



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2023 – 07:02 AM EDT

PDB ID : 3PGS
Title : Phe3Gly mutant of EcFadL
Authors : van den Berg, B.; Lepore, B.W.
Deposited on : 2010-11-02
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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 : 2.35
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) : 2.35

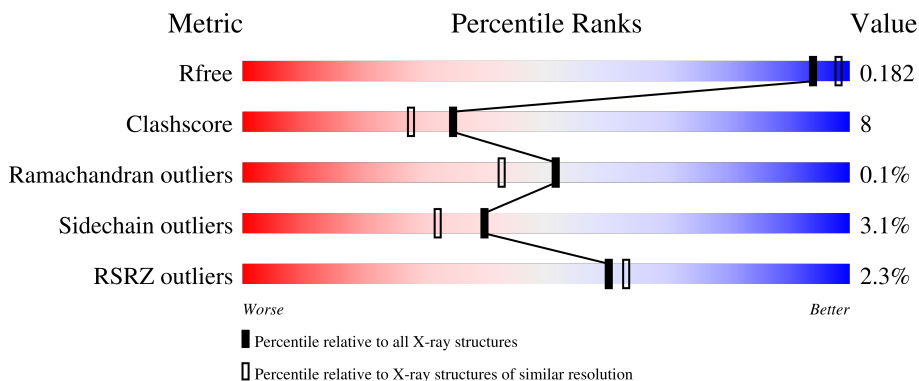
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 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 $\leq 5\%$. 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	427	 2% 87% 12% .
1	B	427	 3% 82% 17% .

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8014 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 Long-chain fatty acid transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	427	Total	C	N	O	S	3	23	0
			3459	2194	592	666	7			
1	B	426	Total	C	N	O	S	5	19	0
			3411	2167	583	654	7			

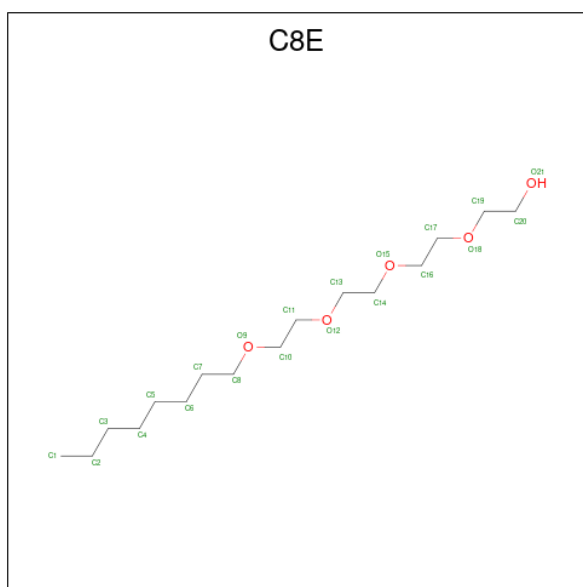
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	GLY	PHE	engineered mutation	UNP P10384
A	422	HIS	-	expression tag	UNP P10384
A	423	HIS	-	expression tag	UNP P10384
A	424	HIS	-	expression tag	UNP P10384
A	425	HIS	-	expression tag	UNP P10384
A	426	HIS	-	expression tag	UNP P10384
A	427	HIS	-	expression tag	UNP P10384
B	3	GLY	PHE	engineered mutation	UNP P10384
B	422	HIS	-	expression tag	UNP P10384
B	423	HIS	-	expression tag	UNP P10384
B	424	HIS	-	expression tag	UNP P10384
B	425	HIS	-	expression tag	UNP P10384
B	426	HIS	-	expression tag	UNP P10384
B	427	HIS	-	expression tag	UNP P10384

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

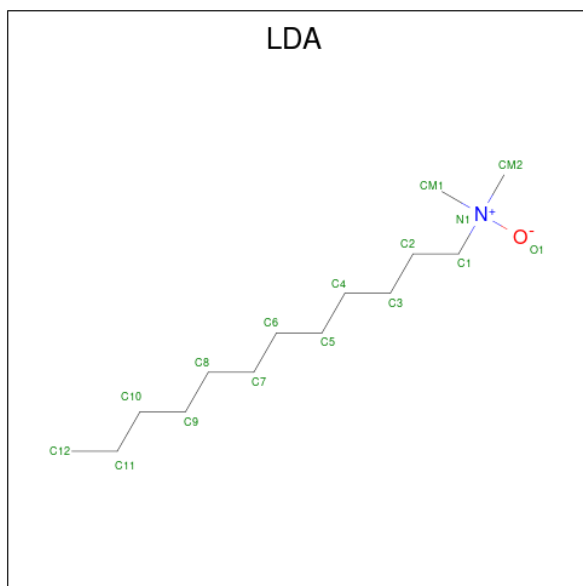
- Molecule 3 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C₁₆H₃₄O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	5		
3	A	1	Total	C	O	0	0
			14	12	2		
3	A	1	Total	C	O	0	0
			20	15	5		
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	A	1	Total	C	O	0	0
			21	16	5		
3	A	1	Total	C	O	0	0
			13	11	2		
3	B	1	Total	C	O	0	0
			21	16	5		
3	B	1	Total	C	O	0	0
			21	16	5		
3	B	1	Total	C	O	0	0
			21	16	5		
3	B	1	Total	C	O	0	0
			15	10	5		
3	B	1	Total	C	O	0	0
			21	16	5		

