Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	4Q35
Title	:	Structure of a membrane protein
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Deposited on	:	2014-04-11
Resolution	:	2.39 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 (i) symbol.

The following versions of software and data (see references (i)) 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 2.39 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.
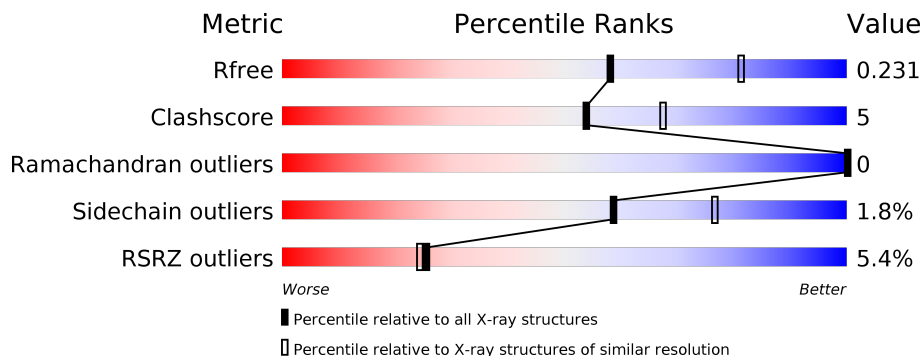
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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	802	5% / 82% / 12% / 5%
2	B	175	5% / 77% / 9% / 14%

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
4	LDA	A	2013	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8165 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 LPS-assembly protein LptD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	758	Total 6198	C 3898	N 1063	O 1217	S 20	0	8	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	785	MET	-	expression tag	UNP Q83SQ0
A	786	ARG	-	expression tag	UNP Q83SQ0
A	787	TYR	-	expression tag	UNP Q83SQ0
A	788	LEU	-	expression tag	UNP Q83SQ0
A	789	ALA	-	expression tag	UNP Q83SQ0
A	790	THR	-	expression tag	UNP Q83SQ0
A	791	LEU	-	expression tag	UNP Q83SQ0
A	792	LEU	-	expression tag	UNP Q83SQ0
A	793	LEU	-	expression tag	UNP Q83SQ0
A	794	SER	-	expression tag	UNP Q83SQ0
A	795	LEU	-	expression tag	UNP Q83SQ0
A	796	ALA	-	expression tag	UNP Q83SQ0
A	797	VAL	-	expression tag	UNP Q83SQ0
A	798	LEU	-	expression tag	UNP Q83SQ0
A	799	ILE	-	expression tag	UNP Q83SQ0
A	800	THR	-	expression tag	UNP Q83SQ0
A	801	ALA	-	expression tag	UNP Q83SQ0
A	802	GLY	-	expression tag	UNP Q83SQ0

- Molecule 2 is a protein called LPS-assembly lipoprotein LptE.

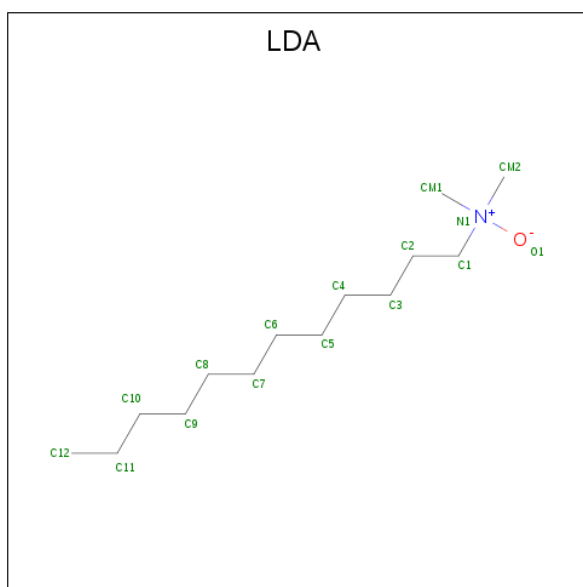| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	150	Total 1181	C 737	N 215	O 222	S 7	0	0	0

- Molecule 3 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code:

C8E) (formula: $C_{16}H_{34}O_5$).
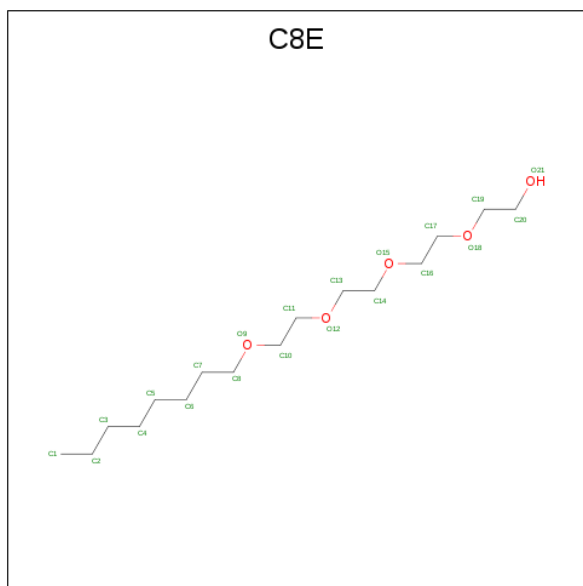
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 21	C 16	O 5	0	0
3	A	1	Total 21	C 16	O 5	0	0
3	A	1	Total 21	C 16	O 5	0	0
3	A	1	Total 21	C 16	O 5	0	0
3	A	1	Total 21	C 16	O 5	0	0
3	A	1	Total 21	C 16	O 5	0	0

• Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).

