



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 07:12 am BST

PDB ID : 5IV8  
Title : The LPS Transporter LptDE from *Klebsiella pneumoniae*, core complex  
Authors : Botos, I.; McCarthy, J.G.; Buchanan, S.K.  
Deposited on : 2016-03-20  
Resolution : 2.94 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.

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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 : 2.11  
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

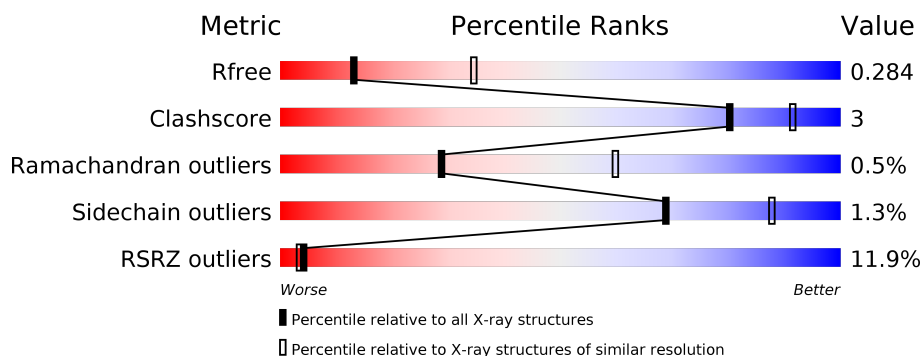
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.94 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	2969 (2.98-2.90)
Clashscore	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)
RSRZ outliers	127900	2902 (2.98-2.90)

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  $\geq 3$ , 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	601	<div> <div>7%</div> <div>84%</div> <div>8%</div> <div>8%</div> </div>
1	C	601	<div> <div>17%</div> <div>80%</div> <div>10%</div> <div>10%</div> </div>
2	B	182	<div> <div>7%</div> <div>75%</div> <div>5%</div> <div>20%</div> </div>
2	D	182	<div> <div>5%</div> <div>73%</div> <div>9%</div> <div>18%</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11347 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 biosynthesis protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4472	2808	766	888	10			
1	C	543	Total	C	N	O	S	0	0	0
			4401	2767	749	875	10			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	MET	-	initiating methionine	UNP A0A0U3IWD2
A	182	SER	-	expression tag	UNP A0A0U3IWD2
A	183	ASN	-	expression tag	UNP A0A0U3IWD2
A	184	HIS	-	expression tag	UNP A0A0U3IWD2
A	185	HIS	-	expression tag	UNP A0A0U3IWD2
A	186	HIS	-	expression tag	UNP A0A0U3IWD2
A	187	HIS	-	expression tag	UNP A0A0U3IWD2
A	188	HIS	-	expression tag	UNP A0A0U3IWD2
A	189	HIS	-	expression tag	UNP A0A0U3IWD2
A	190	HIS	-	expression tag	UNP A0A0U3IWD2
A	191	HIS	-	expression tag	UNP A0A0U3IWD2
A	192	HIS	-	expression tag	UNP A0A0U3IWD2
A	193	HIS	-	expression tag	UNP A0A0U3IWD2
A	194	GLU	-	expression tag	UNP A0A0U3IWD2
A	195	ASN	-	expression tag	UNP A0A0U3IWD2
A	196	LEU	-	expression tag	UNP A0A0U3IWD2
A	197	TYR	-	expression tag	UNP A0A0U3IWD2
A	198	PHE	-	expression tag	UNP A0A0U3IWD2
A	199	GLN	-	expression tag	UNP A0A0U3IWD2
A	200	SER	-	expression tag	UNP A0A0U3IWD2
A	201	MET	-	expression tag	UNP A0A0U3IWD2
C	181	MET	-	initiating methionine	UNP A0A0U3IWD2
C	182	SER	-	expression tag	UNP A0A0U3IWD2
C	183	ASN	-	expression tag	UNP A0A0U3IWD2
C	184	HIS	-	expression tag	UNP A0A0U3IWD2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	185	HIS	-	expression tag	UNP A0A0U3IWD2
C	186	HIS	-	expression tag	UNP A0A0U3IWD2
C	187	HIS	-	expression tag	UNP A0A0U3IWD2
C	188	HIS	-	expression tag	UNP A0A0U3IWD2
C	189	HIS	-	expression tag	UNP A0A0U3IWD2
C	190	HIS	-	expression tag	UNP A0A0U3IWD2
C	191	HIS	-	expression tag	UNP A0A0U3IWD2
C	192	HIS	-	expression tag	UNP A0A0U3IWD2
C	193	HIS	-	expression tag	UNP A0A0U3IWD2
C	194	GLU	-	expression tag	UNP A0A0U3IWD2
C	195	ASN	-	expression tag	UNP A0A0U3IWD2
C	196	LEU	-	expression tag	UNP A0A0U3IWD2
C	197	TYR	-	expression tag	UNP A0A0U3IWD2
C	198	PHE	-	expression tag	UNP A0A0U3IWD2
C	199	GLN	-	expression tag	UNP A0A0U3IWD2
C	200	SER	-	expression tag	UNP A0A0U3IWD2
C	201	MET	-	expression tag	UNP A0A0U3IWD2

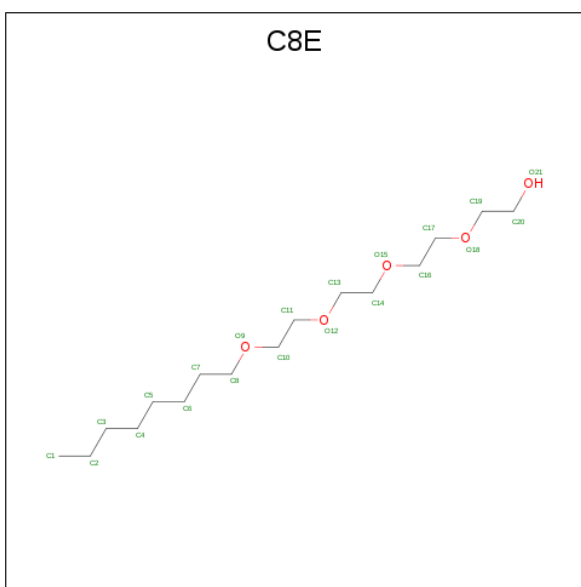
- Molecule 2 is a protein called LPS-assembly lipoprotein LptE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1140	713	201	220	6			
2	D	149	Total	C	N	O	S	0	0	0
			1164	727	205	226	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	15	ALA	-	expression tag	UNP A0A0J4W1Y0
B	16	PRO	-	expression tag	UNP A0A0J4W1Y0
B	17	ASN	-	expression tag	UNP A0A0J4W1Y0
B	18	THR	-	expression tag	UNP A0A0J4W1Y0
B	19	SER	-	expression tag	UNP A0A0J4W1Y0
D	15	ALA	-	expression tag	UNP A0A0J4W1Y0
D	16	PRO	-	expression tag	UNP A0A0J4W1Y0
D	17	ASN	-	expression tag	UNP A0A0J4W1Y0
D	18	THR	-	expression tag	UNP A0A0J4W1Y0
D	19	SER	-	expression tag	UNP A0A0J4W1Y0

- Molecule 3 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C<sub>16</sub>H<sub>34</sub>O<sub>5</sub>).



