.54
1:B:385:GLU:CD	1:B:387:ARG:HH11	2.07	0.53
1:B:367:ARG:NH1	1:B:369:ARG:NH2	2.57	0.53
1:A:63:VAL:HG13	1:A:98:LEU:HD11	1.91	0.53
1:A:24:LEU:HD12	1:A:387:ARG:HD3	1.91	0.53
1:B:136:ARG:NH2	5:B:464:HOH:O	2.41	0.52
1:B:149:THR:HG22	1:B:188:GLU:HB2	1.90	0.52
1:A:6:GLY:N	5:A:471:HOH:O	2.42	0.52
1:B:7:GLN:HG2	1:B:54:GLN:OE1	2.10	0.52
1:B:49:ARG:HD2	5:B:511:HOH:O	2.10	0.52
1:A:162:ASN:ND2	5:A:488:HOH:O	2.42	0.51
1:B:72:ASP:OD1	5:B:500:HOH:O	2.20	0.50
1:B:311:ASP:OD1	1:B:325:MET:HG2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LEU:HB3	1:A:131:LEU:HD13	1.93	0.50
1:A:27:ASN:OD1	1:A:384:ASP:O	2.29	0.49
1:A:200:LEU:CD2	1:A:214:LEU:HD13	2.41	0.49
1:B:317:LEU:N	1:B:317:LEU:HD23	2.28	0.49
1:B:332:ASP:HB2	5:B:471:HOH:O	2.12	0.49
1:A:9:PHE:HD2	1:A:10:LEU:HD13	1.78	0.48
1:B:130:SER:OG	5:B:508:HOH:O	2.18	0.48
1:A:40:TRP:H	1:A:74:GLY:H	1.60	0.48
1:A:314:PHE:CG	1:A:322:LEU:HD23	2.48	0.48
1:A:136:ARG:NH2	5:A:454:HOH:O	2.47	0.48
1:B:248:ASP:CG	1:B:250:ARG:HH22	2.17	0.48
1:B:9:PHE:CD2	1:B:10:LEU:HD13	2.46	0.47
1:A:42:GLN:O	1:A:69:LEU:HD13	2.14	0.47
1:A:149:THR:HG23	1:A:188:GLU:HB2	1.95	0.47
1:A:362:LYS:O	1:A:363:ARG:HB2	2.13	0.47
2:A:408:C8E:H171	2:A:408:C8E:H141	1.37	0.46
1:A:22:PHE:O	1:A:40:TRP:HA	2.14	0.46
1:B:238:ASP:OD2	1:B:246:LYS:HA	2.16	0.46
1:B:161:ARG:NE	3:B:410:SO4:O2	2.41	0.46
1:B:137:GLY:HA3	1:B:155:PHE:HA	1.97	0.46
1:A:49:ARG:HG2	1:A:62:ASP:CG	2.36	0.46
1:B:234:PHE:HZ	1:B:288:THR:HG21	1.80	0.46
1:A:24:LEU:HD12	1:A:387:ARG:CD	2.45	0.46
1:A:259:ARG:NH1	1:A:261:GLY:O	2.49	0.46
1:A:119:VAL:O	1:A:119:VAL:CG2	2.62	0.45
1:B:52:PHE:CE2	1:B:103:LYS:HG3	2.51	0.45
1:A:216:LEU:HB2	1:A:231:LEU:HG	1.97	0.45
1:B:170:SER:HB2	5:B:470:HOH:O	2.16	0.45
1:B:213:TYR:CD1	1:B:234:PHE:CE1	3.04	0.45
1:A:184:PHE:HA	1:A:202:ASN:O	2.16	0.45
1:B:226:LEU:C	1:B:227:LEU:HD23	2.37	0.45
1:A:294:TYR:CE2	1:A:369:ARG:HD3	2.52	0.45
1:B:7:GLN:HA	1:B:12:ASP:OD2	2.17	0.45
1:B:191:PHE:N	1:B:191:PHE:CD2	2.84	0.45
1:B:386:ASN:HD22	2:B:408:C8E:H171	1.82	0.45
1:A:336:LEU:HB3	1:A:339:VAL:HB	1.98	0.45
1:B:218:HIS:NE2	1:B:220:GLN:HB2	2.32	0.45
1:B:64:LEU:HB3	1:B:99:ALA:HB3	2.00	0.44
1:A:305:SER:HA	1:A:330:HIS:O	2.17	0.44
1:A:354:TYR:O	1:A:365:ASN:HA	2.17	0.44
1:A:20:ARG:NH1	1:A:129:ARG:O	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:PHE:HB2	1:B:322:LEU:HB3	2.00	0.44
1:B:319:LEU:HD23	1:B:322:LEU:HD22	1.99	0.44
1:A:154:GLN:HA	1:A:182:PHE:O	2.17	0.44