LDA

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 16	C 14	N 1	O 1	0	0
4	A	1	Total 16	C 14	N 1	O 1	0	0
4	A	1	Total 16	C 14	N 1	O 1	0	0
4	A	1	Total 16	C 14	N 1	O 1	0	0
4	A	1	Total 7	C 7			0	0
4	A	1	Total 7	C 7			0	0
4	A	1	Total 9	C 9			0	0

• Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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

- Molecule 6 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	438	Total 438	O 438	0	0
6	B	90	Total 90	O 90	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: LPS-assembly protein LptD
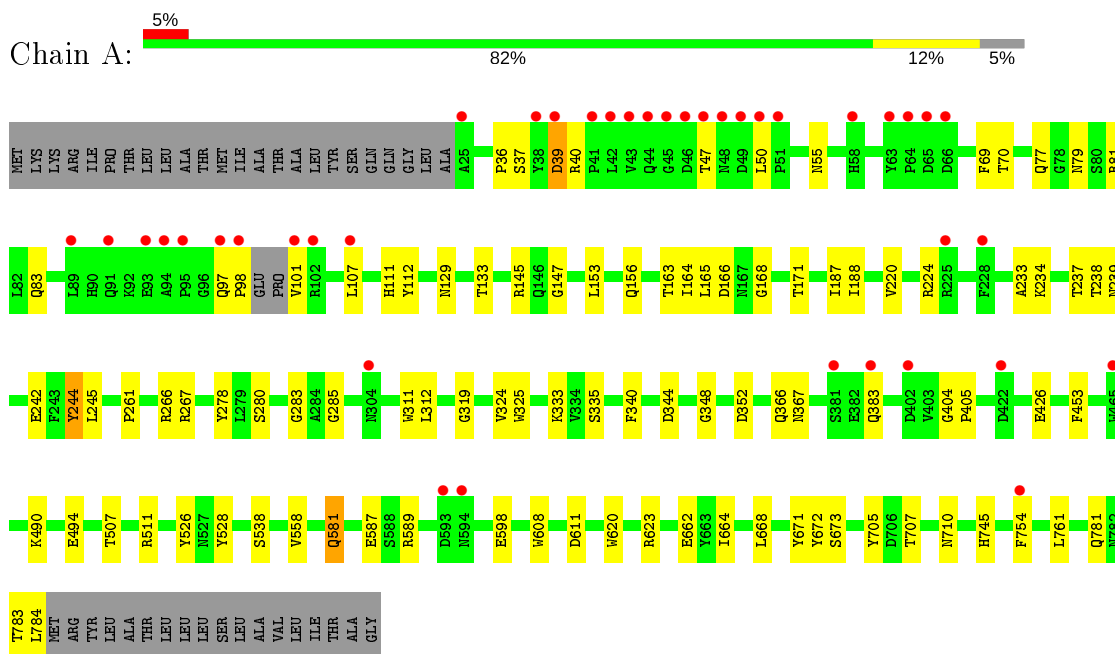
- Molecule 2: LPS-assembly lipoprotein LptE
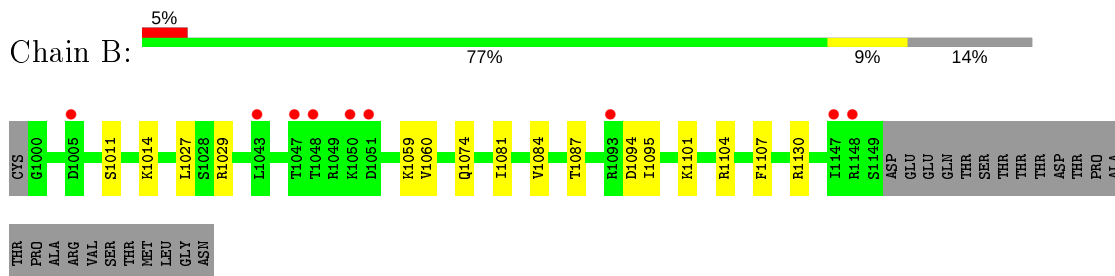
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	240.82Å 116.62Å 68.04Å 90.00° 103.71° 90.00°	Depositor
Resolution (Å)	40.63 – 2.39	Depositor
	40.63 – 2.39	EDS
% Data completeness	98.7 (40.63-2.39)	Depositor
(in resolution range)	98.8 (40.63-2.39)	EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	4.66 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.186 , 0.231	Depositor
	0.189 , 0.231	DCC
R_{free} test set	3667 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å^2)	23.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 57.8	EDS
L-test for twinning[2]	$<|L|>$ = 0.49, $<L^2>$ = 0.32	Xtriage
Estimated twinning fraction	0.021 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8165	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ 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: LDA, C8E, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.39	0/6371	0.62	0/8672
2	B	0.36	0/1198	0.53	0/1617
All	All	0.39	0/7569	0.61	0/10289

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	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	36	PRO	Peptide
1	A	37	SER	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	6198	0	5772	65	0
2	B	1181	0	1212	11	0
3	A	126	0	204	13	0
4	A	87	0	167	9	0
5	A	40	0	0	1	0
5	B	5	0	0	1	0
6	A	438	0	0	7	0
6	B	90	0	0	1	0
All	All	8165	0	7355	79	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 5.

