Full wwPDB X-ray Structure Validation Report (i)

Feb 17, 2025 – 12:14 pm GMT

PDB ID	:	9F2T
Title	:	Ferric-mycobactin receptor (FemA)
Authors	:	Moynie, L.
Deposited on	:	2024-04-24
Resolution	:	2.20 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

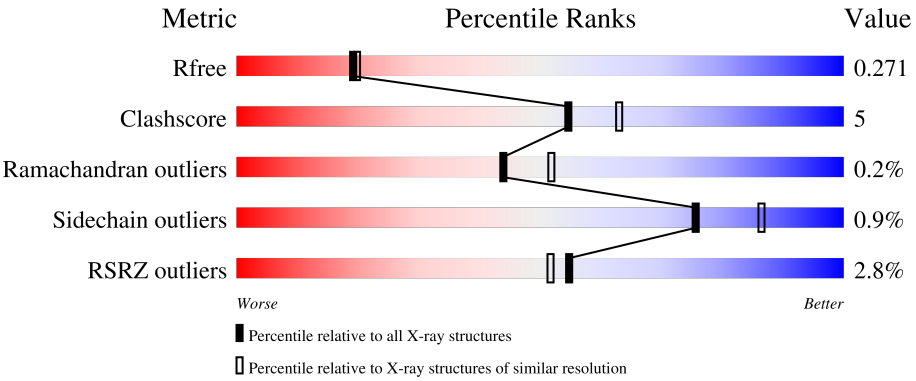
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

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 >=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	780	2% 75% 10% 14%
1	B	780	2% 77% 8% 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
2	EDO	A	801	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10897 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.

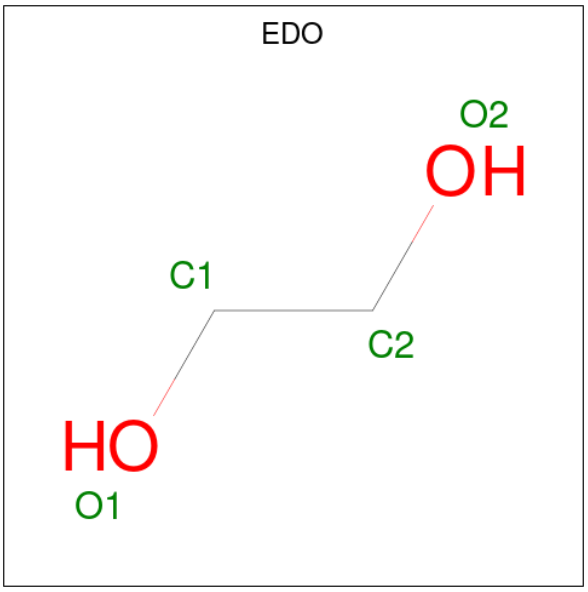
- Molecule 1 is a protein called Ferric-mycobactin receptor, FemA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	670	Total	C	N	O	S	0	0	0
			5141	3205	929	998	9			
1	A	670	Total	C	N	O	S	0	0	0
			5141	3205	929	998	9			

There are 8 discrepancies between the modelled and reference sequences:

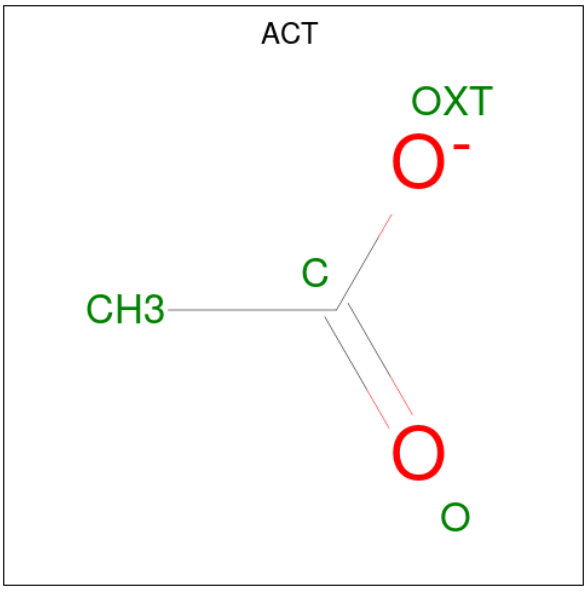
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP Q9I2J4
B	-1	ALA	-	expression tag	UNP Q9I2J4
B	0	MET	-	expression tag	UNP Q9I2J4
B	1	THR	-	expression tag	UNP Q9I2J4
A	-2	GLY	-	expression tag	UNP Q9I2J4
A	-1	ALA	-	expression tag	UNP Q9I2J4
A	0	MET	-	expression tag	UNP Q9I2J4
A	1	THR	-	expression tag	UNP Q9I2J4

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 4 2 2	0	0

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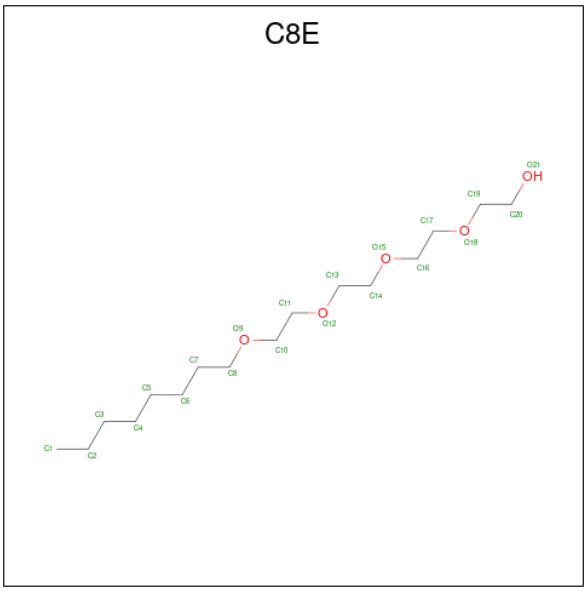
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0

- Molecule 4 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: $C_{16}H_{34}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 12 10 2	0	0
4	B	1	Total C O 15 12 3	0	0
4	B	1	Total C O 16 11 5	0	0
4	B	1	Total C O 15 12 3	0	0
4	A	1	Total C O 15 12 3	0	0
4	A	1	Total C O 15 12 3	0	0
4	A	1	Total C O 21 16 5	0	0

- Molecule 5 is water.

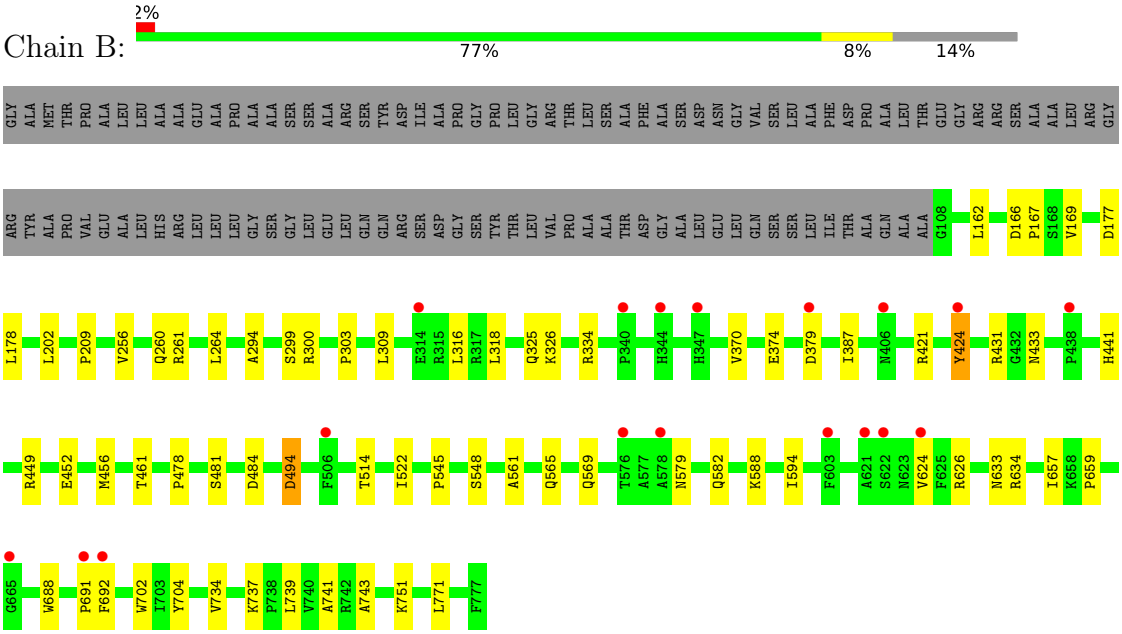
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	246	Total O 246 246	0	0
5	A	236	Total O 236 236	0	0