2:A:408:C8E:H112	2:A:408:C8E:H141	1.66	0.44
1:A:38:GLU:HG2	1:A:39:GLU:N	2.33	0.44
1:B:71:LEU:O	1:B:72:ASP:CB	2.63	0.43
1:B:315:VAL:HG11	5:B:472:HOH:O	2.17	0.43
1:B:135:PHE:CE1	1:B:158:ASN:HB2	2.53	0.43
1:A:63:VAL:CG1	1:A:98:LEU:HD11	2.48	0.43
1:B:70:LYS:HG3	1:B:73:GLY:C	2.38	0.43
1:B:181:ARG:O	1:B:205:LEU:HD12	2.18	0.43
1:A:22:PHE:HE1	5:A:530:HOH:O	2.01	0.43
1:A:234:PHE:O	1:A:250:ARG:HA	2.18	0.43
1:B:213:TYR:HA	1:B:233:GLY:O	2.19	0.43
1:A:353:GLY:HA2	1:A:366:VAL:O	2.19	0.43
1:B:308:LEU:HD13	1:B:309:ARG:N	2.34	0.43
1:A:64:LEU:HB3	1:A:99:ALA:HB3	2.01	0.43
1:B:97:ARG:HD2	1:B:164:ALA:O	2.19	0.42
1:B:72:ASP:HA	1:B:73:GLY:HA2	1.61	0.42
1:B:95:PHE:HB2	1:B:164:ALA:HB2	2.01	0.42
1:B:347:GLY:HA2	1:B:372:SER:O	2.19	0.42
1:A:168:ASP:HB3	1:A:178:THR:HB	2.01	0.42
1:B:156:ARG:HD3	1:B:181:ARG:NH1	2.35	0.42
1:A:162:ASN:OD1	5:A:433:HOH:O	2.22	0.42
1:A:36:LYS:HB3	1:A:36:LYS:HE2	1.73	0.42
1:A:67:TYR:CE1	1:A:94:ASP:OD2	2.73	0.42
1:A:313:ASP:OD2	5:A:440:HOH:O	2.22	0.42
1:B:370:ASN:ND2	2:B:408:C8E:H82	2.34	0.41
1:A:38:GLU:HG2	1:A:39:GLU:H	1.85	0.41
1:A:200:LEU:HD21	1:A:214:LEU:HD13	2.01	0.41
1:B:314:PHE:CG	1:B:322:LEU:HD23	2.55	0.41
1:A:70:LYS:C	1:A:72:ASP:H	2.23	0.41
1:B:20:ARG:HH11	1:B:130:SER:C	2.23	0.41
1:B:326:THR:CG2	2:B:406:C8E:H71	2.43	0.41
1:B:375:ARG:NH1	5:B:462:HOH:O	2.53	0.41
1:A:26:ARG:HD2	1:A:28:PHE:CZ	2.55	0.41
1:A:189:TYR:CE2	1:A:191:PHE:HB3	2.55	0.41
1:A:312:PHE:HE2	1:A:314:PHE:CD1	2.38	0.41
1:B:375:ARG:O	1:B:382:ARG:HD3	2.20	0.41
1:A:68:SER:O	1:A:94:ASP:HB2	2.21	0.41
1:B:370:ASN:HD21	2:B:408:C8E:H101	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:LEU:HD12	1:A:10:LEU:HA	1.88	0.41
1:B:106:VAL:O	1:B:107:SER:HB3	2.20	0.41
1:A:358:SER:HA	1:A:362:LYS:HD2	2.03	0.41
1:B:193:GLY:O	1:B:194:GLU:HB2	2.21	0.41
1:B:248:ASP:OD1	1:B:248:ASP:C	2.59	0.41
1:B:320:PRO:HB2	1:B:357:GLN:HE21	1.83	0.40
2:A:407:C8E:H171	2:A:407:C8E:H142	1.88	0.40
1:A:198:LEU:HD12	1:A:216:LEU:HD23	2.03	0.40
1:A:198:LEU:CD1	1:A:216:LEU:CD2	2.99	0.40
1:B:293:SER:HB2	1:B:349:GLU:OE1	2.22	0.40
1:A:6:GLY:HA2	5:A:496:HOH:O	2.21	0.40
1:A:129:ARG:HB3	1:A:130:SER:H	1.66	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	360/405 (89%)	343 (95%)	16 (4%)	1 (0%)	41	50
1	B	366/405 (90%)	352 (96%)	12 (3%)	2 (0%)	29	35
All	All	726/810 (90%)	695 (96%)	28 (4%)	3 (0%)	34	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	72	ASP
1	A	7	GLN
1	B	129	ARG