- Molecule 4 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula:

C₁₄H₃₁NO).



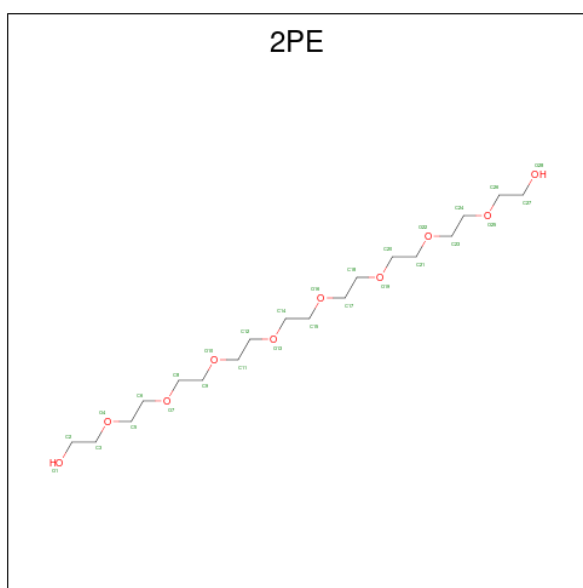
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C 11 11	0	0
4	A	1	Total C 10 10	0	0
4	A	1	Total C 12 12	0	0
4	A	1	Total C 10 10	0	0
4	A	1	Total C 7 7	0	0
4	A	1	Total C 7 7	0	0
4	A	1	Total C 10 10	0	0
4	B	1	Total C 10 10	0	0
4	B	1	Total C 10 10	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

- Molecule 6 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: $C_{18}H_{38}O_{10}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			28	18	10		

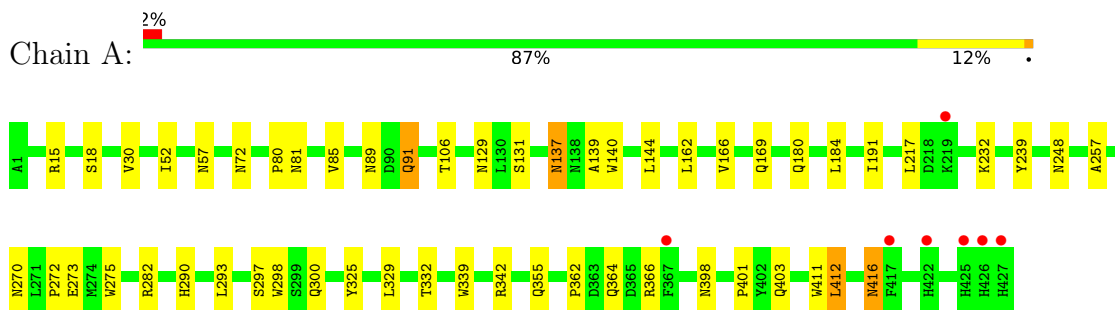
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	394	Total 394	O 394	0	0
7	B	383	Total 383	O 383	0	0

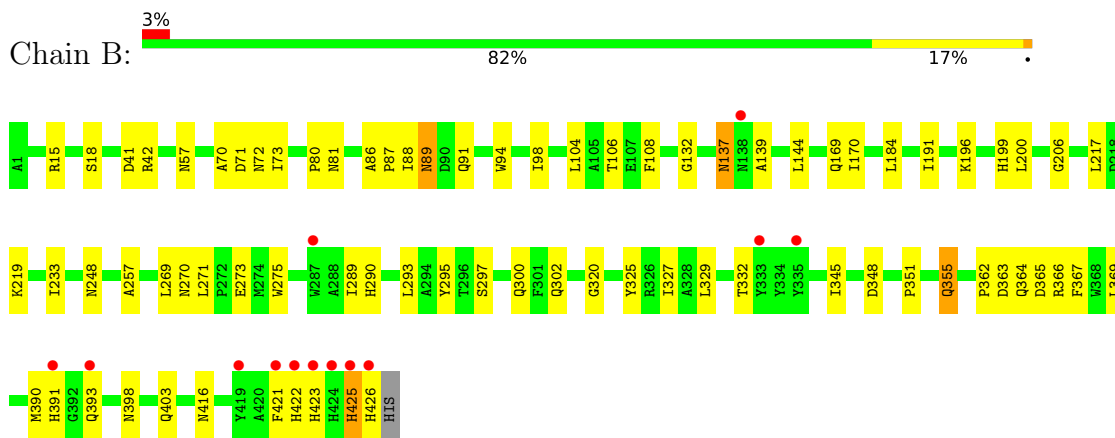
3 Residue-property plots [i](#)