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.

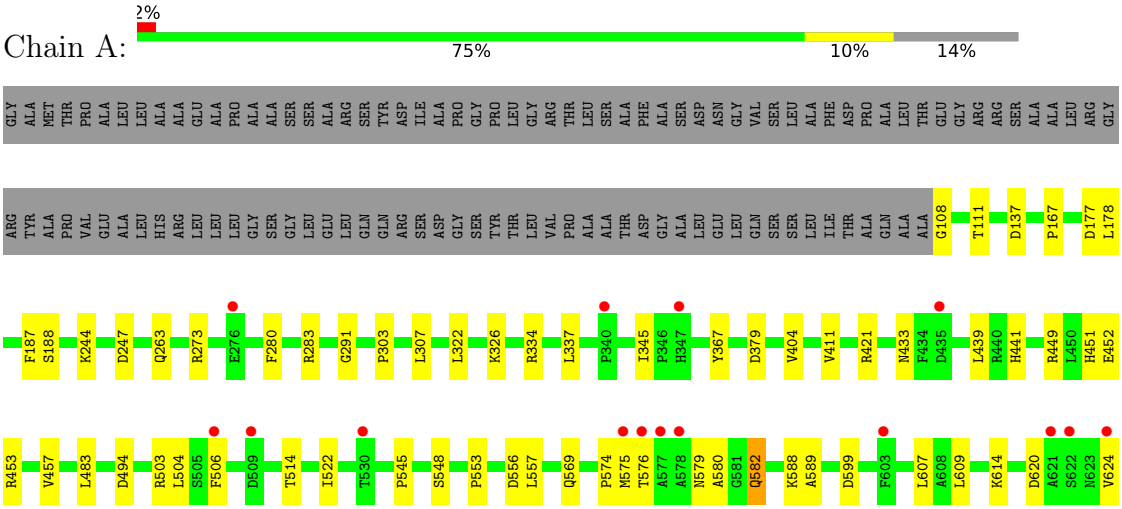
• Molecule 1: Ferric-mycobactin receptor, FemA

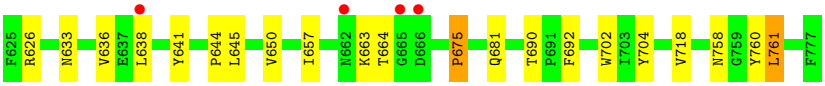
Chain B:



• Molecule 1: Ferric-mycobactin receptor, FemA

Chain A:




F625
R626
N633
V636
E637
L638
Y641
P644
L645
V650
I657
N662
K663
T664
G665
D666
P675
Q681
T690
P691
F692
W702
I703
Y704
V718
N758
G759
Y760
L761
F777

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	83.68Å 84.95Å 86.70Å 89.97° 61.60° 66.26°	Depositor
Resolution (Å)	75.55 – 2.20 75.55 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.3 (75.55-2.20) 98.3 (75.55-2.20)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.225 , 0.271 0.225 , 0.271	Depositor DCC
R_{free} test set	6088 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	28.8	Xtriage
Anisotropy	0.617	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10897	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.43 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.6684e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

5.1 Standard geometry

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

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	0.41	0/5247	0.61	0/7129
1	B	0.42	0/5247	0.61	0/7129
All	All	0.42	0/10494	0.61	0/14258