### 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	288/320 (90%)	271 (94%)	17 (6%)	19	26
1	B	291/320 (91%)	276 (95%)	15 (5%)	23	32
All	All	579/640 (90%)	547 (94%)	32 (6%)	21	29

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	10	LEU
1	B	130	SER
1	B	171	LEU
1	B	202	ASN
1	B	248	ASP
1	B	250	ARG
1	B	304	ARG
1	B	308	LEU
1	B	317	LEU
1	B	375	ARG
1	B	382	ARG
1	B	385	GLU
1	B	387	ARG
1	B	394	LEU
1	B	396	LEU
1	A	10	LEU
1	A	27	ASN
1	A	69	LEU
1	A	149	THR
1	A	171	LEU
1	A	174	ARG
1	A	210	ARG
1	A	235	ARG
1	A	250	ARG
1	A	253	SER
1	A	285	SER
1	A	304	ARG

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Mol	Chain	Res	Type
1	A	336	LEU
1	A	382	ARG
1	A	385	GLU
1	A	394	LEU
1	A	396	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	357	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](#)

13 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	407	-	13,13,20	0.46	0	12,12,19	0.35	0
2	C8E	A	408	-	15,15,20	0.47	0	14,14,19	0.28	0
2	C8E	B	408	-	18,18,20	0.40	0	17,17,19	0.49	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	3PE	A	406	-	19,19,50	1.29	2 (10%)	22,24,55	1.46	3 (13%)
3	SO4	B	412	-	4,4,4	0.19	0	6,6,6	0.27	0
3	SO4	B	411	-	4,4,4	0.13	0	6,6,6	0.33	0
3	SO4	B	413	-	4,4,4	0.15	0	6,6,6	0.21	0
3	SO4	A	409	-	4,4,4	0.10	0	6,6,6	0.36	0
2	C8E	B	406	-	6,6,20	0.31	0	5,5,19	0.40	0
3	SO4	B	410	-	4,4,4	0.19	0	6,6,6	0.28	0
2	C8E	B	407	-	7,7,20	0.44	0	6,6,19	0.19	0
3	SO4	A	410	-	4,4,4	0.13	0	6,6,6	0.21	0
3	SO4	B	409	-	4,4,4	0.15	0	6,6,6	0.25	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	407	-	-	7/11/11/18	-
2	C8E	A	408	-	-	9/13/13/18	-
2	C8E	B	408	-	-	11/16/16/18	-
4	3PE	A	406	-	-	9/22/22/54	-
2	C8E	B	406	-	-	2/4/4/18	-
2	C8E	B	407	-	-	4/5/5/18	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	406	3PE	O21-C2	-3.33	1.38	1.46
4	A	406	3PE	O31-C3	-3.00	1.38	1.45

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	406	3PE	O31-C3-C2	3.79	119.47	108.43
4	A	406	3PE	O21-C21-C22	3.47	120.48	110.80
4	A	406	3PE	O13-C11-C12	2.10	116.95	109.10

There are no chirality outliers.

All (42) torsion outliers are listed below:

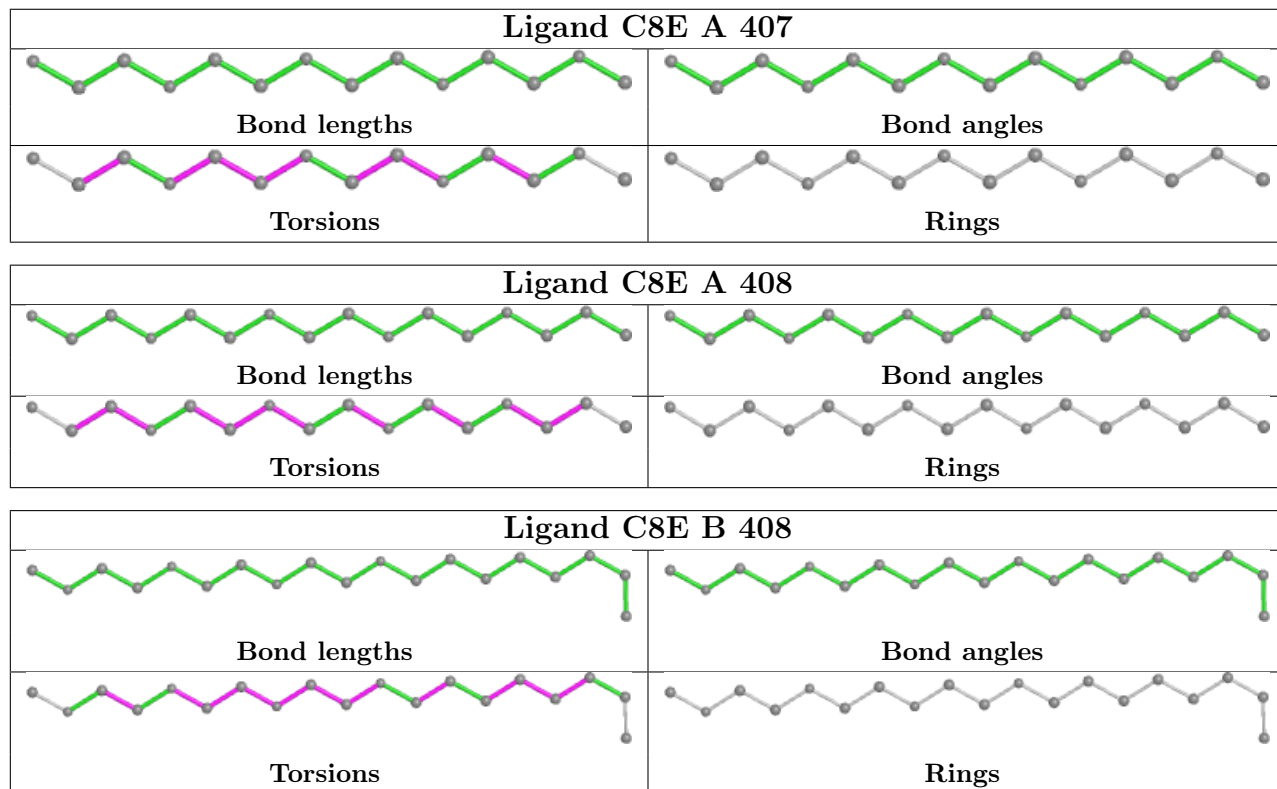
Mol	Chain	Res	Type	Atoms
4	A	406	3PE	O13-C11-C12-N
4	A	406	3PE	C22-C21-O21-C2
2	A	408	C8E	C17-C16-O15-C14
4	A	406	3PE	O22-C21-O21-C2
2	A	407	C8E	O12-C13-C14-O15
2	B	408	C8E	O12-C13-C14-O15
2	A	408	C8E	C6-C7-C8-O9
4	A	406	3PE	O32-C31-O31-C3
2	A	407	C8E	O9-C10-C11-O12
2	B	408	C8E	O9-C10-C11-O12
2	A	407	C8E	O18-C19-C20-O21
2	B	408	C8E	C2-C3-C4-C5
2	B	408	C8E	C3-C4-C5-C6
2	B	408	C8E	C6-C7-C8-O9
2	A	408	C8E	C14-C13-O12-C11
2	B	406	C8E	C7-C8-O9-C10
4	A	406	3PE	O11-C1-C2-O21
2	B	407	C8E	O18-C19-C20-O21
4	A	406	3PE	C32-C31-O31-C3
2	A	407	C8E	C17-C16-O15-C14
4	A	406	3PE	O11-C1-C2-C3
2	B	408	C8E	O15-C16-C17-O18
2	B	407	C8E	O15-C16-C17-O18
2	B	407	C8E	C20-C19-O18-C17
2	A	408	C8E	C13-C14-O15-C16
2	B	407	C8E	C16-C17-O18-C19
2	A	407	C8E	C16-C17-O18-C19
2	B	406	C8E	C5-C6-C7-C8
2	A	408	C8E	C20-C19-O18-C17
4	A	406	3PE	C1-O11-P-O13
2	B	408	C8E	C11-C10-O9-C8
2	B	408	C8E	C14-C13-O12-C11
2	A	408	C8E	O18-C19-C20-O21
2	B	408	C8E	C13-C14-O15-C16
2	B	408	C8E	C10-C11-O12-C13
2	A	407	C8E	C14-C13-O12-C11
2	A	408	C8E	O15-C16-C17-O18
2	A	407	C8E	O15-C16-C17-O18
2	A	408	C8E	O9-C10-C11-O12
2	B	408	C8E	C4-C5-C6-C7
4	A	406	3PE	C1-O11-P-O14
2	A	408	C8E	C7-C8-O9-C10