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: Long-chain fatty acid transport protein



- Molecule 1: Long-chain fatty acid transport protein



4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.07Å 147.51Å 151.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.78 – 1.90 38.78 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.0 (38.78-1.90) 93.9 (38.78-1.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 1.85Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: dev_572)	Depositor
R, R_{free}	0.167 , 0.192 0.161 , 0.182	Depositor DCC
R_{free} test set	1987 reflections (1.66%)	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtrriage
Anisotropy	0.205	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 60.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.007 for -h,l,k	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8014	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 2PE, ACT, LDA, C8E, CA

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	0/3607	0.55	0/4903
1	B	0.37	0/3553	0.54	0/4834
All	All	0.38	0/7160	0.54	0/9737

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	3459	0	3266	44	0
1	B	3411	0	3220	59	0
2	A	1	0	0	0	0
3	A	144	0	226	22	0
3	B	99	0	155	17	0
4	A	67	0	124	5	0
4	B	20	0	38	3	0
5	A	4	0	3	1	0
5	B	4	0	3	0	0
6	B	28	0	38	2	0
7	A	394	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	383	0	0	5	0
All	All	8014	0	7073	118	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 8.

All (118) 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:B:191:ILE:HG21	3:B:434:C8E:H202	1.40	1.02
3:A:443:C8E:H32	1:B:169:GLN:HE22	1.26	0.98
1:B:248:ASN:HD21	1:B:257:ALA:H	1.10	0.97
1:A:248:ASN:HD21	1:A:257:ALA:H	1.15	0.94
1:B:355:GLN:H	1:B:355:GLN:HE21	1.07	0.93
4:A:433:LDA:H111	1:B:170:ILE:HG12	1.52	0.90
1:A:169[A]:GLN:HE22	3:A:442:C8E:H112	1.40	0.85
1:A:166:VAL:HG11	3:A:442:C8E:H191	1.58	0.84
1:A:169[A]:GLN:NE2	3:A:442:C8E:H112	1.97	0.80
1:A:30:VAL:HG21	1:A:85[B]:VAL:HG11	1.63	0.78
3:A:443:C8E:H32	1:B:169:GLN:NE2	2.00	0.76
1:B:365:ASP:H	1:B:393:GLN:HE21	1.31	0.75
1:B:355:GLN:H	1:B:355:GLN:NE2	1.83	0.74
1:B:200:LEU:HB3	3:B:431:C8E:H161	1.69	0.73
1:B:355:GLN:HE21	1:B:355:GLN:N	1.87	0.71
1:A:162:LEU:HD22	3:A:440:C8E:H111	1.73	0.69
1:A:81:ASN:HD21	1:A:416:ASN:HD21	1.40	0.68
1:B:132:GLY:HA3	3:B:433:C8E:H81	1.78	0.66
1:A:57:ASN:ND2	1:A:72:ASN:H	1.96	0.63
5:A:1428:ACT:H2	7:A:772:HOH:O	1.97	0.63
1:A:401:PRO:HA	3:A:442:C8E:H22	1.80	0.63
1:B:41:ASP:O	1:B:425:HIS:HE1	1.82	0.63
1:B:81:ASN:HD21	1:B:416:ASN:HD21	1.48	0.61
1:B:364:GLN:HB2	1:B:393:GLN:HG3	1.82	0.61
1:B:57:ASN:ND2	1:B:72:ASN:H	1.99	0.60
1:B:89:ASN:ND2	1:B:91:GLN:H	2.00	0.60
1:A:239:TYR:HB2	3:A:438:C8E:C2	2.33	0.59
1:B:270:ASN:O	3:B:431:C8E:H11	2.01	0.59
1:A:57:ASN:HD22	1:A:72:ASN:H	1.51	0.58
1:A:137:ASN:ND2	1:A:140:TRP:H	2.01	0.58
1:A:275:TRP:CH2	4:A:432:LDA:H71	2.38	0.58
1:B:57:ASN:HD22	1:B:72:ASN:H	1.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:HIS:HE1	1:B:332:THR:OG1	1.87	0.57
1:B:269:LEU:HD11	3:B:431:C8E:H13	1.87	0.57
1:B:89:ASN:C	1:B:89:ASN:HD22	2.08	0.56
4:A:433:LDA:H81	3:B:435:C8E:H11	1.88	0.55
1:B:365:ASP:H	1:B:393:GLN:NE2	2.01	0.54
3:B:434:C8E:H111	7:B:488:HOH:O	2.08	0.54
1:B:271:LEU:HD23	3:B:431:C8E:H22	1.89	0.54
1:B:422:HIS:C	1:B:423:HIS:HD1	2.10	0.54
1:A:273:GLU:H	1:A:300:GLN:HE22	1.55	0.53
3:A:440:C8E:O15	3:A:440:C8E:H191	2.08	0.53
1:B:73[B]:ILE:HG21	1:B:108:PHE:CZ	2.44	0.52
1:A:137:ASN:C	1:A:137:ASN:HD22	2.13	0.52