All (79) 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:623:ARG:HH21	1:A:784:LEU:HD12	1.52	0.74
1:A:705:TYR:OH	1:A:710:ASN:OD1	2.05	0.70
1:A:234:LYS:NZ	1:A:244[B]:TYR:OH	2.25	0.70
2:B:1087:THR:HB	2:B:1095:ILE:HD11	1.78	0.64
2:B:1059:LYS:O	6:B:1333:HOH:O	2.15	0.64
1:A:97:GLN:HB3	1:A:98:PRO:HD2	1.80	0.63
2:B:1104:ARG:NH2	5:B:1201:SO4:O3	2.32	0.63
1:A:366:GLN:O	2:B:1029:ARG:NH2	2.33	0.61
1:A:238:THR:HG23	1:A:267:ARG:HH21	1.65	0.60
1:A:156:GLN:HG2	3:A:2001:C8E:H202	1.84	0.59
1:A:101:VAL:N	1:A:129:ASN:OD1	2.35	0.59
1:A:233:ALA:HB3	1:A:754[A]:PHE:CE2	2.38	0.59
1:A:133:THR:HG21	3:A:2001:C8E:H41	1.83	0.59
2:B:1060:VAL:HG12	2:B:1084:VAL:HG22	1.84	0.58
1:A:668:LEU:HD13	1:A:672:TYR:CD2	2.39	0.58
1:A:352:ASP:OD1	6:A:2286:HOH:O	2.17	0.56
1:A:761:LEU:O	6:A:2178:HOH:O	2.18	0.56
1:A:145:ARG:HH11	4:A:2005:LDA:H11	1.70	0.55
1:A:707:THR:HB	3:A:2009:C8E:H132	1.89	0.53
1:A:163:THR:HG23	3:A:2001:C8E:H171	1.90	0.53
1:A:145:ARG:HD2	4:A:2005:LDA:HM11	1.92	0.52
1:A:280:SER:HB2	3:A:2011:C8E:O12	2.10	0.52
1:A:69:PHE:O	1:A:70:THR:OG1	2.26	0.52
1:A:145:ARG:NH1	4:A:2005:LDA:H11	2.26	0.50
1:A:340:PHE:CE1	1:A:348:GLY:HA3	2.46	0.49
1:A:47:THR:HA	1:A:50:LEU:HD12	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:TRP:CD1	3:A:2007:C8E:H62	2.48	0.49
1:A:81:ARG:NH1	1:A:83:GLN:OE1	2.34	0.48
6:A:2534:HOH:O	2:B:1074:GLN:HG2	2.12	0.48
1:A:490:LYS:HG2	1:A:511:ARG:HG3	1.95	0.48
1:A:367[B]:ASN:ND2	6:A:2274:HOH:O	2.38	0.47
1:A:47:THR:O	1:A:77:GLN:NE2	2.34	0.47
1:A:283:GLY:HA3	1:A:319:GLY:HA3	1.96	0.47
1:A:112:TYR:CE2	3:A:2001:C8E:H51	2.50	0.47
1:A:238:THR:O	1:A:266:ARG:HD3	2.14	0.47
2:B:1094:ASP:OD1	2:B:1095:ILE:N	2.42	0.47
1:A:707:THR:HG21	3:A:2009:C8E:H111	1.97	0.46
1:A:426:GLU:HG2	6:A:2510:HOH:O	2.15	0.46
1:A:224:ARG:NH1	5:A:2014:SO4:O3	2.39	0.46
1:A:324:VAL:HG23	1:A:325:TRP:CD1	2.51	0.46
3:A:2011:C8E:H111	4:A:2013:LDA:H111	1.97	0.46
1:A:165:LEU:HB2	1:A:187:ILE:HB	1.97	0.46
1:A:781:GLN:HG2	2:B:1081:ILE:HG12	1.98	0.46
1:A:164:ILE:HD12	1:A:188:ILE:HG12	1.98	0.46
1:A:598:GLU:HG3	1:A:662:GLU:HG2	1.98	0.46
1:A:147:GLY:HA2	1:A:171:THR:O	2.16	0.45
1:A:156:GLN:NE2	3:A:2001:C8E:H142	2.31	0.45
1:A:278:TYR:CZ	1:A:285:GLY:HA3	2.52	0.45
4:A:2010:LDA:H81	4:A:2010:LDA:H112	1.64	0.45
1:A:383:GLN:HG3	1:A:671:TYR:CZ	2.51	0.45
4:A:2004:LDA:H22	4:A:2004:LDA:HM21	1.55	0.45
1:A:40:ARG:NH2	1:A:79:ASN:O	2.50	0.45
1:A:581:GLN:HB3	1:A:608:TRP:CD2	2.53	0.44
1:A:244[B]:TYR:OH	1:A:344:ASP:OD2	2.26	0.44
1:A:311:TRP:CD1	1:A:335:SER:HB3	2.53	0.44
2:B:1011:SER:HA	2:B:1014:LYS:HG2	1.99	0.44
1:A:165:LEU:HB3	1:A:168:GLY:HA3	2.00	0.43
1:A:558:VAL:HG11	4:A:2004:LDA:H52	2.00	0.43
1:A:238:THR:CG2	1:A:267:ARG:HH21	2.31	0.43
1:A:526:TYR:HB3	1:A:528:TYR:CZ	2.54	0.43
1:A:673:SER:HB2	6:A:2473:HOH:O	2.18	0.43
1:A:587:GLU:HG2	1:A:589:ARG:HG3	2.00	0.42
1:A:333:LYS:HD3	4:A:2006:LDA:H51	2.00	0.42
1:A:404:GLY:HA3	1:A:405:PRO:HD2	1.83	0.42
1:A:784:LEU:HG	2:B:1101:LYS:NZ	2.35	0.42
1:A:239:ASN:HB2	1:A:242:GLU:OE2	2.20	0.41
1:A:494:GLU:HG2	1:A:507:THR:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:ILE:HG23	1:A:668:LEU:HD12	2.02	0.41
1:A:39:ASP:O	1:A:40:ARG:HB2	2.21	0.41
1:A:239:ASN:OD1	1:A:267:ARG:NE	2.42	0.41
1:A:245:LEU:O	1:A:261:PRO:HD2	2.20	0.41
3:A:2007:C8E:H112	6:A:2237:HOH:O	2.21	0.41
1:A:153:LEU:HB3	1:A:166:ASP:HB2	2.03	0.41
1:A:220:VAL:HG11	4:A:2005:LDA:H122	2.02	0.41
2:B:1027:LEU:HD22	2:B:1060:VAL:HG13	2.02	0.41
3:A:2009:C8E:H51	3:A:2009:C8E:H81	1.85	0.40
3:A:2003:C8E:H12	3:A:2011:C8E:H82	2.04	0.40
1:A:783:THR:O	1:A:784:LEU:HB2	2.20	0.40
1:A:39:ASP:OD1	1:A:39:ASP:N	2.55	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	762/802 (95%)	735 (96%)	27 (4%)	0	100	100
2	B	148/175 (85%)	146 (99%)	2 (1%)	0	100	100
All	All	910/977 (93%)	881 (97%)	29 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	666/695 (96%)	652 (98%)	14 (2%)	53	72
2	B	131/153 (86%)	129 (98%)	2 (2%)	65	80
All	All	797/848 (94%)	781 (98%)	16 (2%)	59	74

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ASP
1	A	55	ASN
1	A	107	LEU
1	A	111[A]	HIS
1	A	111[B]	HIS
1	A	237	THR
1	A	244[A]	TYR
1	A	244[B]	TYR
1	A	312	LEU
1	A	453	PHE
1	A	538	SER
1	A	581	GLN
1	A	611	ASP
1	A	745	HIS
2	B	1107	PHE
2	B	1130	ARG

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)