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

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	5141	0	4999	54	0
1	B	5141	0	4999	43	0
2	A	8	0	12	5	0
2	B	4	0	6	2	0
3	A	8	0	6	1	0
3	B	4	0	3	0	0
4	A	51	0	84	6	0
4	B	58	0	92	8	0
5	A	236	0	0	2	0
5	B	246	0	0	3	0
All	All	10897	0	10201	97	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 (97) 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:337:LEU:HD13	1:A:760:TYR:HB3	1.49	0.92
1:A:404:VAL:HG21	1:A:411:VAL:HG23	1.56	0.88
1:A:307:LEU:HG	4:A:805:C8E:H12	1.65	0.78
1:A:108:GLY:N	1:A:111:THR:HG1	1.87	0.72
1:A:439:LEU:HD23	1:A:504:LEU:HD23	1.75	0.68
1:B:741:ALA:HB1	4:B:804:C8E:H111	1.76	0.68
1:A:718:VAL:HG11	1:A:761:LEU:HD21	1.78	0.65
1:B:633:ASN:HB3	1:B:657:ILE:HD11	1.80	0.64
1:A:607:LEU:HD12	1:A:638:LEU:HD21	1.80	0.64
1:A:334:ARG:HH22	4:A:807:C8E:H101	1.64	0.63
1:A:702:TRP:HB2	3:A:802:ACT:H1	1.82	0.61
1:B:421:ARG:NH1	1:B:452:GLU:OE1	2.32	0.61
1:A:137:ASP:O	5:A:901:HOH:O	2.16	0.60
1:B:771:LEU:HB3	4:B:804:C8E:H71	1.85	0.59
1:A:367:TYR:HD2	4:A:805:C8E:H112	1.68	0.57
1:B:737:LYS:HA	1:B:737:LYS:HE2	1.87	0.57
1:A:322:LEU:HD23	4:A:805:C8E:H72	1.87	0.57
1:B:309:LEU:HB3	4:B:803:C8E:H12	1.86	0.56
1:A:449:ARG:NH1	1:A:494:ASP:OD2	2.35	0.56
1:B:261:ARG:HG3	1:B:294:ALA:HA	1.86	0.56
1:A:421:ARG:NH1	1:A:452:GLU:OE1	2.32	0.55
1:A:188:SER:H	2:A:801:EDO:H12	1.71	0.55
1:A:620:ASP:OD2	1:A:626:ARG:NH2	2.39	0.55
1:B:565:GLN:OE1	1:B:588:LYS:HD2	2.08	0.54
1:B:316:LEU:HD12	1:B:374:GLU:O	2.10	0.52
1:B:256:VAL:HG23	4:B:804:C8E:H42	1.92	0.52
1:B:624:VAL:HG11	1:B:626:ARG:HH11	1.73	0.52
1:A:718:VAL:HG11	1:A:761:LEU:CD2	2.40	0.52
1:B:579:ASN:HB2	1:B:582:GLN:OE1	2.10	0.51
1:A:553:PRO:HG2	1:A:557:LEU:HD23	1.93	0.51
1:A:247:ASP:O	1:A:273:ARG:HG3	2.11	0.51
1:A:609:LEU:HD13	1:A:636:VAL:HB	1.93	0.51
1:B:209:PRO:HG3	1:B:325:GLN:HG3	1.92	0.51
1:B:177:ASP:OD1	1:B:178:LEU:N	2.45	0.50
1:A:575:MET:HA	1:A:580:ALA:HB1	1.94	0.49
1:A:263:GLN:HA	1:A:291:GLY:HA3	1.93	0.49
1:A:574:PRO:HB2	1:A:576:THR:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:PHE:HA	2:A:801:EDO:H11	1.96	0.48
1:B:522:ILE:HG21	1:B:569:GLN:HG3	1.96	0.47
1:B:300:ARG:NH2	5:B:909:HOH:O	2.35	0.47
1:B:514:THR:HB	1:B:548:SER:OG	2.15	0.47
1:B:702:TRP:CZ2	1:B:704:TYR:HB2	2.50	0.47
1:A:439:LEU:HG	1:A:506:PHE:CE2	2.49	0.47
1:B:734:VAL:HG22	1:B:739:LEU:HD13	1.96	0.47
1:B:334:ARG:CZ	4:B:805:C8E:H171	2.44	0.47
1:A:334:ARG:NH2	4:A:807:C8E:H101	2.29	0.47
1:A:188:SER:HB2	2:A:801:EDO:H12	1.97	0.46
1:A:457:VAL:HG23	1:A:483:LEU:HD13	1.98	0.46
1:A:633:ASN:HB3	1:A:657:ILE:HD11	1.97	0.46
1:A:167:PRO:O	1:A:681:GLN:NE2	2.49	0.46
1:A:702:TRP:CZ2	1:A:704:TYR:HB2	2.51	0.45
1:B:481:SER:O	1:B:484:ASP:HB2	2.16	0.45
1:B:561:ALA:HB2	1:B:594:ILE:HG22	1.97	0.45
1:B:264:LEU:HD22	4:B:804:C8E:H11	1.98	0.45
1:B:387:ILE:HG13	1:B:424:TYR:HE2	1.81	0.45
1:A:178:LEU:HD21	4:A:807:C8E:H171	1.98	0.44
1:A:503:ARG:HD2	5:A:1073:HOH:O	2.16	0.44
1:B:162:LEU:HB3	1:B:169:VAL:HG11	1.98	0.44
1:A:690:THR:HB	1:A:692:PHE:CD1	2.52	0.44
1:B:449:ARG:NE	1:B:494:ASP:OD1	2.51	0.43
1:A:439:LEU:CD2	1:A:504:LEU:HD23	2.47	0.43
1:B:691:PRO:HG3	2:B:801:EDO:H11	2.01	0.43
1:B:387:ILE:HD11	1:A:280:PHE:CE2	2.54	0.43
1:B:431:ARG:NH1	5:B:905:HOH:O	2.48	0.43
1:A:641:TYR:HA	1:A:650:VAL:O	2.18	0.43
1:A:345:ILE:HD12	1:A:761:LEU:HD11	2.01	0.43
1:A:663:LYS:HD2	1:A:664:THR:N	2.33	0.43
1:A:675:PRO:HB2	1:A:758:ASN:HA	2.00	0.43
1:B:303:PRO:HD2	1:B:326:LYS:O	2.18	0.43
1:B:688:TRP:HE1	2:B:801:EDO:H12	1.83	0.43
1:B:202:LEU:HD13	1:B:370:VAL:HB	2.00	0.43
1:B:688:TRP:CH2	1:B:692:PHE:HE2	2.37	0.43
1:A:303:PRO:HD2	1:A:326:LYS:O	2.18	0.42
1:A:177:ASP:OD1	1:A:178:LEU:N	2.52	0.42
1:B:433:ASN:HA	1:B:441:HIS:O	2.19	0.42
1:A:514:THR:HB	1:A:548:SER:OG	2.19	0.42
1:A:188:SER:N	2:A:801:EDO:H12	2.35	0.42
1:A:589:ALA:HB2	1:A:614:LYS:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:GLN:HA	1:B:261:ARG:HA	1.73	0.42
4:B:806:C8E:H81	4:B:806:C8E:H52	1.57	0.42
1:A:433:ASN:HA	1:A:441:HIS:O	2.20	0.41
1:B:461:THR:O	1:B:478:PRO:HG2	2.21	0.41
1:A:451:HIS:HD1	1:A:494:ASP:CG	2.20	0.41
1:A:244:LYS:HB3	1:A:283:ARG:HD3	2.02	0.41
1:A:188:SER:H	2:A:801:EDO:C1	2.32	0.41
1:B:743:ALA:HB2	4:B:804:C8E:H131	2.02	0.41
1:A:644:PRO:O	1:A:645:LEU:HD13	2.21	0.41
1:A:579:ASN:O	1:A:582:GLN:HB2	2.20	0.41
1:A:556:ASP:HB2	1:A:599:ASP:O	2.20	0.41
1:A:624:VAL:HG11	1:A:626:ARG:NH1	2.35	0.41
1:B:166:ASP:HA	1:B:167:PRO:HD3	1.94	0.40
1:B:316:LEU:HD11	1:B:318:LEU:HD21	2.03	0.40
1:B:456:MET:HE3	1:B:456:MET:HB3	1.92	0.40
1:B:624:VAL:HG12	1:B:626:ARG:HG3	2.03	0.40
1:A:522:ILE:HG21	1:A:569:GLN:HG2	2.03	0.40
1:B:299:SER:HB2	5:B:1088:HOH:O	2.21	0.40
1:B:634:ARG:HH11	1:B:634:ARG:HD3	1.78	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	668/780 (86%)	647 (97%)	20 (3%)	1 (0%)	48 57
1	B	668/780 (86%)	648 (97%)	18 (3%)	2 (0%)	37 42
All	All	1336/1560 (86%)	1295 (97%)	38 (3%)	3 (0%)	44 52

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	545	PRO
1	B	545	PRO
1	B	659	PRO

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	535/612 (87%)	529 (99%)	6 (1%)	70 82
1	B	535/612 (87%)	531 (99%)	4 (1%)	81 90
All	All	1070/1224 (87%)	1060 (99%)	10 (1%)	75 86

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	379	ASP
1	B	424	TYR
1	B	494	ASP
1	B	751	LYS
1	A	379	ASP
1	A	453	ARG
1	A	582	GLN
1	A	588	LYS
1	A	675	PRO
1	A	761	LEU

Sometimes 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 oligosaccharides 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	$\#\|Z\| > 2$
3	ACT	A	804	-	3,3,3	1.63	1 (33%)	3,3,3	1.28	0
4	C8E	B	805	-	15,15,20	0.41	0	14,14,19	0.42	0
4	C8E	A	806	-	14,14,20	0.41	0	13,13,19	0.38	0
2	EDO	A	801	-	3,3,3	0.47	0	2,2,2	0.44	0
4	C8E	A	807	-	20,20,20	0.38	0	19,19,19	0.56	0
4	C8E	A	805	-	14,14,20	0.31	0	13,13,19	0.80	0
4	C8E	B	803	-	11,11,20	0.37	0	10,10,19	0.48	0
2	EDO	B	801	-	3,3,3	0.53	0	2,2,2	0.26	0
3	ACT	B	802	-	3,3,3	1.50	1 (33%)	3,3,3	1.26	0
4	C8E	B	804	-	14,14,20	0.33	0	13,13,19	0.53	0
3	ACT	A	802	-	3,3,3	1.39	1 (33%)	3,3,3	1.44	0
2	EDO	A	803	-	3,3,3	0.39	0	2,2,2	0.73	0
4	C8E	B	806	-	14,14,20	0.39	0	13,13,19	0.26	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	C8E	B	805	-	-	8/13/13/18	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	C8E	A	806	-	-	9/12/12/18	-
2	EDO	A	801	-	-	0/1/1/1	-
4	C8E	A	807	-	-	8/18/18/18	-
4	C8E	A	805	-	-	10/12/12/18	-
4	C8E	B	803	-	-	3/9/9/18	-
2	EDO	B	801	-	-	0/1/1/1	-
4	C8E	B	804	-	-	9/12/12/18	-
2	EDO	A	803	-	-	0/1/1/1	-
4	C8E	B	806	-	-	8/12/12/18	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	804	ACT	CH3-C	2.53	1.59	1.49
3	B	802	ACT	CH3-C	2.32	1.58	1.49
3	A	802	ACT	CH3-C	2.11	1.57	1.49

There are no bond angle outliers.