1:B:137[A]:ASN:HD22	1:B:139[A]:ALA:H	1.57	0.51
1:A:30:VAL:CG2	1:A:85[B]:VAL:HG11	2.38	0.51
1:A:18:SER:OG	1:A:290:HIS:HD2	1.95	0.50
1:B:73[B]:ILE:HG21	1:B:108:PHE:CE1	2.46	0.50
1:A:290:HIS:HE1	1:A:332:THR:OG1	1.95	0.50
1:A:411:TRP:CZ3	3:A:430:C8E:H82	2.46	0.50
1:B:289:ILE:HD11	6:B:436:2PE:H181	1.94	0.50
1:A:339:TRP:CD1	3:A:441:C8E:H171	2.46	0.49
1:B:366:ARG:HD3	1:B:390:MET:CE	2.43	0.49
1:B:89:ASN:HD22	1:B:91:GLN:H	1.59	0.48
1:A:52:ILE:HG23	1:A:412[A]:LEU:HD13	1.94	0.48
1:A:293:LEU:HD11	1:A:325[B]:TYR:HD2	1.78	0.48
1:B:367[A]:PHE:HD2	1:B:391[A]:HIS:CE1	2.31	0.48
1:B:275:TRP:HH2	4:B:430:LDA:H82	1.79	0.48
1:B:351:PRO:HD2	1:B:363:ASP:OD2	2.13	0.48
3:B:435:C8E:H192	7:B:734:HOH:O	2.13	0.48
3:A:439:C8E:H61	7:A:583:HOH:O	2.14	0.47
1:A:80:PRO:HB2	4:A:434:LDA:H41	1.96	0.47
1:A:52:ILE:HG12	1:A:412[A]:LEU:CD1	2.44	0.47
1:A:298:TRP:CZ3	3:A:438:C8E:H202	2.49	0.47
1:A:180:GLN:HE21	4:A:433:LDA:C1	2.28	0.46
3:B:433:C8E:H111	7:B:599:HOH:O	2.14	0.46
1:B:137[A]:ASN:HD22	1:B:137[A]:ASN:C	2.19	0.46
1:B:273:GLU:H	1:B:300:GLN:HE22	1.63	0.46
1:A:137:ASN:ND2	1:A:139:ALA:H	2.14	0.46
1:B:273:GLU:HG2	1:B:297:SER:HB2	1.96	0.46
1:B:295:TYR:HD1	1:B:325[B]:TYR:CE1	2.34	0.46
1:B:18:SER:OG	1:B:290:HIS:HD2	1.99	0.46
1:B:196:LYS:HD3	1:B:199:HIS:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:441:C8E:H42	3:A:441:C8E:H13	1.53	0.45
1:B:42:ARG:HD2	1:B:421:PHE:O	2.16	0.45
1:A:411:TRP:CH2	3:A:430:C8E:H82	2.52	0.45
1:A:272:PRO:HA	1:A:300:GLN:HE21	1.80	0.45
1:B:275:TRP:CH2	4:B:430:LDA:H82	2.52	0.45
1:A:293:LEU:HD11	1:A:325[B]:TYR:CD2	2.52	0.45
1:A:89:ASN:HB3	1:A:91:GLN:H	1.83	0.44
1:B:70:ALA:HB1	1:B:73[B]:ILE:HD11	1.98	0.44
1:A:30:VAL:HG21	1:A:85[A]:VAL:HG21	1.98	0.44
1:B:106[A]:THR:HG21	1:B:362:PRO:CD	2.47	0.44
1:A:298:TRP:HZ3	3:A:438:C8E:H202	1.83	0.44
3:A:443:C8E:H81	3:B:435:C8E:H41	1.99	0.44
1:B:398:ASN:OD1	1:B:403:GLN:HG2	2.18	0.44
1:A:52:ILE:HG23	1:A:412[A]:LEU:CD1	2.48	0.43
1:B:302:GLN:NE2	1:B:320:GLY:HA2	2.32	0.43
1:A:273:GLU:HG2	1:A:297:SER:HB2	1.99	0.43
3:A:440:C8E:H202	3:A:442:C8E:H12	2.00	0.43
1:B:57:ASN:HD22	1:B:71:ASP:HA	1.83	0.43
1:A:364:GLN:HE21	1:A:366:ARG:HE	1.66	0.43
3:A:440:C8E:H41	3:A:440:C8E:H71	1.63	0.43
1:B:345:ILE:HG22	1:B:369:LEU:HD13	2.00	0.43
1:B:88:ILE:O	1:B:426:HIS:NE2	2.51	0.42
1:A:232:LYS:HG2	1:A:270:ASN:HD22	1.83	0.42
1:B:206:GLY:HA3	1:B:233:ILE:HD13	2.01	0.42
1:A:191:ILE:HG13	3:A:440:C8E:H21	2.01	0.42
3:A:443:C8E:C8	3:B:435:C8E:H41	2.50	0.42
1:A:15[B]:ARG:HG3	1:A:342:ARG:HD3	2.01	0.42
1:B:293:LEU:HD11	1:B:325[B]:TYR:CD1	2.55	0.42
3:B:431:C8E:H13	3:B:431:C8E:H42	1.61	0.42
1:B:80:PRO:HD2	3:B:432:C8E:H202	2.02	0.41
1:A:191:ILE:HG21	3:A:440:C8E:H21	2.03	0.41
1:A:272:PRO:HA	1:A:300:GLN:NE2	2.36	0.41
1:B:98:ILE:HG13	4:B:429:LDA:H91	2.01	0.41
3:B:434:C8E:H81	7:B:624:HOH:O	2.21	0.41
3:B:432:C8E:H142	7:B:619:HOH:O	2.21	0.41
1:B:137[A]:ASN:ND2	1:B:139[A]:ALA:H	2.18	0.41
1:A:106[B]:THR:HG21	1:A:362:PRO:HD3	2.03	0.41
1:A:398:ASN:OD1	1:A:403:GLN:HG2	2.20	0.41
1:B:86:ALA:HA	1:B:87:PRO:HD3	1.94	0.41
1:B:327:ILE:HD11	6:B:436:2PE:H92	2.03	0.40
1:B:94:TRP:HB3	3:B:433:C8E:H101	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ASN:HD21	1:A:131:SER:HG	1.66	0.40
1:B:422:HIS:C	1:B:423:HIS:ND1	2.75	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	449/427 (105%)	444 (99%)	5 (1%)	0	100	100
1	B	443/427 (104%)	437 (99%)	5 (1%)	1 (0%)	47	38
All	All	892/854 (104%)	881 (99%)	10 (1%)	1 (0%)	51	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	425	HIS