22 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	#$|Z| > 2$
4	LDA	A	2013	-	8,8,15	0.29	0	7,7,17	0.49	0
3	C8E	A	2007	-	20,20,20	0.39	0	19,19,19	0.38	0
4	LDA	A	2010	-	6,6,15	0.26	0	5,5,17	0.42	0
4	LDA	A	2005	-	12,15,15	2.15	1 (8%)	14,17,17	0.47	0
3	C8E	A	2002	-	20,20,20	0.41	0	19,19,19	0.29	0
4	LDA	A	2006	-	12,15,15	2.02	1 (8%)	14,17,17	0.57	0
5	SO4	A	2018	-	4,4,4	0.13	0	6,6,6	0.12	0
3	C8E	A	2009	-	20,20,20	0.41	0	19,19,19	0.37	0
5	SO4	A	2020	-	4,4,4	0.14	0	6,6,6	0.06	0
4	LDA	A	2008	-	12,15,15	2.09	1 (8%)	14,17,17	0.44	0
5	SO4	A	2021	-	4,4,4	0.14	0	6,6,6	0.06	0
3	C8E	A	2003	-	20,20,20	0.41	0	19,19,19	0.39	0
5	SO4	B	1201	-	4,4,4	0.17	0	6,6,6	0.18	0
5	SO4	A	2016	-	4,4,4	0.17	0	6,6,6	0.06	0
4	LDA	A	2012	-	6,6,15	0.26	0	5,5,17	0.49	0
3	C8E	A	2011	-	20,20,20	0.39	0	19,19,19	0.36	0
5	SO4	A	2015	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	A	2014	-	4,4,4	0.14	0	6,6,6	0.05	0
3	C8E	A	2001	-	20,20,20	0.41	0	19,19,19	0.37	0
4	LDA	A	2004	-	12,15,15	2.07	1 (8%)	14,17,17	0.49	0
5	SO4	A	2017	-	4,4,4	0.16	0	6,6,6	0.06	0
5	SO4	A	2019	-	4,4,4	0.14	0	6,6,6	0.11	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
4	LDA	A	2012	-	-	3/4/4/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	C8E	A	2002	-	-	13/18/18/18	-
4	LDA	A	2013	-	-	3/6/6/13	-
3	C8E	A	2011	-	-	13/18/18/18	-
3	C8E	A	2007	-	-	12/18/18/18	-
4	LDA	A	2010	-	-	2/4/4/13	-
4	LDA	A	2006	-	-	7/13/13/13	-
3	C8E	A	2003	-	-	10/18/18/18	-
3	C8E	A	2001	-	-	7/18/18/18	-
4	LDA	A	2005	-	-	5/13/13/13	-
4	LDA	A	2004	-	-	8/13/13/13	-
3	C8E	A	2009	-	-	10/18/18/18	-
4	LDA	A	2008	-	-	7/13/13/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2005	LDA	O1-N1	-7.38	1.24	1.42
4	A	2008	LDA	O1-N1	-7.13	1.25	1.42
4	A	2004	LDA	O1-N1	-7.10	1.25	1.42
4	A	2006	LDA	O1-N1	-6.92	1.26	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (100) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2006	LDA	C2-C1-N1-O1
4	A	2006	LDA	C2-C1-N1-CM1
4	A	2006	LDA	C2-C1-N1-CM2
4	A	2004	LDA	C2-C1-N1-O1
4	A	2004	LDA	C2-C1-N1-CM2
3	A	2001	C8E	O18-C19-C20-O21
4	A	2008	LDA	C6-C7-C8-C9
3	A	2007	C8E	C7-C8-O9-C10
3	A	2001	C8E	O12-C13-C14-O15
3	A	2002	C8E	O12-C13-C14-O15
3	A	2002	C8E	C17-C16-O15-C14
3	A	2011	C8E	O12-C13-C14-O15