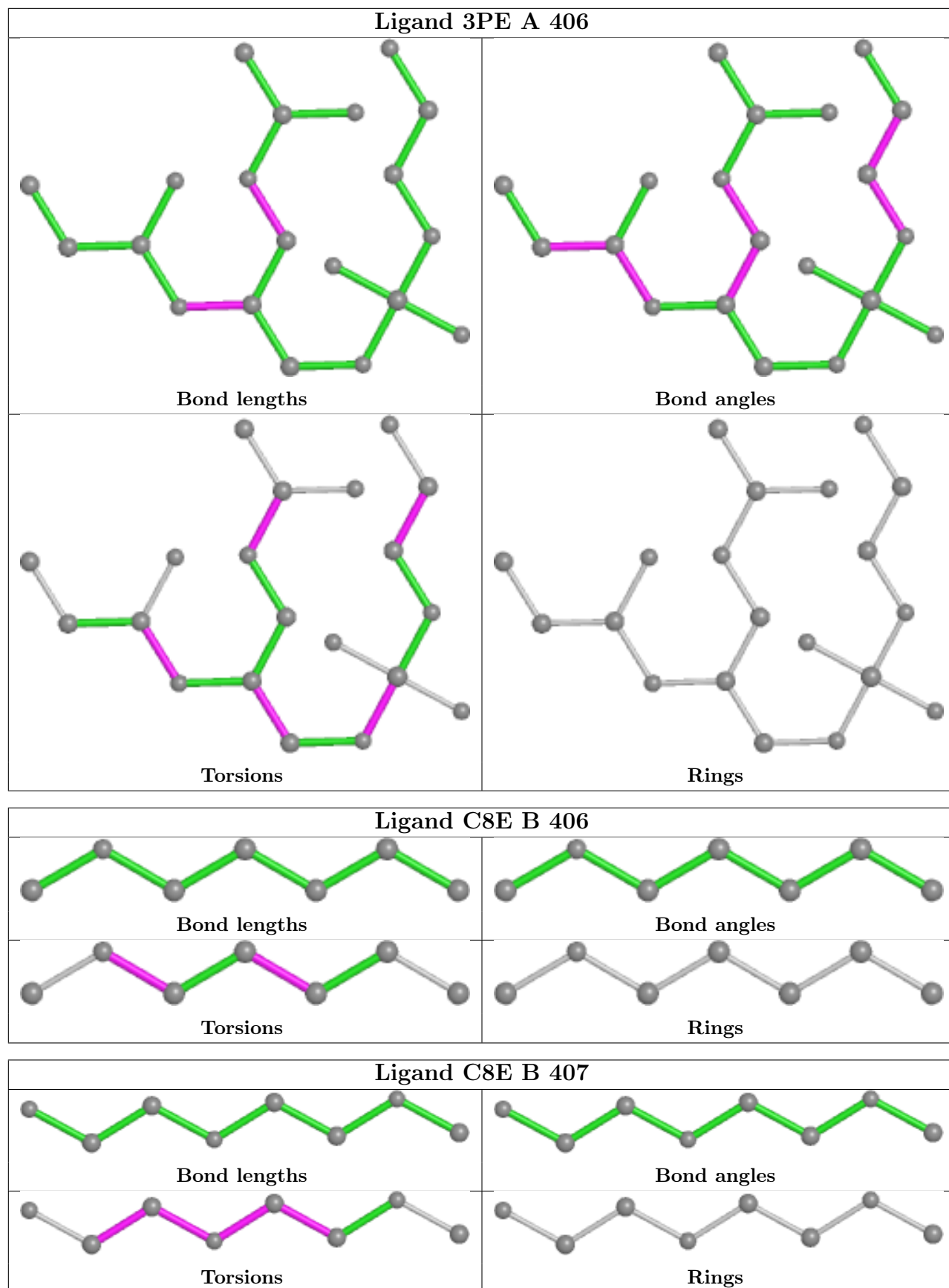
There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	407	C8E	1	0
2	A	408	C8E	3	0
2	B	408	C8E	7	0
2	B	406	C8E	2	0
3	B	410	SO4	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, 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	368/405 (90%)	0.26	12 (3%) 46 53	15, 24, 43, 63	0
1	B	371/405 (91%)	0.29	6 (1%) 72 78	11, 23, 39, 54	0
All	All	739/810 (91%)	0.28	18 (2%) 59 66	11, 24, 41, 63	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	29	VAL	5.4
1	B	7	GLN	4.5
1	A	30	GLY	4.3
1	A	92	ALA	3.7
1	A	73	GLY	3.1
1	A	231	LEU	2.8
1	A	28	PHE	2.7
1	A	224	ASP	2.7
1	B	145	ILE	2.5
1	B	318	GLY	2.4
1	A	222	LEU	2.4
1	A	35	GLY	2.3
1	A	74	GLY	2.3
1	B	73	GLY	2.3
1	B	193	GLY	2.2
1	B	146	ALA	2.2
1	A	361	PHE	2.1
1	A	221	PRO	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](#)