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	360/336 (107%)	349 (97%)	11 (3%)	40	32
1	B	353/336 (105%)	341 (97%)	12 (3%)	37	28
All	All	713/672 (106%)	690 (97%)	23 (3%)	40	30

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	137	ASN
1	A	144	LEU
1	A	184	LEU
1	A	217	LEU
1	A	282	ARG
1	A	329	LEU
1	A	355	GLN
1	A	412[A]	LEU
1	A	412[B]	LEU
1	A	416	ASN
1	B	15	ARG
1	B	89	ASN
1	B	104	LEU
1	B	137[A]	ASN
1	B	137[B]	ASN
1	B	144	LEU
1	B	184	LEU
1	B	217	LEU
1	B	219	LYS
1	B	329	LEU
1	B	348	ASP
1	B	355	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	57	ASN
1	A	83	HIS
1	A	127	ASN
1	A	129	ASN
1	A	137	ASN
1	A	138	ASN
1	A	180	GLN
1	A	248	ASN
1	A	270	ASN
1	A	281	ASN
1	A	290	HIS
1	A	300	GLN
1	A	302	GLN

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Mol	Chain	Res	Type
1	A	303	GLN
1	A	316	GLN
1	A	356	ASN
1	A	364	GLN
1	A	416	ASN
1	A	418	ASN
1	B	57	ASN
1	B	83	HIS
1	B	89	ASN
1	B	127	ASN
1	B	129	ASN
1	B	169	GLN
1	B	180	GLN
1	B	248	ASN
1	B	270	ASN
1	B	281	ASN
1	B	290	HIS
1	B	300	GLN
1	B	302	GLN
1	B	303	GLN
1	B	316	GLN
1	B	355	GLN
1	B	356	ASN
1	B	393	GLN
1	B	416	ASN
1	B	418	ASN
1	B	425	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 26 ligands modelled in this entry, 1 is monoatomic - leaving 25 for Mogul analysis.