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Mol	Chain	Res	Type	Atoms
3	A	2003	C8E	O12-C13-C14-O15
3	A	2007	C8E	C6-C7-C8-O9
4	A	2004	LDA	C1-C2-C3-C4
3	A	2007	C8E	O18-C19-C20-O21
3	A	2002	C8E	O18-C19-C20-O21
3	A	2002	C8E	O15-C16-C17-O18
3	A	2002	C8E	C6-C7-C8-O9
3	A	2001	C8E	C6-C7-C8-O9
3	A	2011	C8E	C6-C7-C8-O9
3	A	2009	C8E	C2-C3-C4-C5
4	A	2008	LDA	C5-C6-C7-C8
4	A	2013	LDA	C11-C10-C9-C8
4	A	2005	LDA	C5-C6-C7-C8
3	A	2001	C8E	C2-C3-C4-C5
3	A	2011	C8E	C2-C3-C4-C5
4	A	2004	LDA	C7-C8-C9-C10
4	A	2005	LDA	C6-C7-C8-C9
3	A	2011	C8E	C5-C6-C7-C8
3	A	2003	C8E	C3-C4-C5-C6
3	A	2003	C8E	O9-C10-C11-O12
3	A	2009	C8E	C6-C7-C8-O9
4	A	2005	LDA	C1-C2-C3-C4
4	A	2008	LDA	C1-C2-C3-C4
4	A	2008	LDA	C9-C10-C11-C12
3	A	2007	C8E	C5-C6-C7-C8
4	A	2013	LDA	C7-C8-C9-C10
4	A	2010	LDA	C7-C8-C9-C10
4	A	2006	LDA	C7-C8-C9-C10
4	A	2008	LDA	C7-C8-C9-C10
3	A	2002	C8E	O9-C10-C11-O12
4	A	2005	LDA	C7-C8-C9-C10
3	A	2011	C8E	C3-C4-C5-C6
3	A	2001	C8E	C3-C4-C5-C6
3	A	2007	C8E	C4-C5-C6-C7
4	A	2006	LDA	C4-C5-C6-C7
4	A	2006	LDA	C9-C10-C11-C12
4	A	2006	LDA	C1-C2-C3-C4
3	A	2001	C8E	C1-C2-C3-C4
4	A	2012	LDA	C9-C10-C11-C12
3	A	2003	C8E	O15-C16-C17-O18
4	A	2010	LDA	C11-C10-C9-C8
4	A	2005	LDA	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
3	A	2003	C8E	C5-C6-C7-C8
3	A	2009	C8E	O15-C16-C17-O18
4	A	2008	LDA	C11-C10-C9-C8
3	A	2001	C8E	C14-C13-O12-C11
3	A	2003	C8E	C10-C11-O12-C13
3	A	2007	C8E	C13-C14-O15-C16
3	A	2003	C8E	C16-C17-O18-C19
3	A	2002	C8E	C16-C17-O18-C19
3	A	2009	C8E	C17-C16-O15-C14
3	A	2011	C8E	C10-C11-O12-C13
3	A	2003	C8E	C20-C19-O18-C17
3	A	2009	C8E	C20-C19-O18-C17
3	A	2007	C8E	C20-C19-O18-C17
3	A	2002	C8E	C20-C19-O18-C17
3	A	2007	C8E	C11-C10-O9-C8
3	A	2002	C8E	C7-C8-O9-C10
3	A	2007	C8E	C14-C13-O12-C11
3	A	2007	C8E	C17-C16-O15-C14
4	A	2012	LDA	C7-C8-C9-C10
3	A	2011	C8E	C7-C8-O9-C10
3	A	2002	C8E	C1-C2-C3-C4
3	A	2011	C8E	C20-C19-O18-C17
3	A	2011	C8E	C11-C10-O9-C8
3	A	2011	C8E	C16-C17-O18-C19
4	A	2004	LDA	C9-C10-C11-C12
3	A	2002	C8E	C13-C14-O15-C16
3	A	2009	C8E	C4-C5-C6-C7
3	A	2011	C8E	C17-C16-O15-C14
3	A	2009	C8E	O18-C19-C20-O21
3	A	2002	C8E	C14-C13-O12-C11
3	A	2003	C8E	C6-C7-C8-O9
3	A	2009	C8E	C3-C4-C5-C6
3	A	2011	C8E	C4-C5-C6-C7
4	A	2012	LDA	C11-C10-C9-C8
4	A	2004	LDA	C5-C6-C7-C8
3	A	2009	C8E	C13-C14-O15-C16
4	A	2004	LDA	C3-C4-C5-C6
3	A	2011	C8E	O18-C19-C20-O21
3	A	2003	C8E	O18-C19-C20-O21
4	A	2008	LDA	C4-C5-C6-C7
3	A	2002	C8E	C10-C11-O12-C13
3	A	2009	C8E	O12-C13-C14-O15

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Mol	Chain	Res	Type	Atoms
4	A	2013	LDA	C9-C10-C11-C12
3	A	2007	C8E	O9-C10-C11-O12
4	A	2004	LDA	C2-C3-C4-C5
3	A	2007	C8E	C3-C4-C5-C6

There are no ring outliers.

12 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2013	LDA	1	0
3	A	2007	C8E	2	0
4	A	2010	LDA	1	0
4	A	2005	LDA	4	0
4	A	2006	LDA	1	0
3	A	2009	C8E	3	0
3	A	2003	C8E	1	0
5	B	1201	SO4	1	0
3	A	2011	C8E	3	0
5	A	2014	SO4	1	0
3	A	2001	C8E	5	0
4	A	2004	LDA	2	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 then 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.