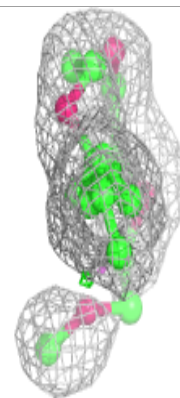
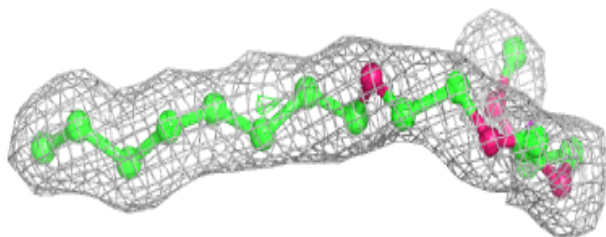
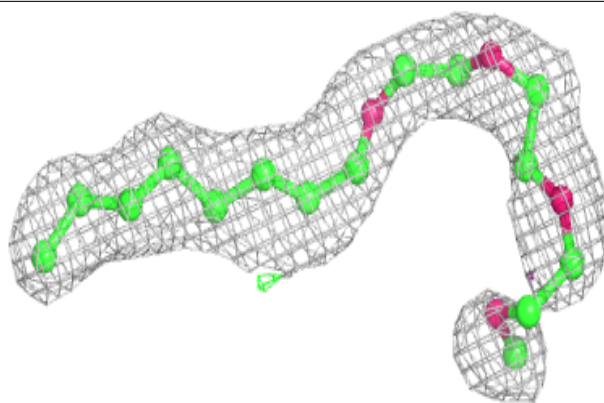
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	C8E	B	408	19/21	0.86	0.20	24,31,47,50	0
2	C8E	A	407	14/21	0.86	0.16	27,35,41,42	0
2	C8E	A	408	16/21	0.87	0.17	22,27,32,38	0
3	SO4	B	412	5/5	0.89	0.17	35,40,41,61	0
4	3PE	A	406	20/51	0.89	0.17	63,69,76,82	0
2	C8E	B	407	8/21	0.91	0.12	30,34,36,40	0
3	SO4	A	410	5/5	0.92	0.13	38,48,52,58	0
3	SO4	B	410	5/5	0.93	0.17	32,41,54,60	0
2	C8E	B	406	7/21	0.94	0.19	15,19,23,25	0
3	SO4	B	413	5/5	0.94	0.21	46,57,64,73	0
3	SO4	A	409	5/5	0.96	0.28	30,40,43,50	0
3	SO4	B	409	5/5	0.96	0.17	35,41,45,46	0
3	SO4	B	411	5/5	0.96	0.20	35,43,58,59	0

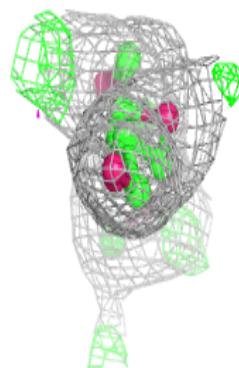
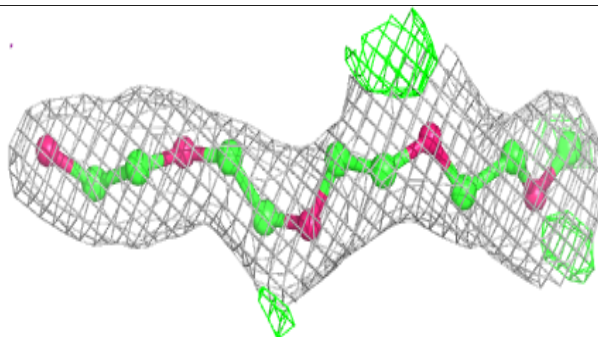
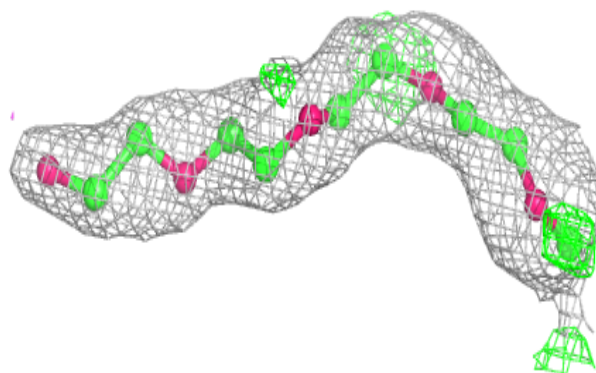
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around C8E B 408:**