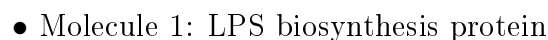
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	16	5		
3	A	1	Total	C	O	0	0
			21	16	5		
3	A	1	Total	C	O	0	0
			21	16	5		
3	C	1	Total	C	O	0	0
			21	16	5		
3	C	1	Total	C	O	0	0
			21	16	5		
3	C	1	Total	C	O	0	0
			21	16	5		
3	C	1	Total	C	O	0	0
			21	16	5		
3	D	1	Total	C	O	0	0
			21	16	5		

- Molecule 4 is water.

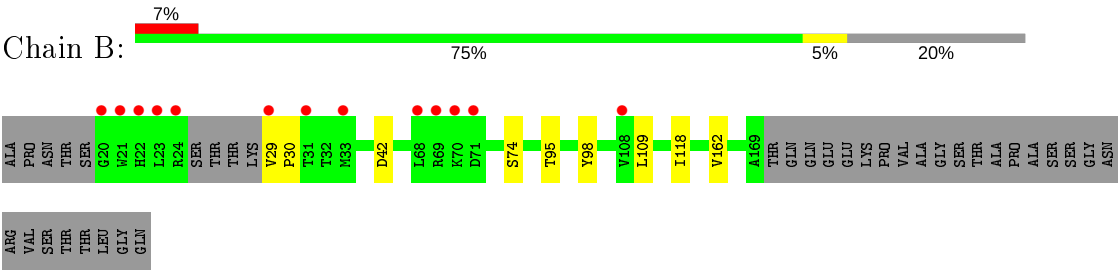
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O	0	0
			2	2		



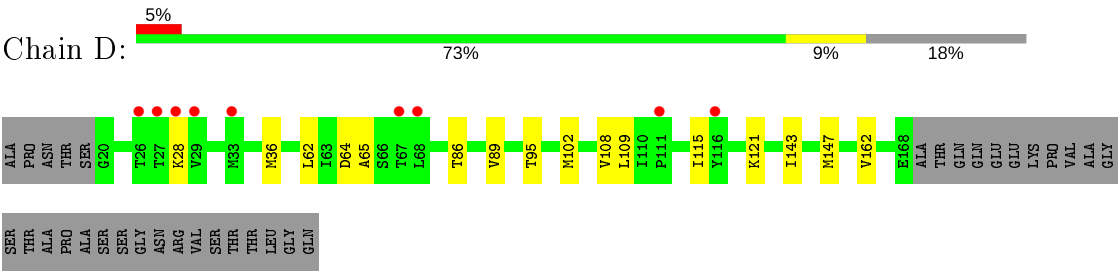
- Molecule 1: LPS biosynthesis protein



● Molecule 2: LPS-assembly lipoprotein LptE



● Molecule 2: LPS-assembly lipoprotein LptE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	75.02Å 173.05Å 84.76Å 90.00° 111.26° 90.00°	Depositor
Resolution (Å)	41.41 – 2.94 46.58 – 2.94	Depositor EDS
% Data completeness (in resolution range)	83.7 (41.41-2.94) 83.7 (46.58-2.94)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.03 (at 2.96Å)	Xtriage
Refinement program	PHENIX (1.10 _2155: ???)	Depositor
R, $R_{free}$	0.235 , 0.284 0.235 , 0.284	Depositor DCC
$R_{free}$ test set	1991 reflections (5.55%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.0	Xtriage
Anisotropy	0.284	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 48.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	11347	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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

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	0.24	0/4588	0.43	0/6240
1	C	0.24	0/4517	0.45	0/6147
2	B	0.24	0/1158	0.41	0/1569
2	D	0.24	0/1183	0.41	0/1604
All	All	0.24	0/11446	0.43	0/15560