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	439	-	20,20,20	0.36	0	19,19,19	0.40	0
4	LDA	A	432	-	9,9,15	0.27	0	8,8,17	0.52	0
3	C8E	B	433	-	20,20,20	0.36	0	19,19,19	0.40	0
3	C8E	A	441	-	20,20,20	0.37	0	19,19,19	0.49	0
4	LDA	A	435	-	6,6,15	0.27	0	5,5,17	0.42	0
4	LDA	B	430	-	9,9,15	0.27	0	8,8,17	0.53	0
4	LDA	A	434	-	9,9,15	0.24	0	8,8,17	0.57	0
3	C8E	B	435	-	20,20,20	0.34	0	19,19,19	0.56	0
6	2PE	B	436	-	27,27,27	0.69	0	26,26,26	1.54	0
4	LDA	A	437	-	9,9,15	0.27	0	8,8,17	0.49	0
3	C8E	A	443	-	12,12,20	0.33	0	11,11,19	0.38	0
5	ACT	B	1428	-	3,3,3	0.82	0	3,3,3	1.42	0
3	C8E	A	430	-	13,13,20	0.39	0	12,12,19	0.41	0
4	LDA	B	429	-	9,9,15	0.27	0	8,8,17	0.55	0
3	C8E	A	440	-	20,20,20	0.34	0	19,19,19	0.54	0
4	LDA	A	433	-	11,11,15	0.28	0	10,10,17	0.49	0
3	C8E	B	434	-	14,14,20	0.42	0	13,13,19	0.45	0
4	LDA	A	431	-	10,10,15	0.27	0	9,9,17	0.51	0
3	C8E	B	431	-	20,20,20	0.38	0	19,19,19	0.62	0
3	C8E	A	438	-	19,19,20	0.40	0	18,18,19	0.53	0
3	C8E	A	442	-	20,20,20	0.38	0	19,19,19	0.47	0
3	C8E	B	432	-	20,20,20	0.39	0	19,19,19	0.33	0
5	ACT	A	1428	-	3,3,3	0.79	0	3,3,3	1.12	0
3	C8E	A	429	-	12,12,20	0.39	0	11,11,19	0.47	0
4	LDA	A	436	-	6,6,15	0.27	0	5,5,17	0.47	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	439	-	-	12/18/18/18	-
4	LDA	A	432	-	-	5/7/7/13	-
3	C8E	B	433	-	-	14/18/18/18	-
3	C8E	A	441	-	-	11/18/18/18	-
4	LDA	A	435	-	-	3/4/4/13	-
4	LDA	B	430	-	-	3/7/7/13	-
4	LDA	A	434	-	-	5/7/7/13	-
3	C8E	B	435	-	-	6/18/18/18	-
6	2PE	B	436	-	-	12/25/25/25	-
4	LDA	A	437	-	-	3/7/7/13	-
3	C8E	A	443	-	-	7/10/10/18	-
3	C8E	A	430	-	-	7/11/11/18	-
4	LDA	B	429	-	-	1/7/7/13	-
3	C8E	A	440	-	-	14/18/18/18	-
4	LDA	A	433	-	-	6/9/9/13	-
3	C8E	B	434	-	-	8/12/12/18	-
4	LDA	A	431	-	-	3/8/8/13	-
3	C8E	B	431	-	-	12/18/18/18	-
3	C8E	A	438	-	-	6/17/17/18	-
3	C8E	A	442	-	-	14/18/18/18	-
3	C8E	B	432	-	-	12/18/18/18	-
3	C8E	A	429	-	-	6/10/10/18	-
4	LDA	A	436	-	-	2/4/4/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (172) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	433	C8E	C16-C17-O18-C19
3	A	442	C8E	C3-C4-C5-C6
3	B	431	C8E	C4-C5-C6-C7
3	A	440	C8E	O12-C13-C14-O15
3	A	439	C8E	O9-C10-C11-O12
3	A	440	C8E	O9-C10-C11-O12
3	A	442	C8E	O9-C10-C11-O12