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	806	C8E	O12-C13-C14-O15
4	B	806	C8E	C5-C6-C7-C8
4	B	806	C8E	C3-C4-C5-C6
4	A	805	C8E	O9-C10-C11-O12
4	B	805	C8E	C6-C7-C8-O9
4	A	807	C8E	O9-C10-C11-O12
4	B	804	C8E	C6-C7-C8-O9
4	B	806	C8E	C6-C7-C8-O9
4	A	807	C8E	C6-C7-C8-O9
4	A	805	C8E	C6-C7-C8-O9
4	A	805	C8E	O12-C13-C14-O15
4	A	807	C8E	O18-C19-C20-O21
4	A	807	C8E	C3-C4-C5-C6
4	B	805	C8E	O9-C10-C11-O12
4	A	807	C8E	C2-C3-C4-C5
4	A	805	C8E	C2-C3-C4-C5
4	A	806	C8E	C2-C3-C4-C5
4	B	806	C8E	O12-C13-C14-O15

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Mol	Chain	Res	Type	Atoms
4	B	804	C8E	C2-C3-C4-C5
4	B	804	C8E	C3-C4-C5-C6
4	A	806	C8E	O9-C10-C11-O12
4	B	804	C8E	C5-C6-C7-C8
4	A	806	C8E	C4-C5-C6-C7
4	B	806	C8E	C1-C2-C3-C4
4	B	803	C8E	C4-C5-C6-C7
4	A	807	C8E	C4-C5-C6-C7
4	B	805	C8E	O15-C16-C17-O18
4	B	803	C8E	C1-C2-C3-C4
4	B	806	C8E	O9-C10-C11-O12
4	A	805	C8E	C1-C2-C3-C4
4	A	805	C8E	C4-C5-C6-C7
4	B	803	C8E	C6-C7-C8-O9
4	B	804	C8E	O12-C13-C14-O15
4	B	805	C8E	C16-C17-O18-C19
4	B	806	C8E	C10-C11-O12-C13
4	B	806	C8E	C11-C10-O9-C8
4	A	805	C8E	C10-C11-O12-C13
4	A	805	C8E	C3-C4-C5-C6
4	B	805	C8E	C20-C19-O18-C17
4	A	805	C8E	C7-C8-O9-C10
4	A	806	C8E	C1-C2-C3-C4
4	A	806	C8E	C3-C4-C5-C6
4	A	807	C8E	O12-C13-C14-O15
4	B	805	C8E	C14-C13-O12-C11
4	B	804	C8E	C4-C5-C6-C7
4	A	805	C8E	C5-C6-C7-C8
4	A	807	C8E	C14-C13-O12-C11
4	B	804	C8E	O9-C10-C11-O12
4	B	805	C8E	C17-C16-O15-C14
4	B	804	C8E	C14-C13-O12-C11
4	B	804	C8E	C7-C8-O9-C10
4	A	806	C8E	C5-C6-C7-C8
4	A	806	C8E	C10-C11-O12-C13
4	B	805	C8E	O18-C19-C20-O21
4	A	806	C8E	C7-C8-O9-C10

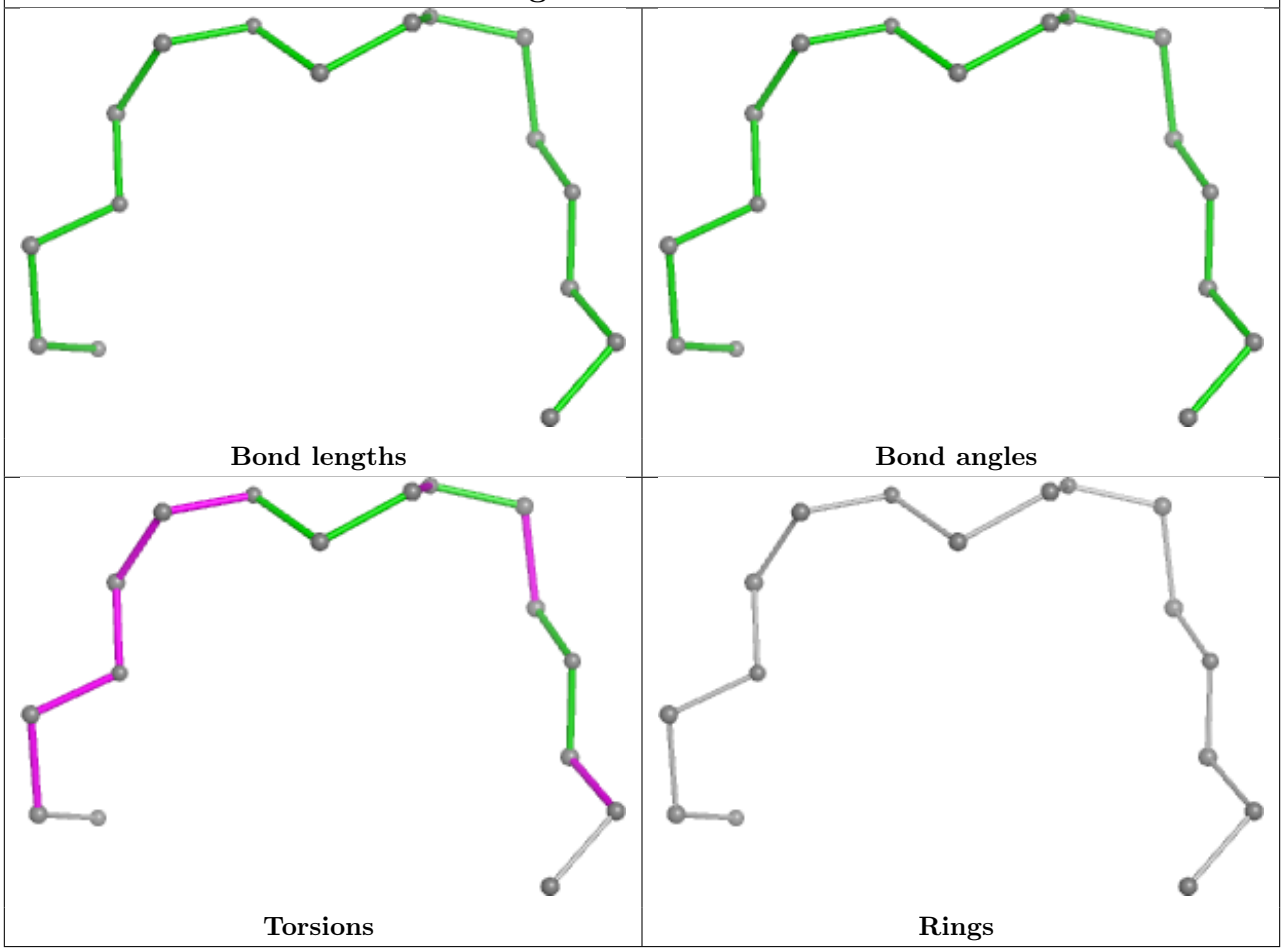
There are no ring outliers.