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	4472	0	4149	21	0
1	C	4401	0	4074	27	0
2	B	1140	0	1147	5	0
2	D	1164	0	1175	8	0
3	A	63	0	102	2	0
3	C	84	0	136	1	0
3	D	21	0	34	0	0
4	A	2	0	0	0	0
All	All	11347	0	10817	60	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (60) 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:C:642:ARG:HE	1:C:646:ARG:HD3	1.52	0.74
1:C:646:ARG:HA	1:C:685:SER:O	1.91	0.70
1:C:251:ALA:HB3	1:C:254:PHE:HB2	1.78	0.64
1:A:774:ILE:HG13	1:A:775:LEU:HD12	1.82	0.62
2:D:109:LEU:HG	2:D:115:ILE:HG22	1.83	0.60
1:C:453:LEU:HD13	1:C:548:ILE:HD13	1.85	0.58
1:C:320:ILE:HG13	1:C:324:TRP:HB2	1.87	0.56
1:C:233:LYS:HD2	1:C:750:GLY:HA3	1.88	0.56
1:A:452:LEU:HB2	3:A:801:C8E:H62	1.89	0.54
1:A:409:LEU:HB2	3:A:801:C8E:H171	1.89	0.54
2:D:108:VAL:HG11	2:D:162:VAL:HG21	1.90	0.53
1:C:775:LEU:HD21	2:D:89:VAL:HG13	1.89	0.53
1:C:562:VAL:HB	1:C:571:PHE:HB3	1.91	0.53
2:B:118:ILE:HD11	2:B:162:VAL:HG21	1.92	0.52
1:C:529:LEU:HD21	1:C:543:SER:HB3	1.92	0.51
1:A:361:GLY:HA3	1:A:370:THR:HG22	1.92	0.51
1:A:536:LEU:HD11	1:A:605:ALA:HB3	1.93	0.51
1:C:230:PRO:HB3	1:C:244:LEU:HD23	1.91	0.51
2:D:102:MET:O	2:D:121:LYS:HA	2.11	0.50
1:C:255:ASP:HB3	1:C:276:ARG:HB2	1.93	0.49
1:A:562:VAL:HG22	1:A:571:PHE:HB3	1.95	0.49
2:B:74:SER:HB3	2:B:109:LEU:HB2	1.94	0.48
1:A:277:TYR:CZ	1:A:284:GLY:HA3	2.49	0.47
1:A:448:THR:HG22	1:A:486:VAL:HG12	1.96	0.47
1:A:325:ARG:NH2	2:B:42:ASP:OD2	2.47	0.47
1:C:371:VAL:HG22	1:C:393:LEU:HD13	1.97	0.47
1:C:232:ALA:HA	1:C:241:GLU:O	2.15	0.46
1:A:436:ASN:HD22	1:A:449:GLU:HB2	1.80	0.46
1:C:622:ILE:HD11	1:C:631:VAL:HG11	1.97	0.46
1:A:481:MET:HG2	1:A:516:ARG:HG3	1.98	0.45
1:A:549:ALA:HA	1:A:586:THR:HG22	1.97	0.45
2:B:95:THR:HG21	2:B:98:TYR:CZ	2.51	0.45
1:A:430:HIS:CG	1:A:545:LEU:HD13	2.51	0.45
1:C:688:ILE:HG13	1:C:689:VAL:HG23	1.99	0.45
3:C:801:C8E:H82	3:C:801:C8E:H51	1.84	0.45
1:A:583:GLU:HG3	1:A:585:ARG:HG3	2.00	0.44
1:C:628:LEU:HD22	1:C:658:GLU:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:536:LEU:HD11	1:C:605:ALA:HB3	2.00	0.43
2:D:86:THR:HG23	2:D:95:THR:HG23	2.00	0.42
1:A:241:GLU:HB3	1:A:261:HIS:HE1	1.84	0.42
1:A:504:LEU:HG	1:A:558:LEU:HD11	2.01	0.42
1:A:228:LEU:HB2	1:A:245:PRO:HB2	2.00	0.42
1:C:418:ASN:OD1	1:C:419:SER:N	2.53	0.42
1:C:554:VAL:HG13	1:C:579:TYR:HB3	2.00	0.42
1:A:240:VAL:HG22	1:A:264:ASN:HB2	2.02	0.42
1:C:486:VAL:O	1:C:509:GLN:HA	2.20	0.41
1:C:719:CYS:SG	1:C:720:CYS:N	2.88	0.41
2:B:29:VAL:HA	2:B:30:PRO:HD3	1.96	0.41
1:C:521:ILE:O	1:C:547:ARG:NH2	2.53	0.41
1:A:583:GLU:HB3	1:A:598:THR:HB	2.00	0.41
1:C:564:ASP:HB3	1:C:570:ARG:HD2	2.02	0.41
2:D:143:ILE:O	2:D:147:MET:HG3	2.20	0.41
1:C:244:LEU:O	1:C:260:PRO:HD2	2.21	0.41
1:C:667:TYR:O	1:C:673:TYR:HB2	2.20	0.41
2:D:36:MET:O	2:D:62:LEU:HA	2.21	0.41
1:A:502:GLN:HA	1:A:562:VAL:HA	2.02	0.40
1:C:424:PRO:HB3	1:C:462:LEU:HD23	2.03	0.40
2:D:64:ASP:OD1	2:D:65:ALA:N	2.50	0.40
1:C:774:ILE:HD12	1:C:774:ILE:HA	1.94	0.40
1:A:694:VAL:HG22	1:A:714:VAL:HG12	2.03	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	548/601 (91%)	510 (93%)	35 (6%)	3 (0%)	29 60
1	C	539/601 (90%)	497 (92%)	38 (7%)	4 (1%)	22 52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	142/182 (78%)	139 (98%)	3 (2%)	0	100	100
2	D	147/182 (81%)	141 (96%)	6 (4%)	0	100	100
All	All	1376/1566 (88%)	1287 (94%)	82 (6%)	7 (0%)	29	60

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	666	SER
1	A	365	GLN
1	C	629	ASP
1	C	365	GLN
1	C	239	GLY
1	A	221	ASP
1	C	552	ASN

### 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	480/526 (91%)	474 (99%)	6 (1%)	69	88
1	C	473/526 (90%)	464 (98%)	9 (2%)	57	81
2	B	127/156 (81%)	127 (100%)	0	100	100
2	D	131/156 (84%)	130 (99%)	1 (1%)	81	93
All	All	1211/1364 (89%)	1195 (99%)	16 (1%)	69	88

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

Mol	Chain	Res	Type
1	A	406	ASP
1	A	437	LEU
1	A	552	ASN
1	A	589	ASP
1	A	673	TYR

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Mol	Chain	Res	Type
1	A	721	TYR
1	C	290	TYR
1	C	394	ASP
1	C	421	ASN
1	C	425	GLU
1	C	516	ARG
1	C	589	ASP
1	C	677	ILE
1	C	692	TRP
1	C	749	PHE
2	D	28	LYS

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

Mol	Chain	Res	Type
2	B	91	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 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
3	C8E	A	801	-	20,20,20	0.38	0	19,19,19	0.33	0
3	C8E	C	801	-	20,20,20	0.38	0	19,19,19	0.35	0
3	C8E	D	201	-	20,20,20	0.39	0	19,19,19	0.34	0
3	C8E	A	802	-	20,20,20	0.37	0	19,19,19	0.40	0
3	C8E	C	802	-	20,20,20	0.38	0	19,19,19	0.40	0
3	C8E	C	803	-	20,20,20	0.37	0	19,19,19	0.40	0
3	C8E	A	803	-	20,20,20	0.38	0	19,19,19	0.37	0
3	C8E	C	804	-	20,20,20	0.38	0	19,19,19	0.38	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
3	C8E	A	801	-	-	8/18/18/18	-
3	C8E	C	801	-	-	14/18/18/18	-
3	C8E	D	201	-	-	10/18/18/18	-
3	C8E	A	802	-	-	11/18/18/18	-
3	C8E	C	802	-	-	14/18/18/18	-
3	C8E	C	803	-	-	13/18/18/18	-
3	C8E	A	803	-	-	8/18/18/18	-
3	C8E	C	804	-	-	9/18/18/18	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	803	C8E	O12-C13-C14-O15
3	D	201	C8E	O12-C13-C14-O15
3	A	802	C8E	O12-C13-C14-O15
3	C	803	C8E	O12-C13-C14-O15
3	C	804	C8E	O9-C10-C11-O12
3	A	801	C8E	O18-C19-C20-O21
3	C	804	C8E	O15-C16-C17-O18
3	A	801	C8E	O9-C10-C11-O12
3	C	804	C8E	O12-C13-C14-O15