Ligand C8E A 2007

Bond lengths

Bond angles

Torsions

Rings

Ligand C8E A 2002

Bond lengths

Bond angles

Torsions

Rings

Ligand C8E A 2009

Bond lengths

Bond angles

Torsions

Rings

Ligand C8E A 2003

Bond lengths

Bond angles

Torsions

Rings

Ligand C8E A 2011

Bond lengths

Bond angles

Torsions

Rings

Ligand C8E A 2001

Bond lengths

Bond angles

Torsions

Rings
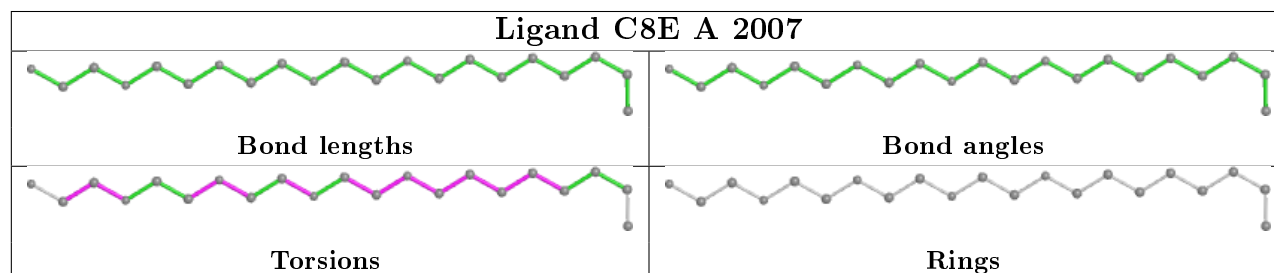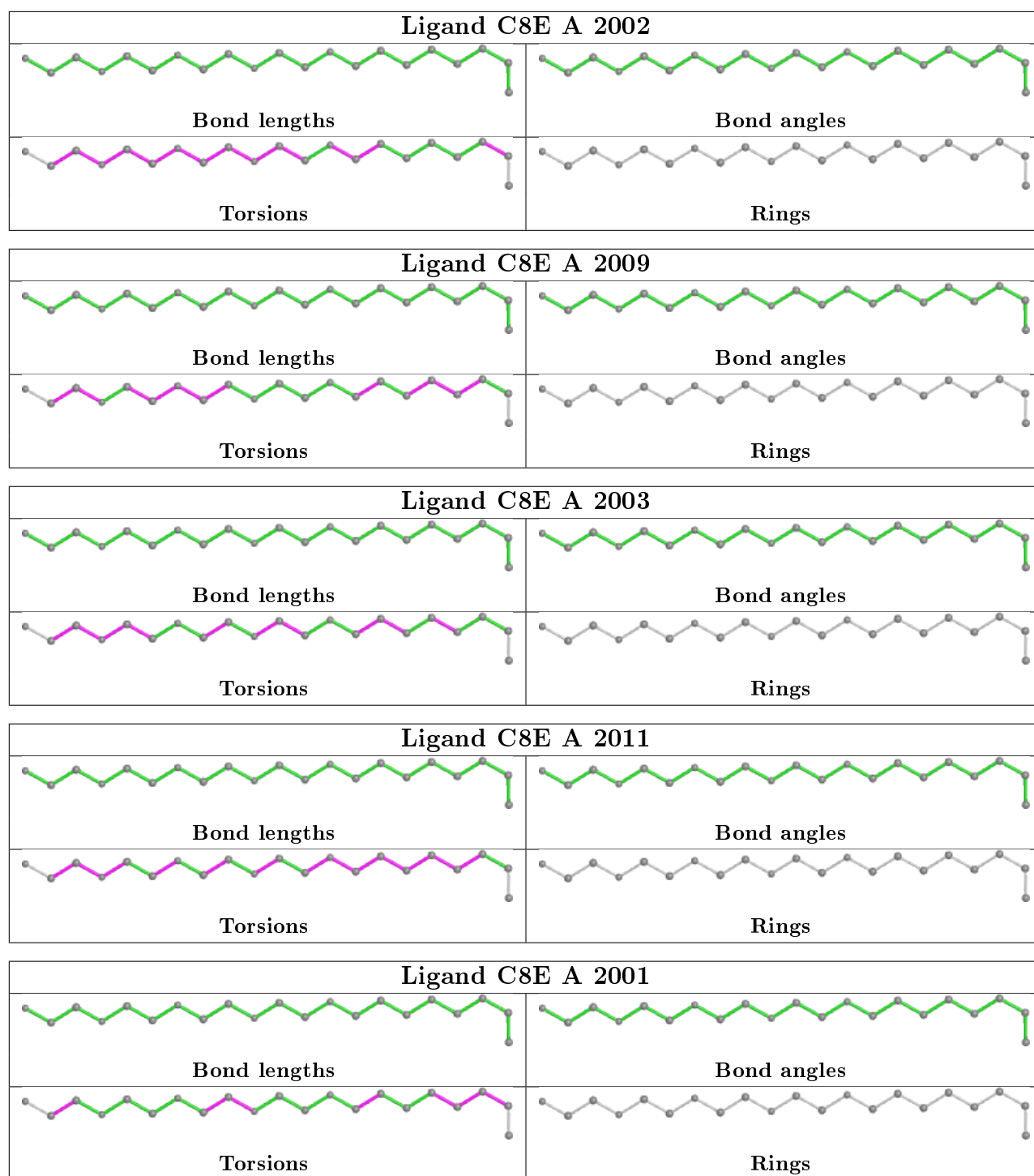
5.7 Other polymers (i)

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(Å²)	Q<0.9
1	A	758/802 (94%)	0.07	40 (5%)	26	25	6, 24, 75, 134	0
2	B	150/175 (85%)	0.36	9 (6%)	21	20	9, 28, 74, 98	0
All	All	908/977 (92%)	0.12	49 (5%)	25	24	6, 24, 75, 134	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	94	ALA	6.3
1	A	47	THR	6.1
1	A	63	TYR	6.0
1	A	95	PRO	5.6
1	A	49	ASP	5.0
2	B	1050	LYS	4.7
1	A	107	LEU	4.4
1	A	44	GLN	4.2
1	A	93	GLU	3.8
1	A	98	PRO	3.7
1	A	383	GLN	3.5
1	A	46	ASP	3.4
1	A	48	ASN	3.4
1	A	102	ARG	3.4
1	A	41	PRO	3.3
2	B	1051	ASP	3.2
1	A	89	LEU	3.1
1	A	228	PHE	3.1
2	B	1043	LEU	3.1
1	A	45	GLY	3.1
1	A	39	ASP	3.1
1	A	38	TYR	2.9
1	A	42	LEU	2.9
2	B	1048	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	43	VAL	2.9
1	A	25	ALA	2.8
2	B	1148	ARG	2.8
2	B	1005	ASP	2.8
1	A	304	ASN	2.7
2	B	1147	ILE	2.7
1	A	594	ASN	2.7
1	A	97	GLN	2.7
1	A	66	ASP	2.6
1	A	65	ASP	2.6
1	A	754[A]	PHE	2.6
1	A	381	SER	2.6
1	A	91	GLN	2.6
1	A	593	ASP	2.5
1	A	64	PRO	2.5
1	A	101	VAL	2.4
1	A	225	ARG	2.4
1	A	58	HIS	2.4
2	B	1093	ARG	2.4
1	A	465	TRP	2.3
1	A	50	LEU	2.2
1	A	51	PRO	2.2
1	A	422	ASP	2.2
2	B	1047	THR	2.1
1	A	402	ASP	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 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(Å²)	Q<0.9
5	SO4	A	2017	5/5	0.74	0.25	56,56,67,76	2
4	LDA	A	2013	9/16	0.77	0.43	46,55,65,67	0
3	C8E	A	2009	21/21	0.78	0.30	38,58,68,80	0
4	LDA	A	2006	16/16	0.78	0.28	27,47,63,88	0
4	LDA	A	2004	16/16	0.80	0.33	18,45,89,107	0
4	LDA	A	2008	16/16	0.80	0.33	17,41,65,92	0
3	C8E	A	2011	21/21	0.82	0.31	24,61,88,94	0
3	C8E	A	2007	21/21	0.85	0.32	26,65,97,99	0
5	SO4	A	2021	5/5	0.86	0.30	84,93,96,100	0
4	LDA	A	2005	16/16	0.86	0.24	23,59,97,98	0
3	C8E	A	2002	21/21	0.87	0.29	17,54,78,86	0
3	C8E	A	2003	21/21	0.88	0.22	8,32,67,71	0
3	C8E	A	2001	21/21	0.89	0.26	40,50,65,73	0
4	LDA	A	2010	7/16	0.93	0.19	32,37,49,52	0
4	LDA	A	2012	7/16	0.94	0.20	30,34,44,62	0
5	SO4	A	2018	5/5	0.94	0.15	27,27,28,46	3
5	SO4	A	2015	5/5	0.94	0.18	38,40,43,53	5
5	SO4	A	2019	5/5	0.94	0.14	61,71,84,103	0
5	SO4	A	2020	5/5	0.95	0.12	62,80,83,91	0
5	SO4	A	2014	5/5	0.96	0.10	53,58,63,64	2
5	SO4	A	2016	5/5	0.97	0.25	48,56,62,67	4
5	SO4	B	1201	5/5	0.99	0.10	18,19,21,27	4