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Mol	Chain	Res	Type	Atoms
3	A	442	C8E	O12-C13-C14-O15
6	B	436	2PE	O4-C5-C6-O7
6	B	436	2PE	O19-C20-C21-O22
3	B	433	C8E	O12-C13-C14-O15
3	B	431	C8E	O12-C13-C14-O15
3	A	439	C8E	O15-C16-C17-O18
6	B	436	2PE	O10-C11-C12-O13
3	A	441	C8E	O12-C13-C14-O15
3	A	440	C8E	C4-C5-C6-C7
3	A	442	C8E	C6-C7-C8-O9
3	A	441	C8E	C6-C7-C8-O9
3	A	439	C8E	O18-C19-C20-O21
3	A	441	C8E	O18-C19-C20-O21
3	B	432	C8E	O18-C19-C20-O21
3	B	433	C8E	O18-C19-C20-O21
3	B	434	C8E	O18-C19-C20-O21
6	B	436	2PE	O13-C14-C15-O16
3	B	432	C8E	C6-C7-C8-O9
3	A	429	C8E	O12-C13-C14-O15
3	A	440	C8E	C6-C7-C8-O9
3	B	431	C8E	C6-C7-C8-O9
3	B	434	C8E	O15-C16-C17-O18
3	A	440	C8E	O18-C19-C20-O21
3	B	435	C8E	O18-C19-C20-O21
3	A	439	C8E	C2-C3-C4-C5
3	A	442	C8E	C2-C3-C4-C5
3	A	443	C8E	C3-C4-C5-C6
4	A	431	LDA	C7-C8-C9-C10
4	A	435	LDA	C11-C10-C9-C8
3	A	441	C8E	C2-C3-C4-C5
3	A	440	C8E	C2-C3-C4-C5
3	B	432	C8E	C2-C3-C4-C5
3	B	433	C8E	C2-C3-C4-C5
3	B	433	C8E	C6-C7-C8-O9
4	A	433	LDA	C7-C8-C9-C10
6	B	436	2PE	O1-C2-C3-O4
4	A	437	LDA	C11-C10-C9-C8
3	B	435	C8E	C2-C3-C4-C5
4	A	432	LDA	C4-C5-C6-C7
6	B	436	2PE	C8-C9-O10-C11
3	B	431	C8E	C2-C3-C4-C5
3	A	441	C8E	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
3	A	439	C8E	C3-C4-C5-C6
3	A	443	C8E	C2-C3-C4-C5
3	A	438	C8E	O18-C19-C20-O21
3	B	432	C8E	C16-C17-O18-C19
4	B	429	LDA	C9-C10-C11-C12
3	B	431	C8E	C1-C2-C3-C4
4	B	430	LDA	C11-C10-C9-C8
3	A	441	C8E	C1-C2-C3-C4
4	A	431	LDA	C5-C6-C7-C8
3	A	443	C8E	C5-C6-C7-C8
3	A	442	C8E	O18-C19-C20-O21
3	B	431	C8E	C5-C6-C7-C8
3	B	431	C8E	C3-C4-C5-C6
3	A	440	C8E	C3-C4-C5-C6
4	A	434	LDA	C7-C8-C9-C10
3	A	442	C8E	C1-C2-C3-C4
3	A	440	C8E	C1-C2-C3-C4
3	B	433	C8E	C3-C4-C5-C6
3	A	430	C8E	C1-C2-C3-C4
4	A	435	LDA	C7-C8-C9-C10
3	B	432	C8E	O12-C13-C14-O15
3	A	443	C8E	C1-C2-C3-C4
3	A	438	C8E	O9-C10-C11-O12
4	A	433	LDA	C2-C3-C4-C5
4	A	433	LDA	C1-C2-C3-C4
4	A	434	LDA	C1-C2-C3-C4
3	B	435	C8E	C1-C2-C3-C4
4	A	436	LDA	C9-C10-C11-C12
4	B	430	LDA	C7-C8-C9-C10
3	B	435	C8E	O12-C13-C14-O15
4	A	433	LDA	C6-C7-C8-C9
3	B	433	C8E	O9-C10-C11-O12
4	A	432	LDA	C7-C8-C9-C10
3	A	439	C8E	C4-C5-C6-C7
3	B	434	C8E	C7-C8-O9-C10
6	B	436	2PE	O7-C8-C9-O10
4	A	434	LDA	C4-C5-C6-C7
3	A	442	C8E	C5-C6-C7-C8
4	A	432	LDA	C9-C10-C11-C12
3	A	429	C8E	C13-C14-O15-C16
3	B	435	C8E	C20-C19-O18-C17
3	B	433	C8E	C17-C16-O15-C14