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Mol	Chain	Res	Type	Atoms
3	C	801	C8E	O12-C13-C14-O15
3	D	201	C8E	O15-C16-C17-O18
3	A	802	C8E	O15-C16-C17-O18
3	C	803	C8E	O15-C16-C17-O18
3	A	802	C8E	O18-C19-C20-O21
3	A	803	C8E	O18-C19-C20-O21
3	C	804	C8E	O18-C19-C20-O21
3	D	201	C8E	C6-C7-C8-O9
3	A	801	C8E	O15-C16-C17-O18
3	C	801	C8E	O18-C19-C20-O21
3	D	201	C8E	O18-C19-C20-O21
3	C	802	C8E	O18-C19-C20-O21
3	C	804	C8E	C2-C3-C4-C5
3	A	803	C8E	C2-C3-C4-C5
3	D	201	C8E	C2-C3-C4-C5
3	A	801	C8E	C2-C3-C4-C5
3	C	803	C8E	C6-C7-C8-O9
3	C	803	C8E	C2-C3-C4-C5
3	C	802	C8E	C2-C3-C4-C5
3	A	802	C8E	C2-C3-C4-C5
3	A	803	C8E	C3-C4-C5-C6
3	D	201	C8E	C3-C4-C5-C6
3	C	802	C8E	C6-C7-C8-O9
3	C	801	C8E	C4-C5-C6-C7
3	C	803	C8E	C3-C4-C5-C6
3	C	803	C8E	O18-C19-C20-O21
3	A	803	C8E	O9-C10-C11-O12
3	C	802	C8E	C17-C16-O15-C14
3	C	803	C8E	C17-C16-O15-C14
3	C	801	C8E	C3-C4-C5-C6
3	C	802	C8E	O12-C13-C14-O15
3	A	802	C8E	C4-C5-C6-C7
3	A	802	C8E	C3-C4-C5-C6
3	C	802	C8E	C3-C4-C5-C6
3	A	801	C8E	C3-C4-C5-C6
3	C	801	C8E	C2-C3-C4-C5
3	C	803	C8E	C4-C5-C6-C7
3	A	803	C8E	C6-C7-C8-O9
3	D	201	C8E	C1-C2-C3-C4
3	A	802	C8E	C6-C7-C8-O9
3	C	802	C8E	C20-C19-O18-C17
3	D	201	C8E	C11-C10-O9-C8

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Mol	Chain	Res	Type	Atoms
3	C	803	C8E	C10-C11-O12-C13
3	C	804	C8E	C20-C19-O18-C17
3	C	801	C8E	C13-C14-O15-C16
3	C	802	C8E	C13-C14-O15-C16
3	A	802	C8E	C1-C2-C3-C4
3	C	803	C8E	C13-C14-O15-C16
3	C	804	C8E	C7-C8-O9-C10
3	A	801	C8E	C13-C14-O15-C16
3	A	803	C8E	C7-C8-O9-C10
3	C	802	C8E	C11-C10-O9-C8
3	D	201	C8E	C10-C11-O12-C13
3	C	804	C8E	C10-C11-O12-C13
3	C	801	C8E	C10-C11-O12-C13
3	C	801	C8E	C11-C10-O9-C8
3	D	201	C8E	C20-C19-O18-C17
3	A	801	C8E	C10-C11-O12-C13
3	C	801	C8E	C1-C2-C3-C4
3	C	804	C8E	C6-C7-C8-O9
3	C	801	C8E	C20-C19-O18-C17
3	C	801	C8E	C17-C16-O15-C14
3	A	802	C8E	C11-C10-O9-C8
3	C	803	C8E	C11-C10-O9-C8
3	C	802	C8E	C14-C13-O12-C11
3	C	801	C8E	C14-C13-O12-C11
3	A	802	C8E	C20-C19-O18-C17
3	C	801	C8E	C5-C6-C7-C8
3	A	802	C8E	O9-C10-C11-O12
3	C	802	C8E	O9-C10-C11-O12
3	C	801	C8E	O15-C16-C17-O18
3	C	803	C8E	C14-C13-O12-C11
3	C	802	C8E	C7-C8-O9-C10
3	A	803	C8E	C20-C19-O18-C17
3	C	803	C8E	C1-C2-C3-C4
3	A	801	C8E	C1-C2-C3-C4
3	C	802	C8E	C1-C2-C3-C4
3	C	802	C8E	O15-C16-C17-O18