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 2009:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
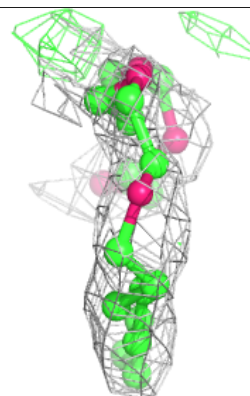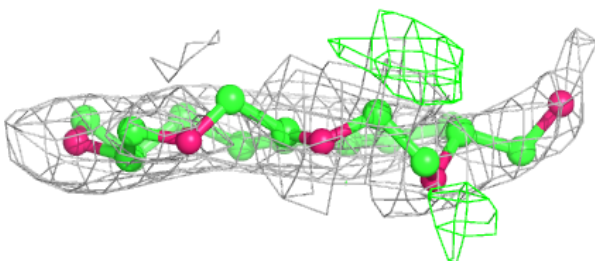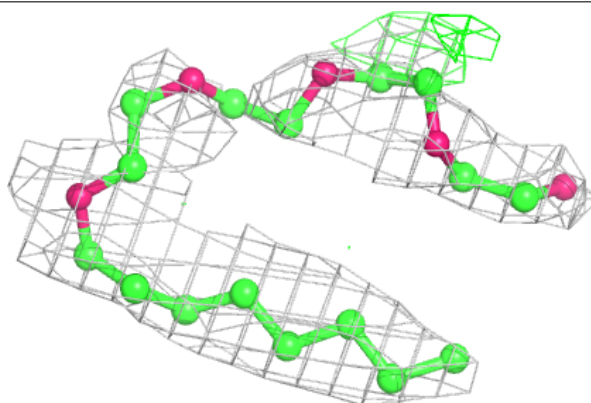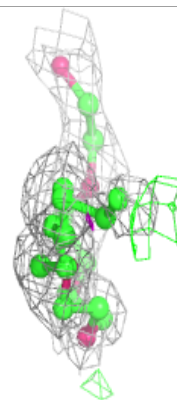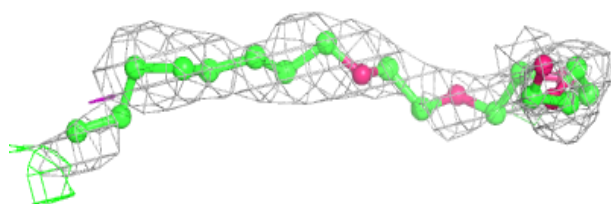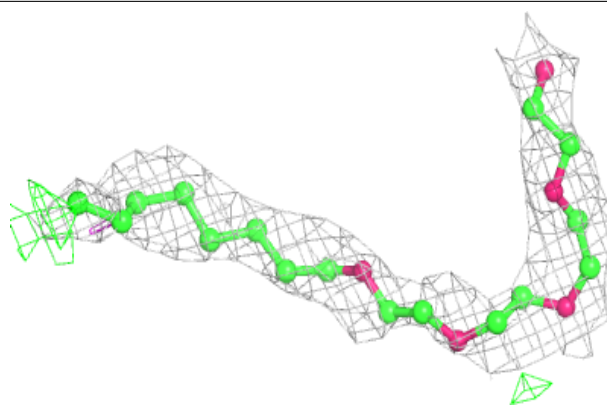and green (positive)
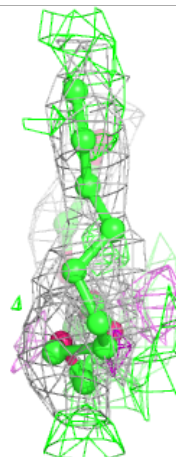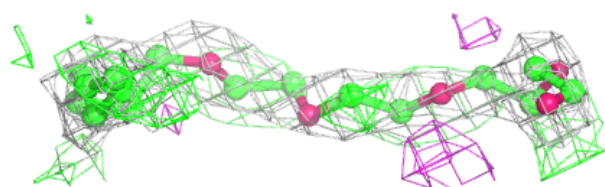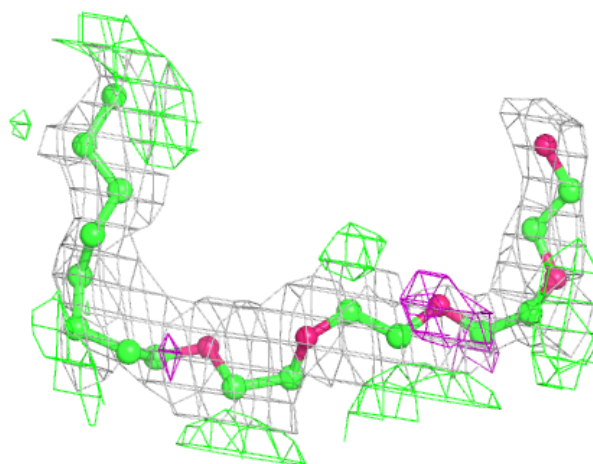
Electron density around C8E A 2011:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
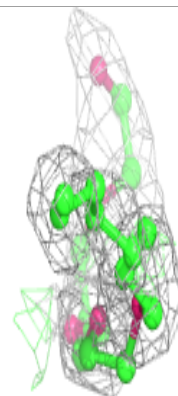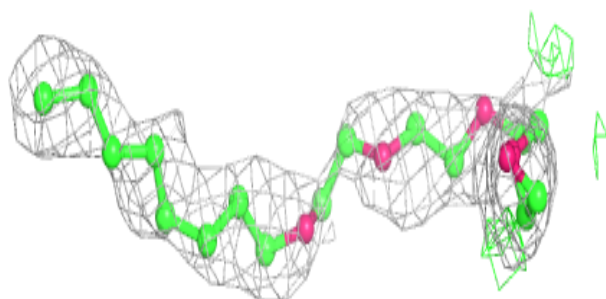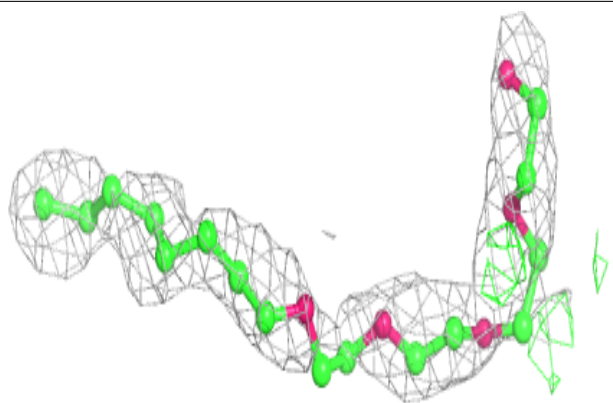
Electron density around C8E A 2007:

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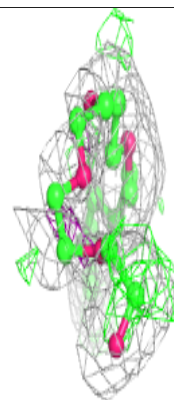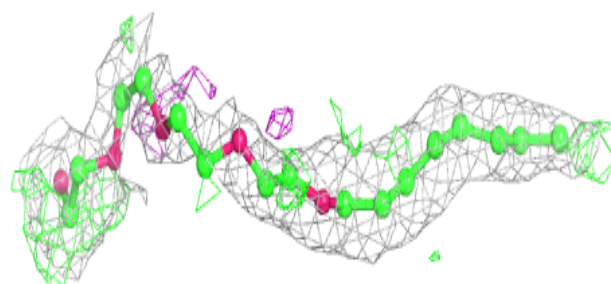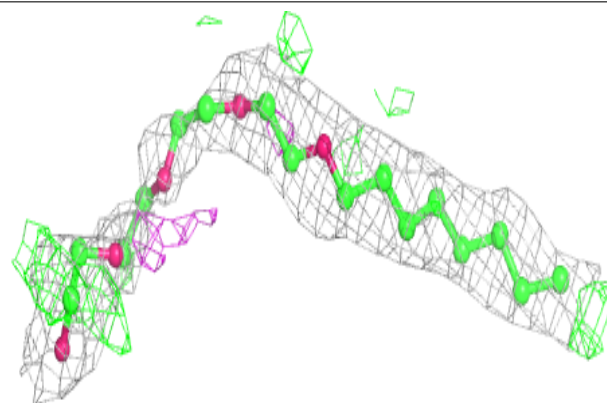mF_o-DF_c (at 3 rmsd) in purple (negative)
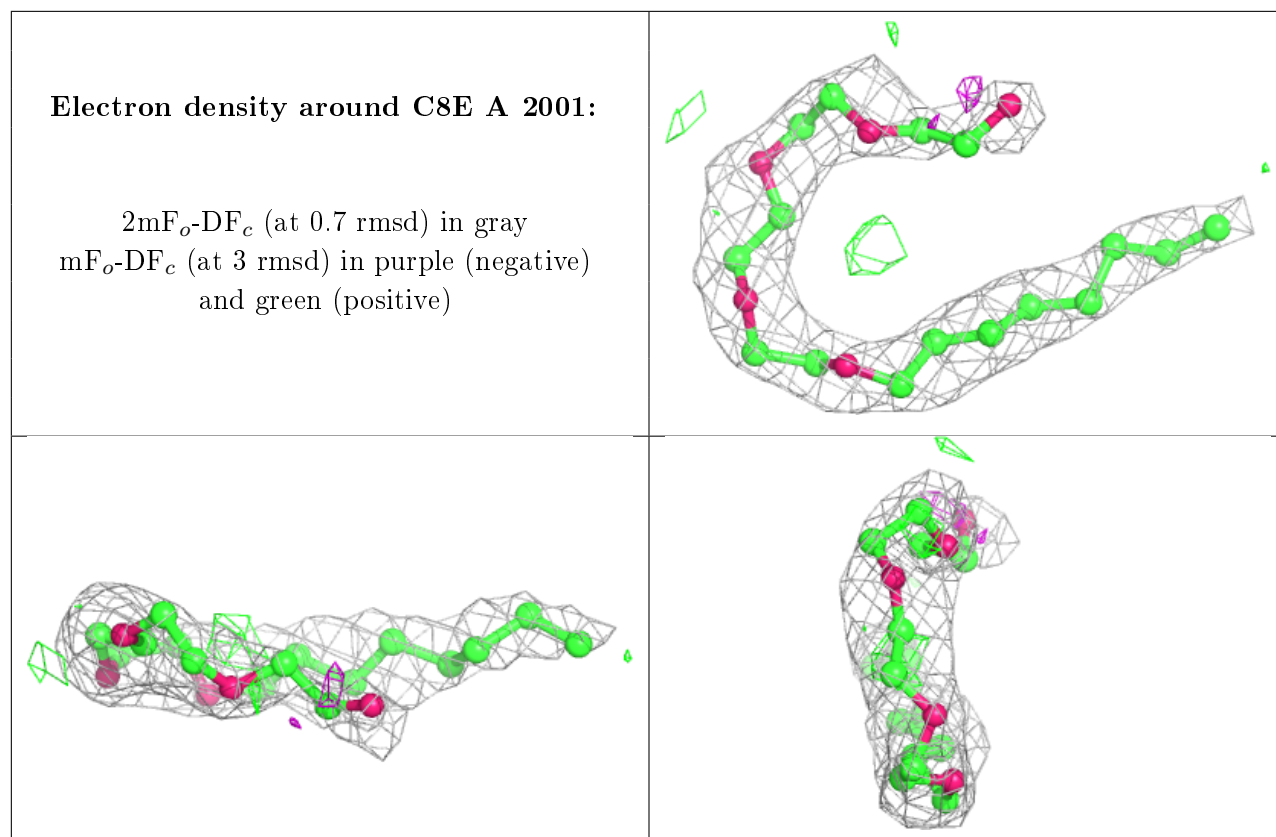and green (positive)

Electron density around C8E A 2002:

$2mF_o$-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 2003:

$2mF_o$-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 2001:

$2mF_o$-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.