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

**Electron density around C8E A 407:**

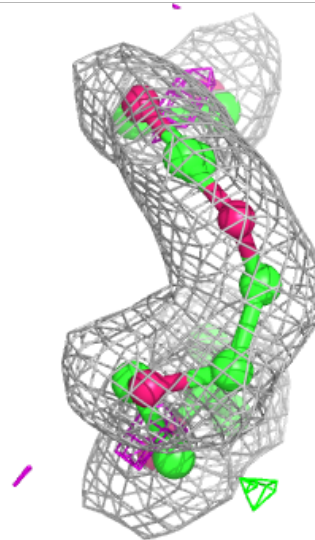
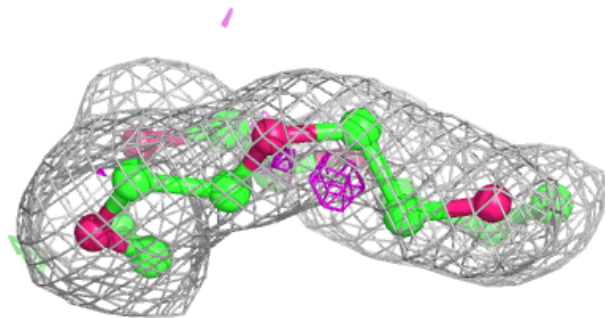
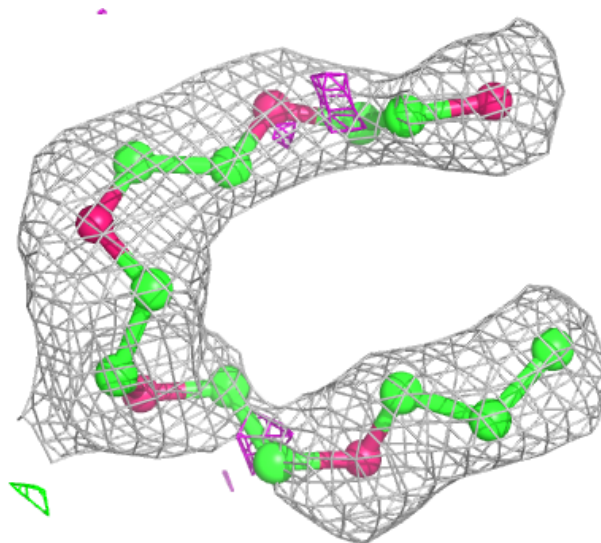
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





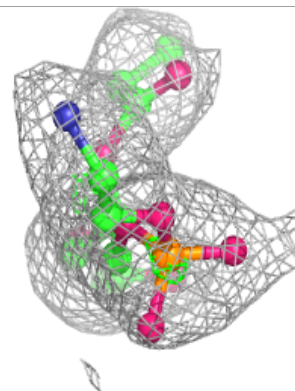
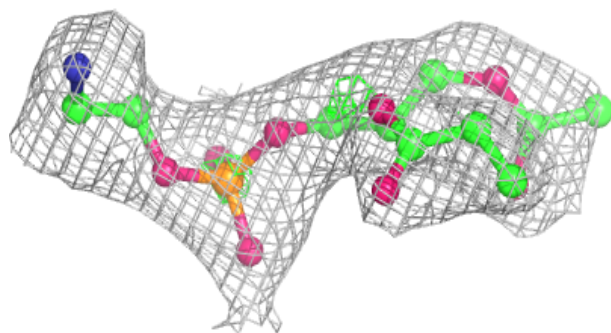
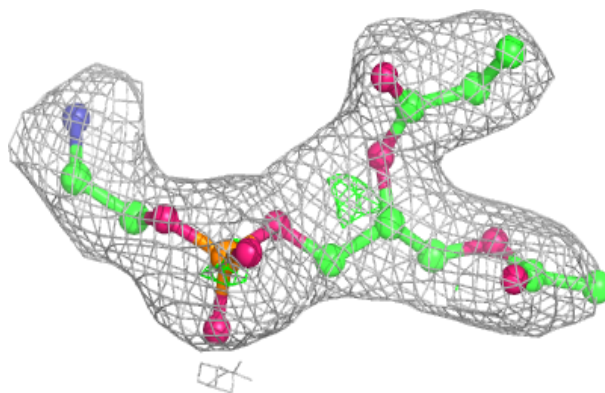
**Electron density around C8E A 408:**