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	C8E	2	0

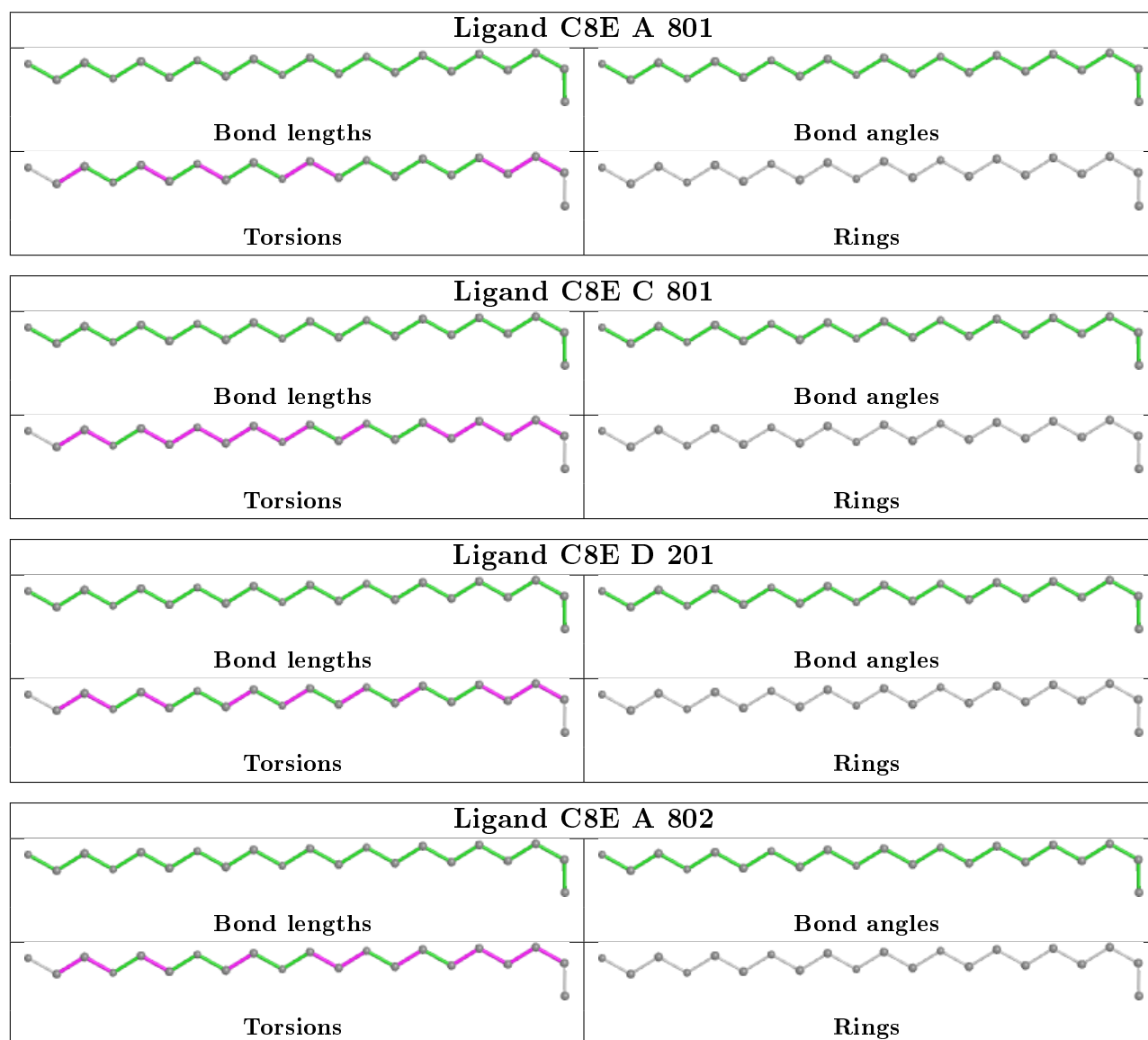
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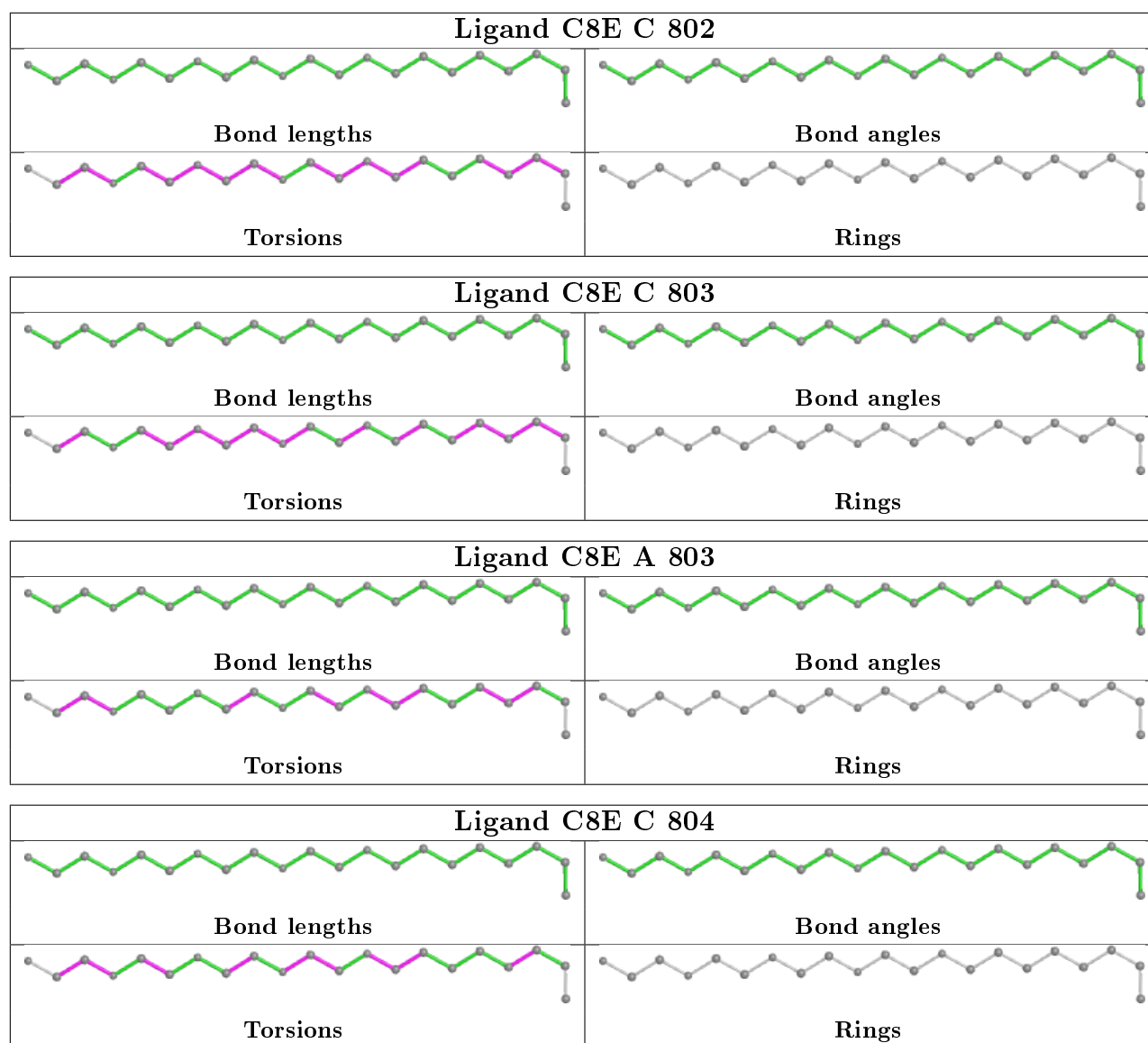


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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	801	C8E	1	0

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

### 6.1 Protein, DNA and RNA chains

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	552/601 (91%)	0.43	41 (7%) 14 12	14, 62, 120, 154	0
1	C	543/601 (90%)	0.86	102 (18%) 1 1	21, 72, 157, 211	0
2	B	146/182 (80%)	0.54	13 (8%) 9 8	21, 63, 126, 164	0
2	D	149/182 (81%)	0.42	9 (6%) 21 20	29, 62, 134, 180	0
All	All	1390/1566 (88%)	0.61	165 (11%) 4 3	14, 65, 144, 211	0