9 monomers are involved in 22 short contacts:

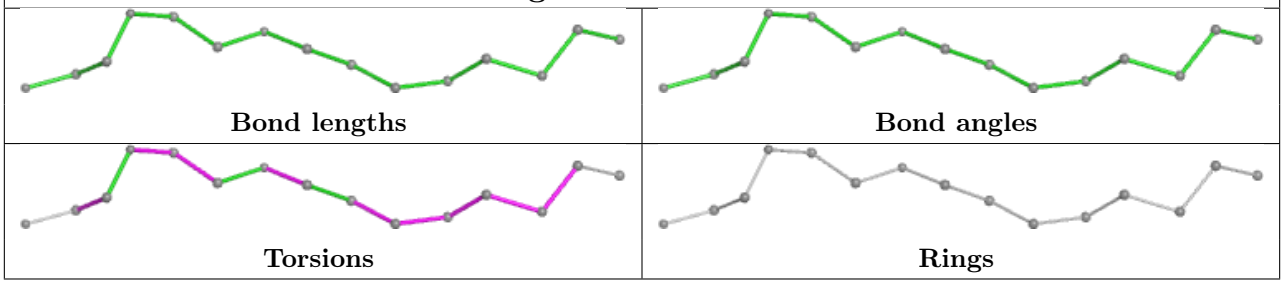
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	805	C8E	1	0
2	A	801	EDO	5	0
4	A	807	C8E	3	0
4	A	805	C8E	3	0
4	B	803	C8E	1	0
2	B	801	EDO	2	0
4	B	804	C8E	5	0
3	A	802	ACT	1	0
4	B	806	C8E	1	0

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 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.