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

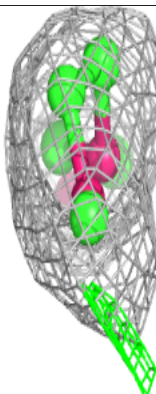
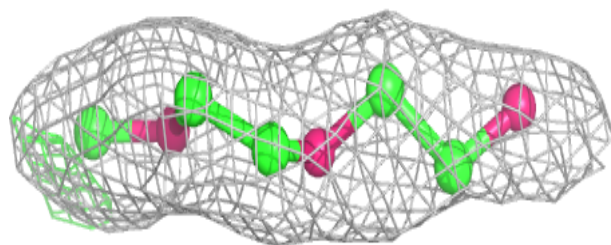
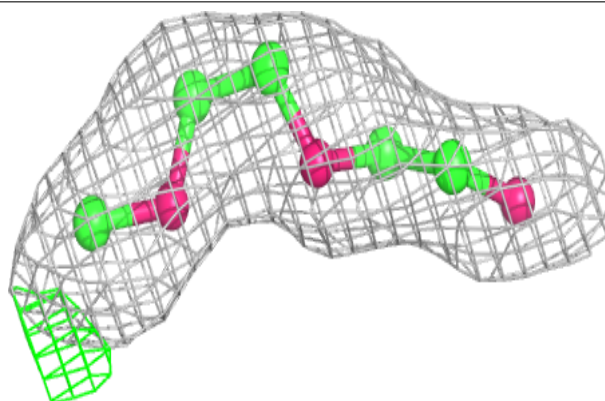


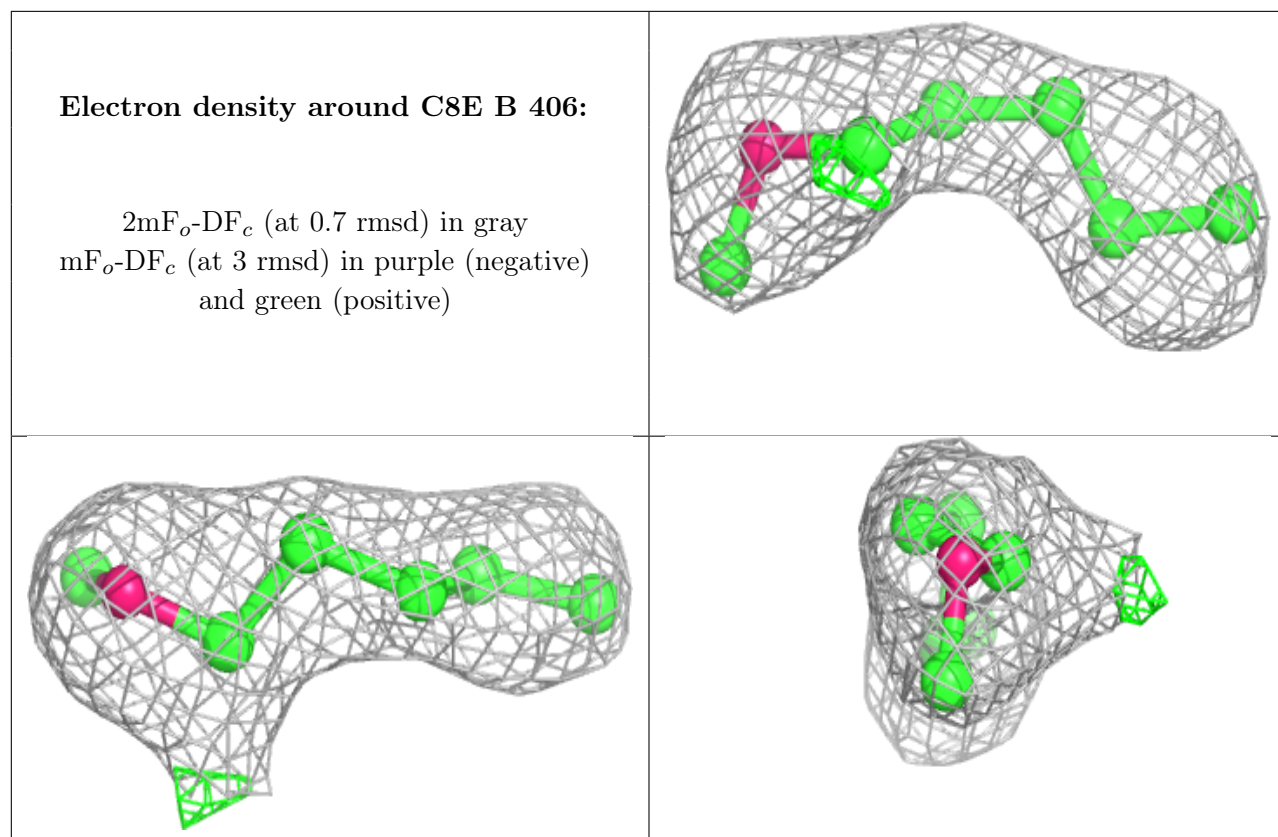
**Electron density around 3PE A 406:**

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

**Electron density around C8E B 407:**

$2mF_o-DF_c$  (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.