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	753	ILE	8.0
1	C	688	ILE	7.5
1	C	723	ILE	6.4
1	C	267	GLY	6.1
1	C	301	HIS	6.1
1	A	722	ALA	6.1
1	C	694	VAL	5.7
1	C	275	PHE	5.6
1	C	269	VAL	5.5
2	B	29	VAL	5.4
1	C	230	PRO	5.3
1	C	716	TYR	5.2
1	C	304	ASP	5.1
1	C	717	ASN	4.9
1	C	689	VAL	4.8
1	C	751	ILE	4.8
1	C	244	LEU	4.7
2	B	69	ARG	4.7
1	C	344	SER	4.7
1	C	695	VAL	4.6
1	A	720	CYS	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	382	GLU	4.6
2	D	27	THR	4.6
1	C	306	ASN	4.5
1	C	312	PHE	4.5
1	C	693	SER	4.5
1	C	692	TRP	4.4
1	C	240	VAL	4.3
2	B	22	HIS	4.3
1	C	229	ILE	4.3
1	C	690	ASP	4.3
1	C	263	MET	4.2
2	D	26	THR	4.2
1	C	228	LEU	4.2
2	B	23	LEU	4.1
1	C	725	LEU	4.1
1	C	719	CYS	4.1
1	A	596	ASN	4.1
2	B	20	GLY	4.0
2	B	68	LEU	4.0
1	C	232	ALA	4.0
1	C	302	SER	4.0
1	A	723	ILE	4.0
1	C	255	ASP	4.0
1	C	718	SER	4.0
1	C	262	TYR	3.9
1	C	256	ALA	3.9
1	C	686	TRP	3.9
1	C	721	TYR	3.8
1	C	752	ASN	3.8
1	C	271	TRP	3.7
1	A	690	ASP	3.7
1	C	720	CYS	3.7
1	C	288	PHE	3.6
1	C	714	VAL	3.6
1	C	242	PHE	3.6
2	B	21	TRP	3.5
1	C	781	LEU	3.5
2	D	29	VAL	3.5
1	C	687	PRO	3.5
1	C	260	PRO	3.4
1	C	724	ARG	3.4
1	C	249	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	492	PHE	3.4
1	C	712	LEU	3.4
2	D	33	MET	3.3
1	C	297	TYR	3.3
2	B	33	MET	3.3
1	C	264	ASN	3.3
1	A	220	GLY	3.3
1	C	276	ARG	3.3
1	A	565	ALA	3.3
1	C	749	PHE	3.2
1	C	227	PHE	3.2
1	C	684	ALA	3.2
1	C	293	SER	3.2
1	C	247	TYR	3.2
1	A	472	ASP	3.2
2	B	70	LYS	3.1
2	D	68	LEU	3.1
2	D	67	THR	3.1
1	A	688	ILE	3.1
1	C	736	SER	3.1
1	C	722	ALA	3.1
1	A	595	ASN	3.1
1	C	231	ASN	3.1
1	A	691	ARG	3.1
1	C	333	VAL	3.0
2	B	24	ARG	3.0
1	C	342	PHE	3.0
1	A	714	VAL	3.0
1	C	467	ALA	2.9
1	C	729	ARG	2.9
1	C	305	SER	2.9
1	C	682	MET	2.9
1	C	691	ARG	2.9
1	C	258	ILE	2.8
1	A	719	CYS	2.8
1	A	615	GLU	2.8
1	C	298	GLU	2.8
1	C	246	TYR	2.8
1	C	233	LYS	2.8
1	C	727	TYR	2.8
2	B	71	ASP	2.8
1	C	252	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	305	SER	2.7
1	C	234	TYR	2.7
1	C	698	TYR	2.7
1	A	739	ASN	2.7
1	A	712	LEU	2.7
1	C	303	SER	2.7
1	C	346	TYR	2.7
1	C	685	SER	2.7
1	C	612	ILE	2.7
1	C	331	THR	2.7
2	D	116	TYR	2.6
1	C	253	ASN	2.6
1	C	286	THR	2.6
1	A	225	SER	2.6
1	C	381	ARG	2.5
1	A	234	TYR	2.5
1	C	248	TRP	2.5
1	C	311	LEU	2.5
2	B	31	THR	2.5
1	C	250	ILE	2.5
1	C	746	ASP	2.4
1	C	257	THR	2.4
1	A	721	TYR	2.4
1	C	700	TYR	2.4
1	C	254	PHE	2.4
2	D	28	LYS	2.4
1	C	259	THR	2.4
1	A	702	THR	2.4
1	A	717	ASN	2.4
1	A	737	ASN	2.4
1	C	265	LYS	2.3
1	A	740	GLY	2.3
1	A	753	ILE	2.3
1	A	224	ARG	2.3
1	A	594	GLU	2.3
1	A	265	LYS	2.3
1	A	678	SER	2.2
1	C	310	TRP	2.2
1	A	495	ASP	2.2
1	C	261	HIS	2.2
1	A	221	ASP	2.1
1	C	251	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	707	ALA	2.1
1	A	223	ARG	2.1
1	C	291	LEU	2.1
1	A	500	PHE	2.1
1	A	708	ALA	2.1
1	C	498	GLU	2.1
1	A	686	TRP	2.1
2	B	108	VAL	2.1
1	C	713	GLY	2.1
1	C	697	ALA	2.1
1	A	724	ARG	2.1
2	D	111	PRO	2.1
1	C	769	MET	2.0
1	A	602	LEU	2.0
1	C	266	ARG	2.0
1	C	747	ASN	2.0
1	A	752	ASN	2.0
1	A	689	VAL	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	C8E	A	803	21/21	0.76	0.28	32,74,93,100	0
3	C8E	C	803	21/21	0.86	0.31	42,80,130,132	0
3	C8E	A	802	21/21	0.88	0.39	22,53,94,110	0
3	C8E	A	801	21/21	0.88	0.30	31,69,97,99	0
3	C8E	D	201	21/21	0.88	0.37	19,62,96,105	0