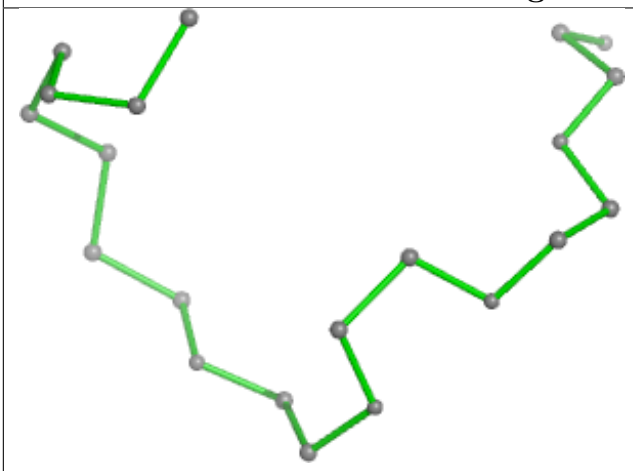
Ligand C8E B 805



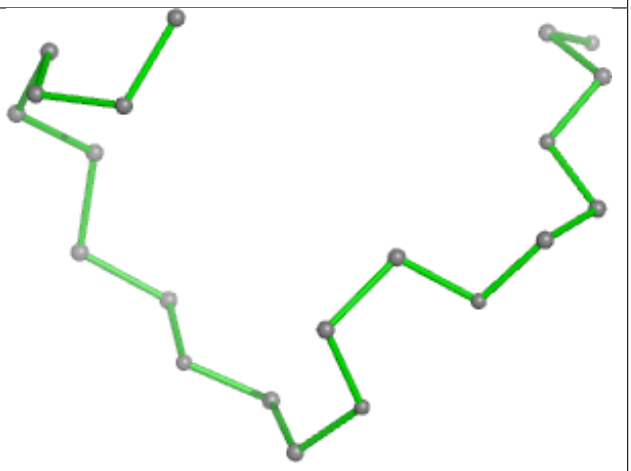
Ligand C8E A 806



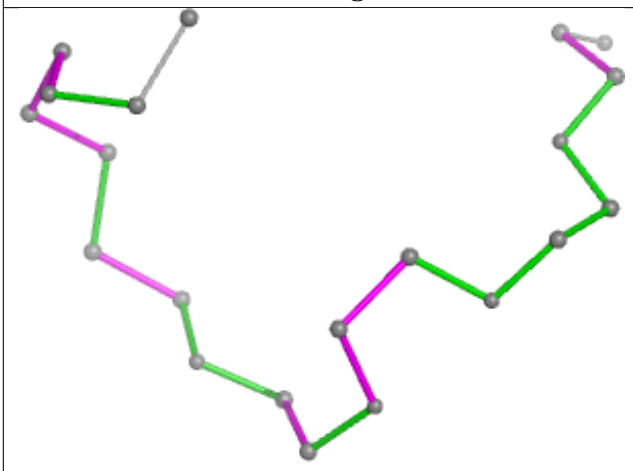
Ligand C8E A 807



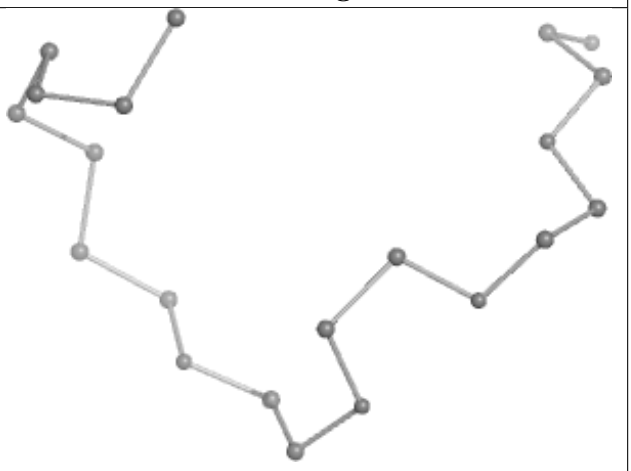
Bond lengths



Bond angles

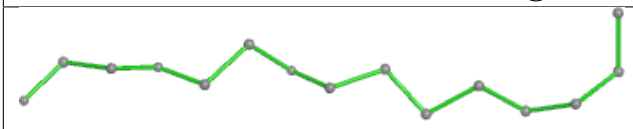


Torsions

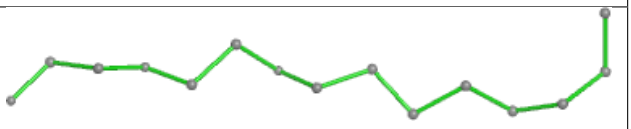


Rings

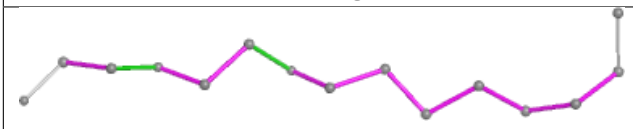
Ligand C8E A 805



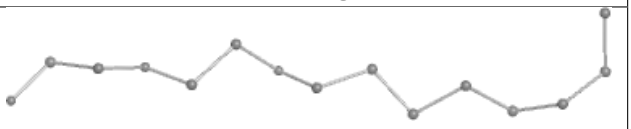
Bond lengths



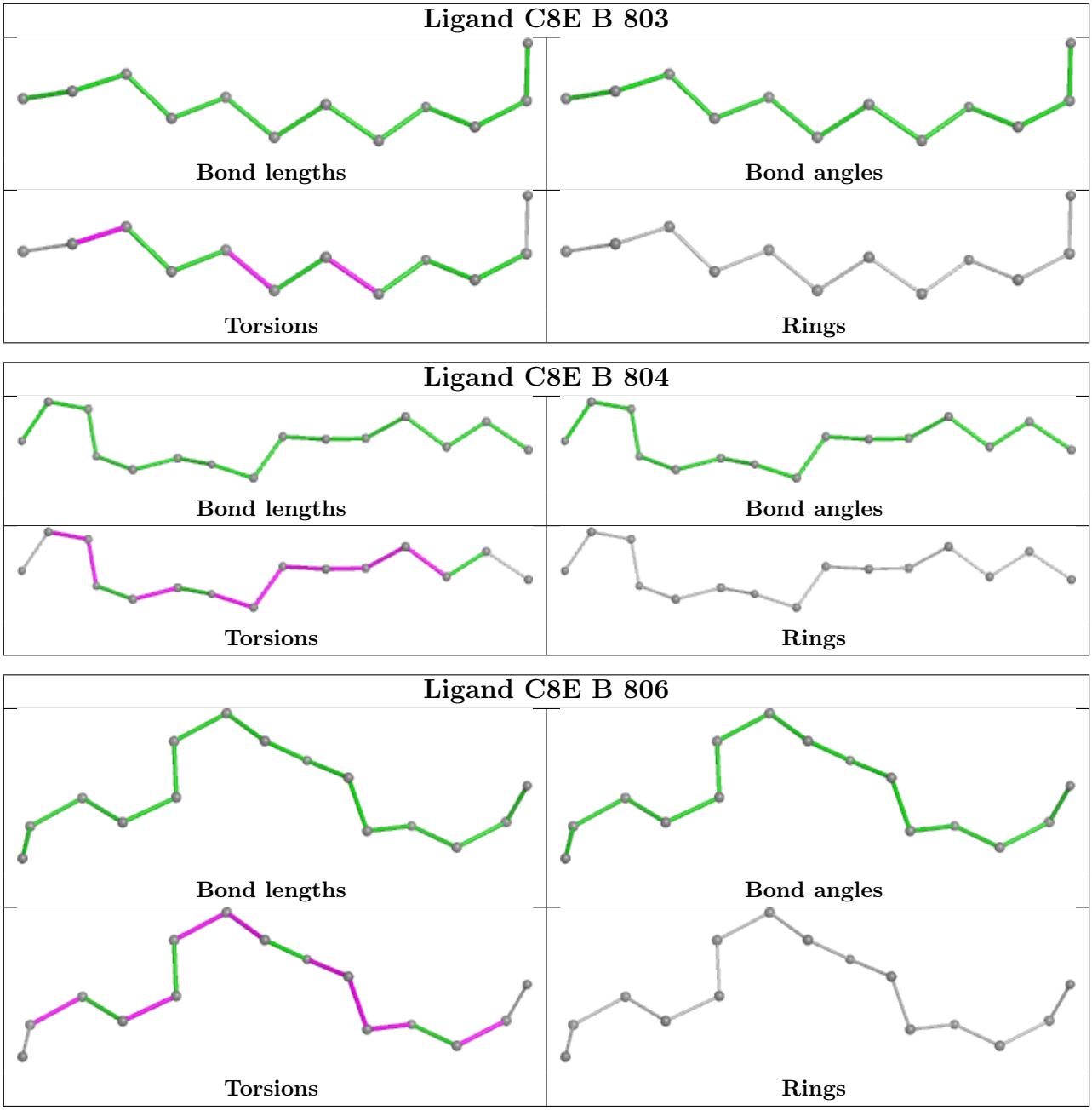
Bond angles



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

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	670/780 (85%)	0.17	19 (2%) 55 52	18, 30, 52, 74	0
1	B	670/780 (85%)	0.10	18 (2%) 56 53	19, 29, 51, 66	0
All	All	1340/1560 (85%)	0.13	37 (2%) 55 52	18, 30, 52, 74	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	621	ALA	4.6
1	B	424	TYR	3.9
1	B	621	ALA	3.6
1	A	575	MET	3.4
1	A	506	PHE	3.4
1	B	344	HIS	3.0
1	B	347	HIS	3.0
1	B	576	THR	3.0
1	A	576	THR	2.9
1	A	530	THR	2.9
1	B	691	PRO	2.8
1	A	622	SER	2.8
1	A	624	VAL	2.8
1	A	276	GLU	2.8
1	A	578	ALA	2.7
1	A	347	HIS	2.6
1	B	603	PHE	2.5
1	B	406	ASN	2.5
1	B	692	PHE	2.4
1	B	578	ALA	2.4
1	A	577	ALA	2.4
1	B	340	PRO	2.3
1	A	603	PHE	2.3
1	A	638	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	506	PHE	2.3
1	B	665	GLY	2.3
1	B	438	PRO	2.2
1	A	509	ASP	2.2
1	B	624	VAL	2.2
1	B	379	ASP	2.2
1	B	314	GLU	2.2
1	A	662	ASN	2.2
1	A	666	ASP	2.1
1	A	340	PRO	2.1
1	A	665	GLY	2.1
1	A	435	ASP	2.0
1	B	622	SER	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^{th} 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^2)	Q<0.9
3	ACT	A	804	4/4	0.75	0.14	39,40,43,43	0
4	C8E	B	806	15/21	0.77	0.18	36,46,56,57	0
2	EDO	A	801	4/4	0.83	0.14	33,35,39,44	0
4	C8E	B	804	15/21	0.84	0.14	31,37,48,48	0
4	C8E	A	806	15/21	0.84	0.13	25,33,42,53	0
3	ACT	B	802	4/4	0.85	0.14	33,39,39,41	0
4	C8E	B	805	16/21	0.85	0.15	31,40,45,47	0
2	EDO	A	803	4/4	0.87	0.13	35,37,39,45	0
4	C8E	A	807	21/21	0.87	0.15	32,42,51,53	0
4	C8E	B	803	12/21	0.88	0.11	29,36,43,47	0

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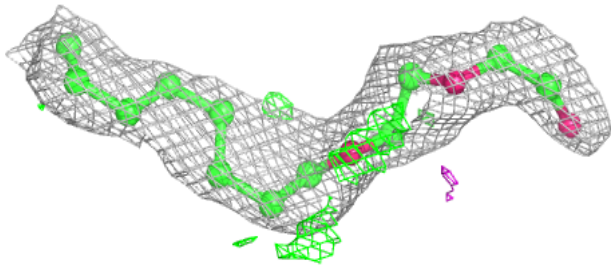
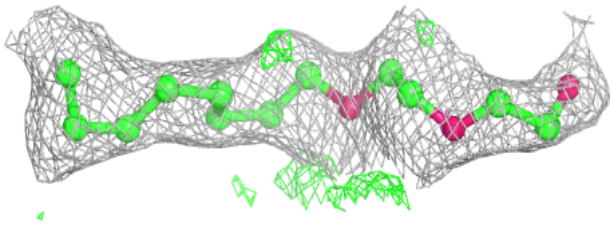
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ACT	A	802	4/4	0.88	0.13	35,37,42,45	0
4	C8E	A	805	15/21	0.90	0.10	25,31,40,40	0
2	EDO	B	801	4/4	0.92	0.11	38,43,43,46	0

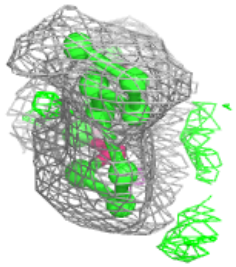
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around C8E B 806:

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

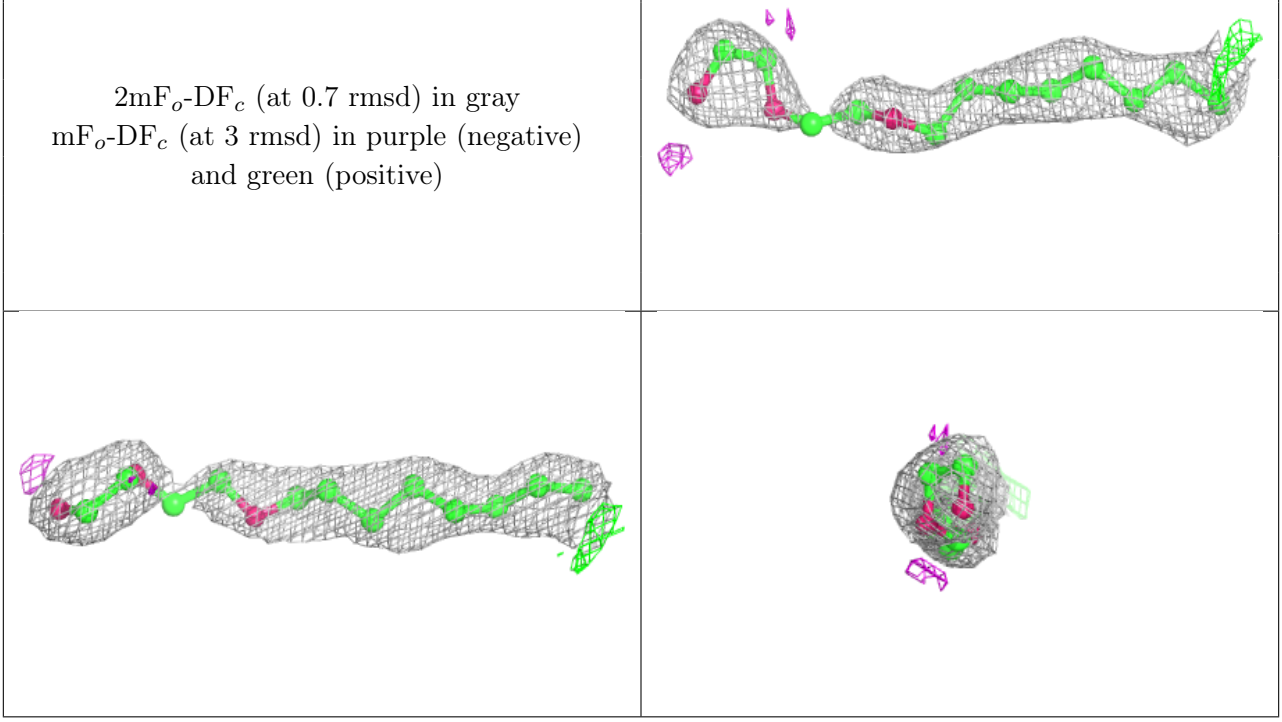






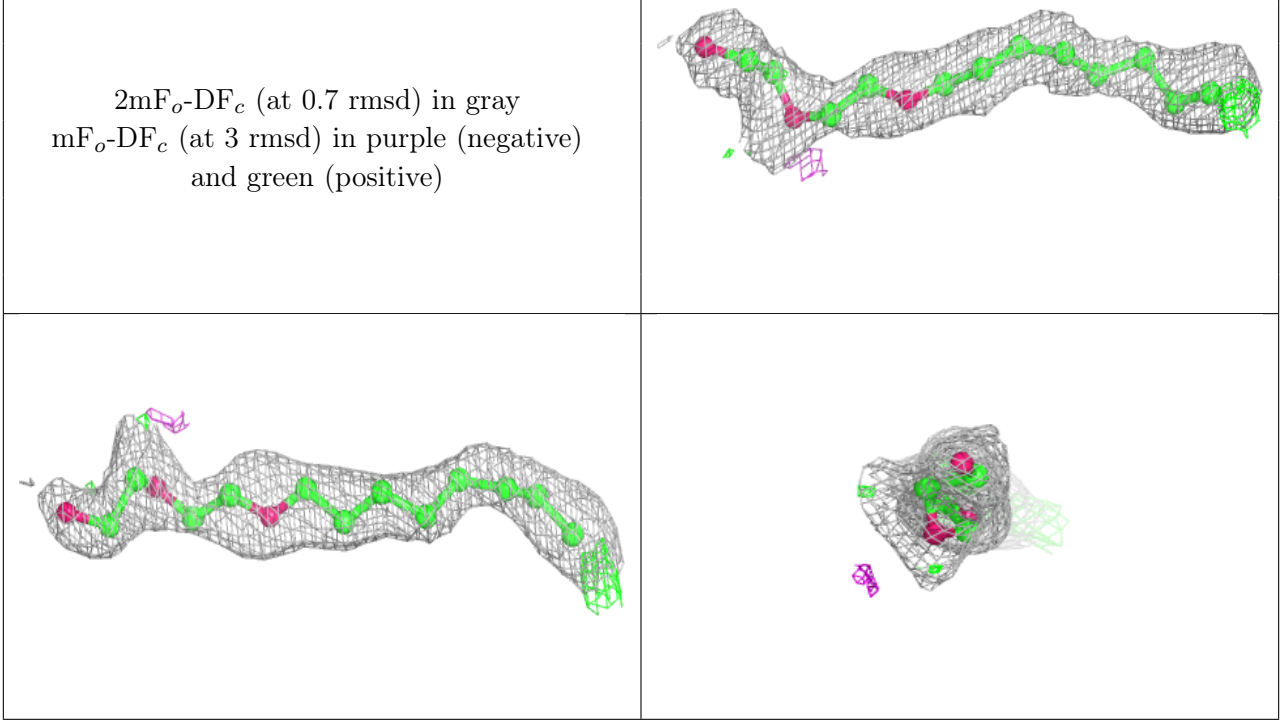
Electron density around C8E B 804:

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



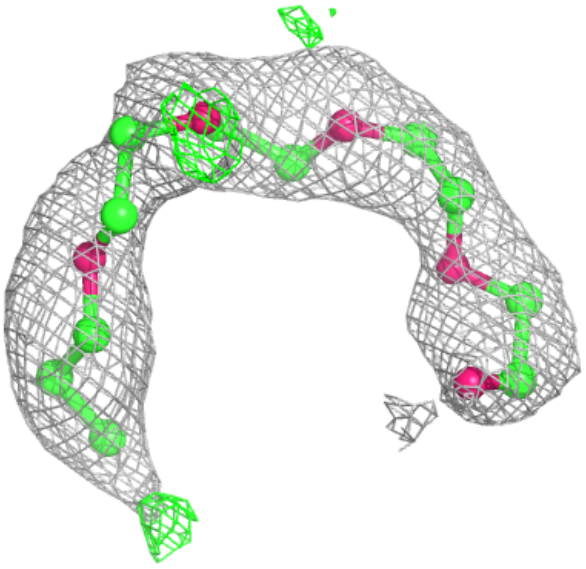
Electron density around C8E A 806:

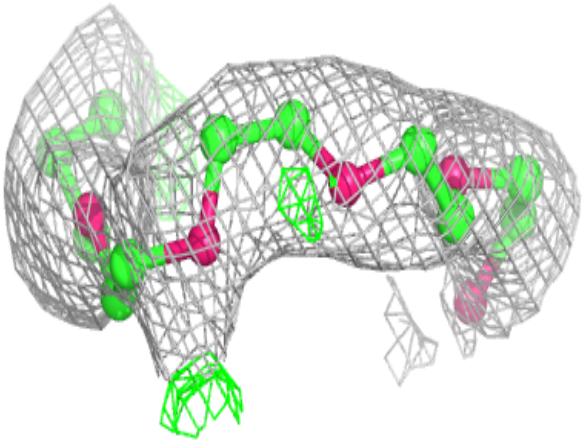
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

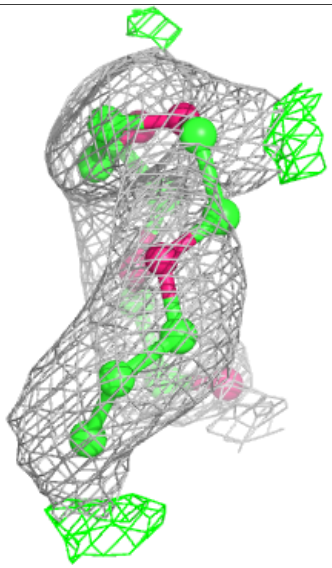


Electron density around C8E B 805:

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

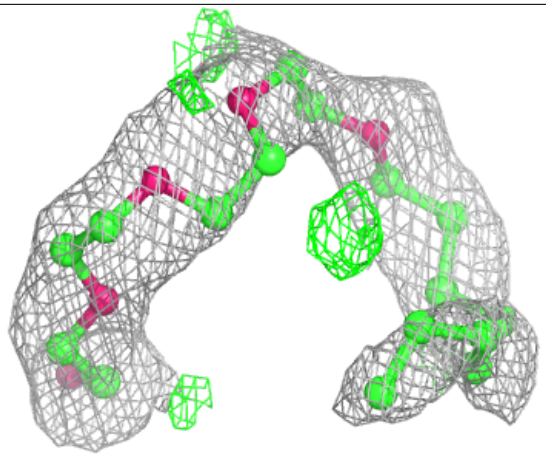


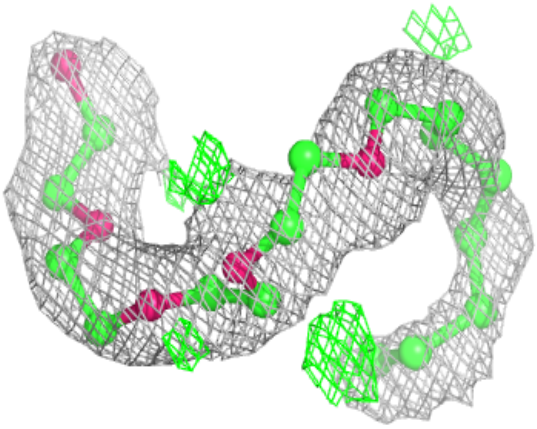


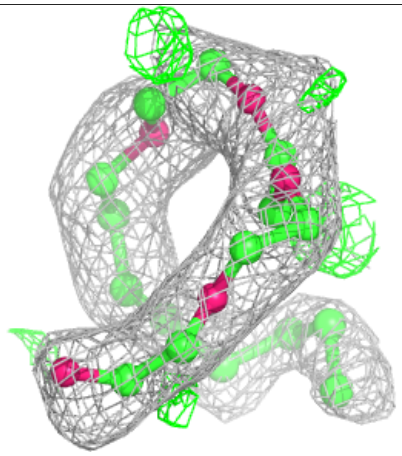


Electron density around C8E A 807:

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

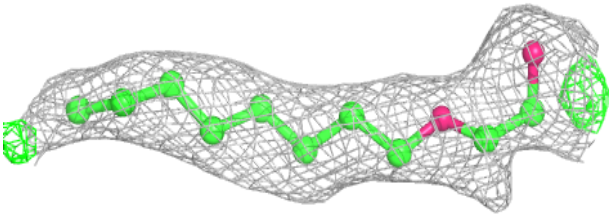


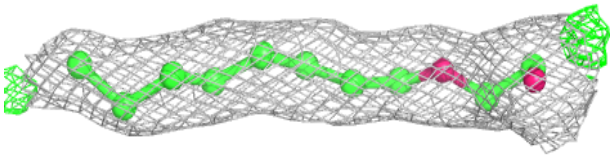


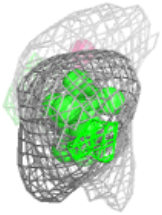


Electron density around C8E B 803:

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

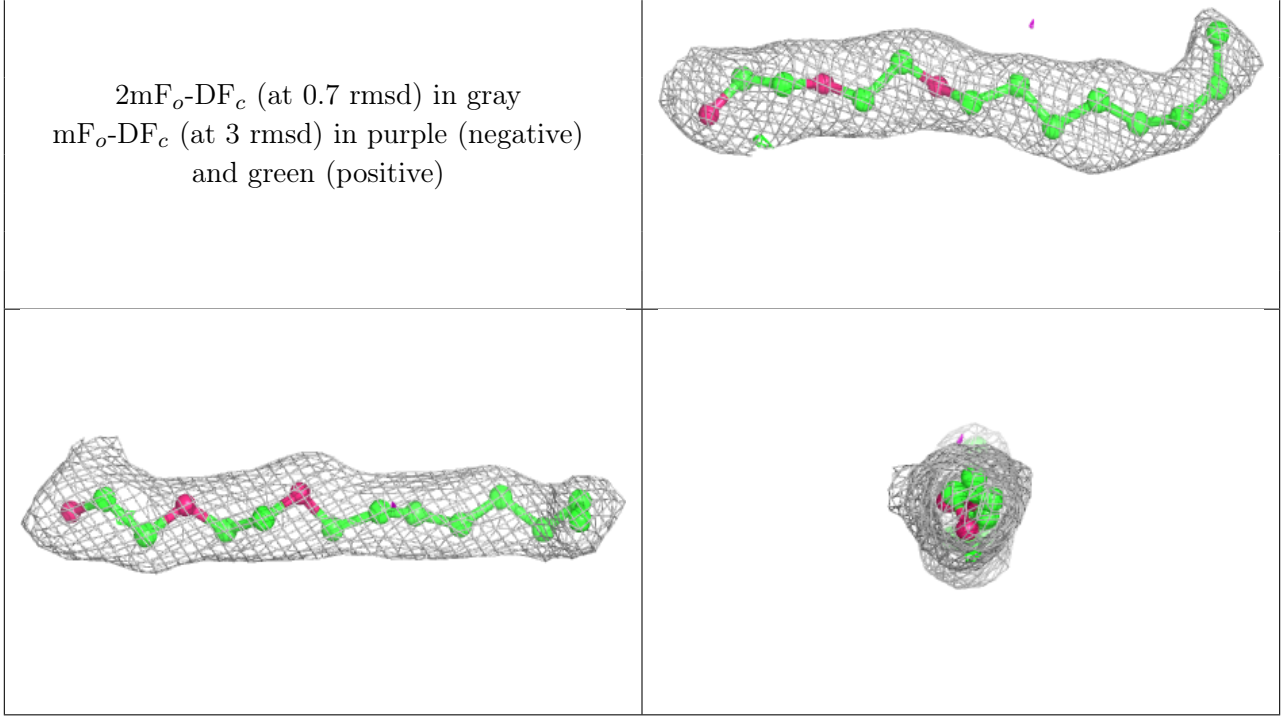






Electron density around C8E A 805:

$2mF_o$-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.