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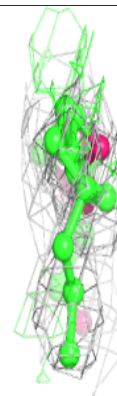
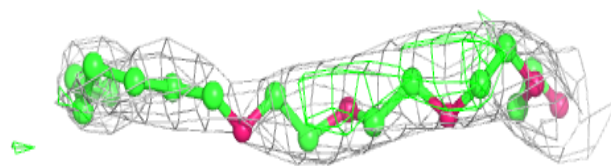
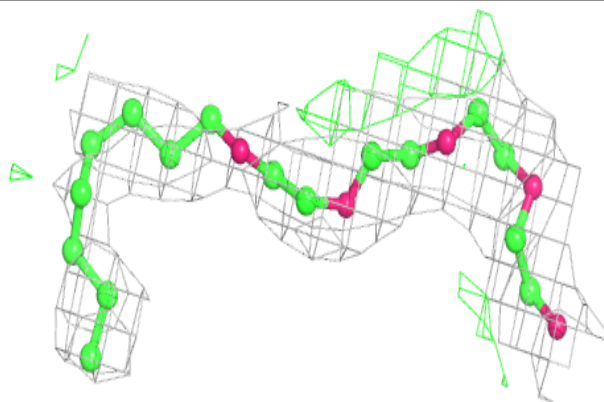
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	C8E	C	802	21/21	0.92	0.26	22,48,72,79	0
3	C8E	C	804	21/21	0.92	0.34	28,45,61,65	0
3	C8E	C	801	21/21	0.93	0.27	16,46,75,84	0

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 803:**

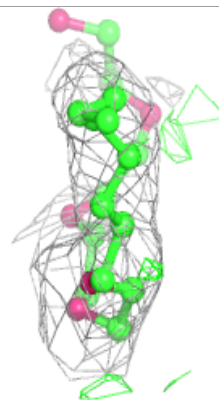
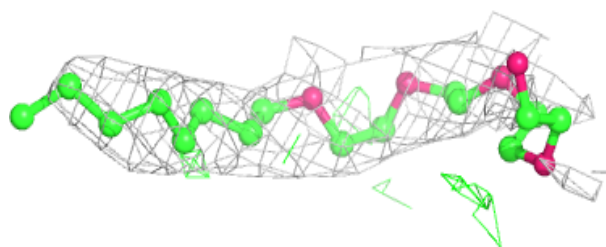
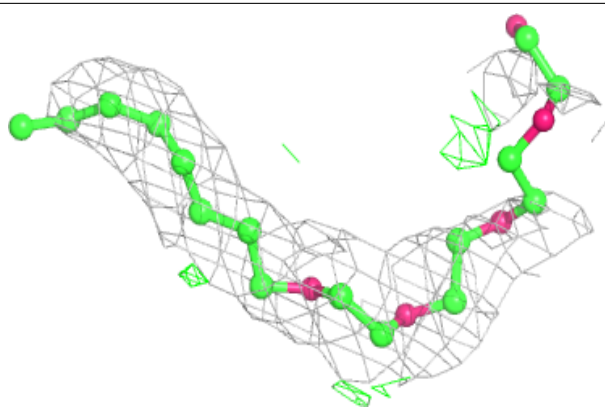
2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



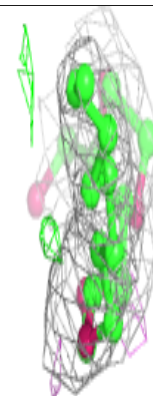
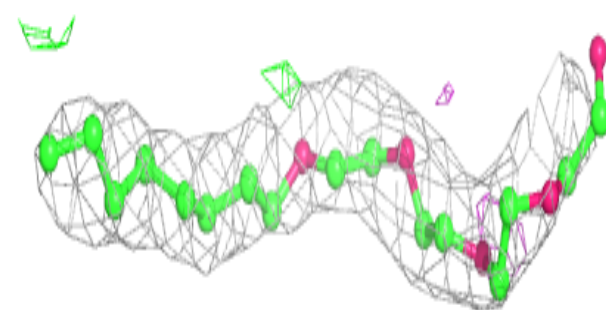
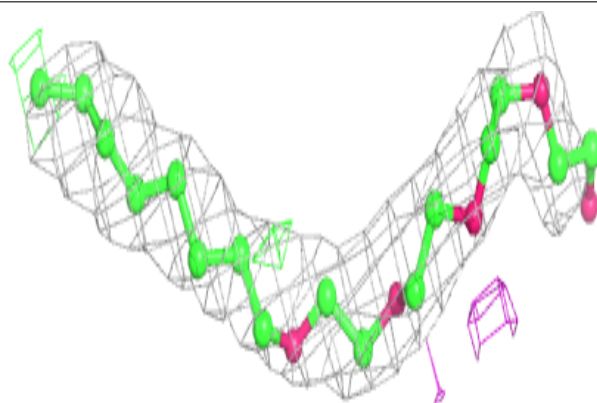


**Electron density around C8E C 803:**

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

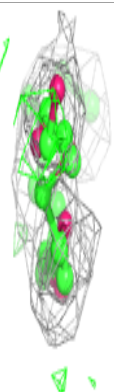
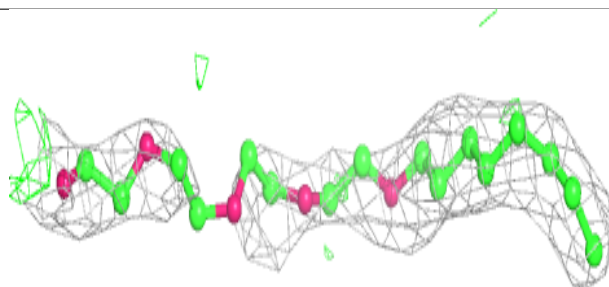
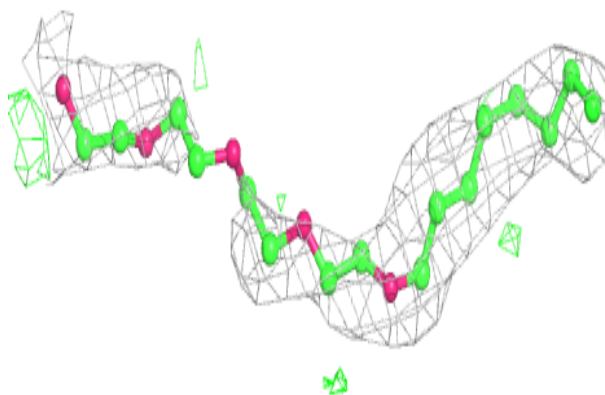
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and green (positive)

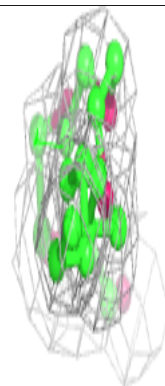
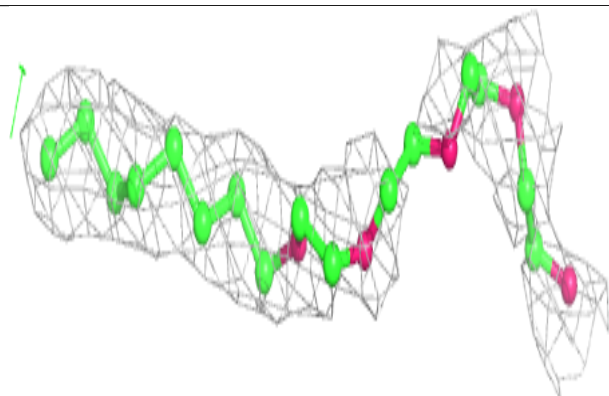
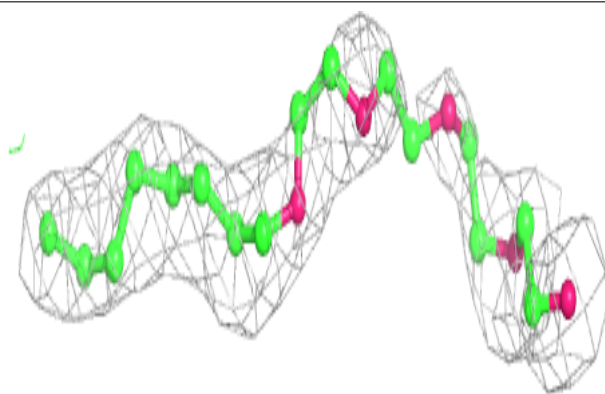


**Electron density around C8E A 801:**

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

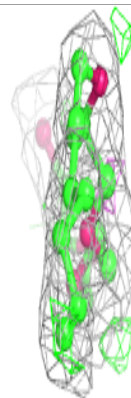
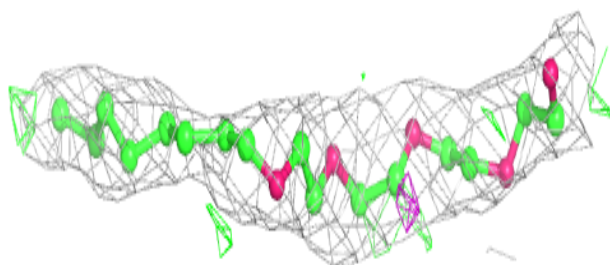
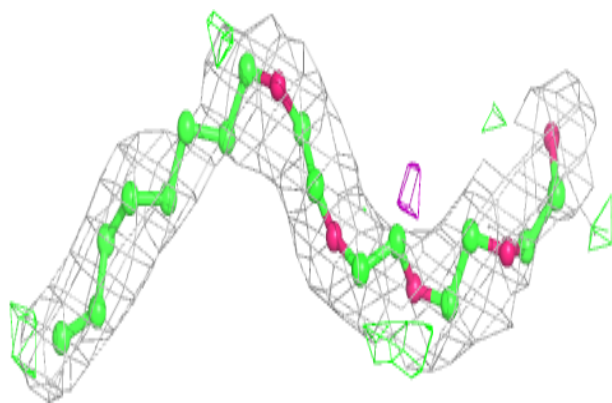
**Electron density around C8E D 201:**

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

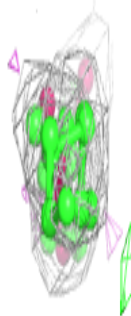
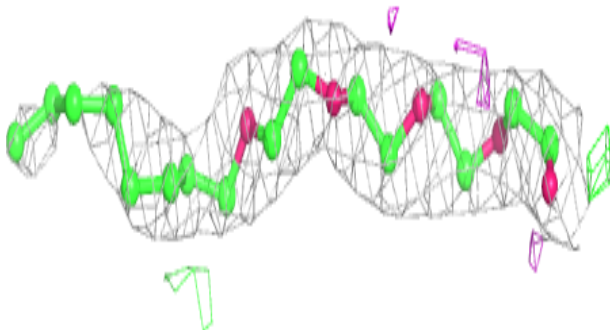
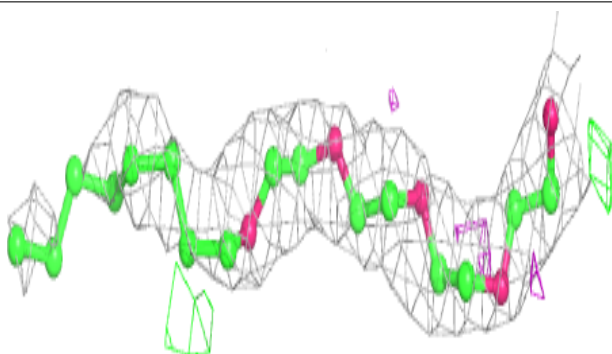


**Electron density around C8E C 802:**

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

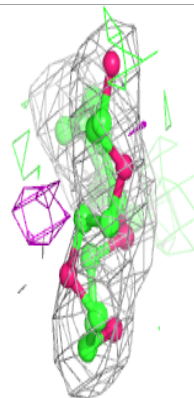
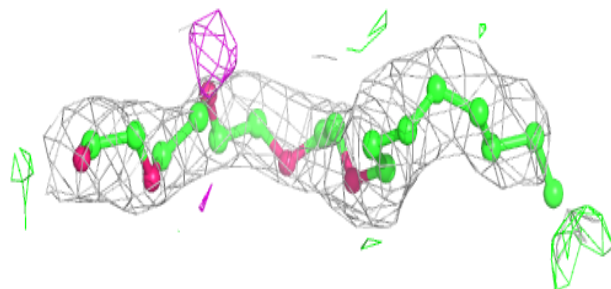
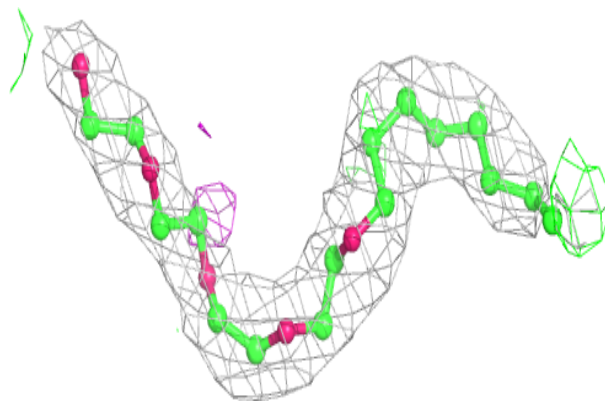
**Electron density around C8E C 804:**

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



**Electron density around C8E C 801:**

$2mF_o-DF_c$  (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.