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Mol	Chain	Res	Type	Atoms
3	B	432	C8E	C13-C14-O15-C16
3	A	440	C8E	C11-C10-O9-C8
3	A	440	C8E	C14-C13-O12-C11
3	A	441	C8E	O15-C16-C17-O18
3	A	430	C8E	C10-C11-O12-C13
6	B	436	2PE	O16-C17-C18-O19
3	A	441	C8E	C20-C19-O18-C17
3	A	441	C8E	C13-C14-O15-C16
3	A	430	C8E	C2-C3-C4-C5
4	A	437	LDA	C7-C8-C9-C10
3	A	442	C8E	C20-C19-O18-C17
3	B	434	C8E	C11-C10-O9-C8
3	A	438	C8E	C17-C16-O15-C14
3	A	429	C8E	C17-C16-O15-C14
3	A	430	C8E	C7-C8-O9-C10
3	B	432	C8E	C20-C19-O18-C17
3	B	431	C8E	C16-C17-O18-C19
3	B	434	C8E	C13-C14-O15-C16
3	A	443	C8E	C10-C11-O12-C13
4	A	433	LDA	C11-C10-C9-C8
3	A	442	C8E	C7-C8-O9-C10
6	B	436	2PE	O22-C23-C24-O25
3	A	443	C8E	C7-C8-O9-C10
3	B	432	C8E	C7-C8-O9-C10
3	B	433	C8E	C7-C8-O9-C10
3	A	429	C8E	O18-C19-C20-O21
3	A	440	C8E	C16-C17-O18-C19
3	B	433	C8E	C13-C14-O15-C16
3	B	433	C8E	C20-C19-O18-C17
3	A	440	C8E	C7-C8-O9-C10
3	A	429	C8E	C20-C19-O18-C17
3	A	439	C8E	C13-C14-O15-C16
3	A	439	C8E	O12-C13-C14-O15
3	A	439	C8E	C10-C11-O12-C13
3	A	440	C8E	C20-C19-O18-C17
3	A	439	C8E	C7-C8-O9-C10
3	A	430	C8E	C14-C13-O12-C11
3	B	431	C8E	C7-C8-O9-C10
3	A	438	C8E	C13-C14-O15-C16
3	B	434	C8E	O12-C13-C14-O15
4	A	434	LDA	C5-C6-C7-C8
4	A	436	LDA	C7-C8-C9-C10

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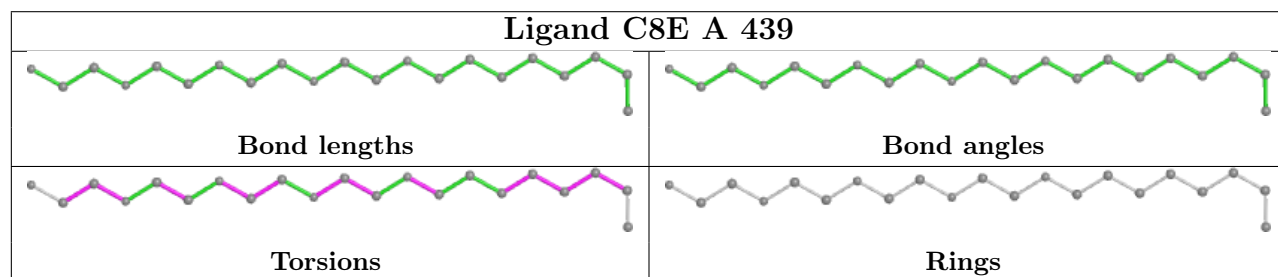
Mol	Chain	Res	Type	Atoms
3	B	432	C8E	C14-C13-O12-C11
3	A	439	C8E	C20-C19-O18-C17
3	A	442	C8E	O15-C16-C17-O18
3	A	439	C8E	C1-C2-C3-C4
3	B	433	C8E	C14-C13-O12-C11
4	A	433	LDA	C4-C5-C6-C7
3	B	431	C8E	O18-C19-C20-O21
4	A	435	LDA	C9-C10-C11-C12
4	A	432	LDA	C6-C7-C8-C9
3	B	432	C8E	O15-C16-C17-O18
4	A	432	LDA	C11-C10-C9-C8
4	B	430	LDA	C5-C6-C7-C8
3	A	442	C8E	C16-C17-O18-C19
3	A	443	C8E	O9-C10-C11-O12
6	B	436	2PE	C24-C23-O22-C21
4	A	434	LDA	C3-C4-C5-C6
3	A	442	C8E	C14-C13-O12-C11
6	B	436	2PE	C12-C11-O10-C9
3	A	441	C8E	C16-C17-O18-C19
3	A	440	C8E	C10-C11-O12-C13
3	B	431	C8E	O9-C10-C11-O12
3	A	438	C8E	C6-C7-C8-O9
3	B	434	C8E	C16-C17-O18-C19
3	A	442	C8E	C10-C11-O12-C13
3	A	441	C8E	C14-C13-O12-C11
3	A	429	C8E	C16-C17-O18-C19
3	B	432	C8E	C10-C11-O12-C13
3	A	438	C8E	C7-C8-O9-C10
3	A	430	C8E	O9-C10-C11-O12
3	B	433	C8E	C4-C5-C6-C7
3	B	434	C8E	O9-C10-C11-O12
3	A	430	C8E	C6-C7-C8-O9
3	B	433	C8E	O15-C16-C17-O18
6	B	436	2PE	C5-C6-O7-C8
3	B	435	C8E	O9-C10-C11-O12
4	A	431	LDA	C11-C10-C9-C8
4	A	437	LDA	C9-C10-C11-C12
3	B	431	C8E	C20-C19-O18-C17
3	B	432	C8E	O9-C10-C11-O12

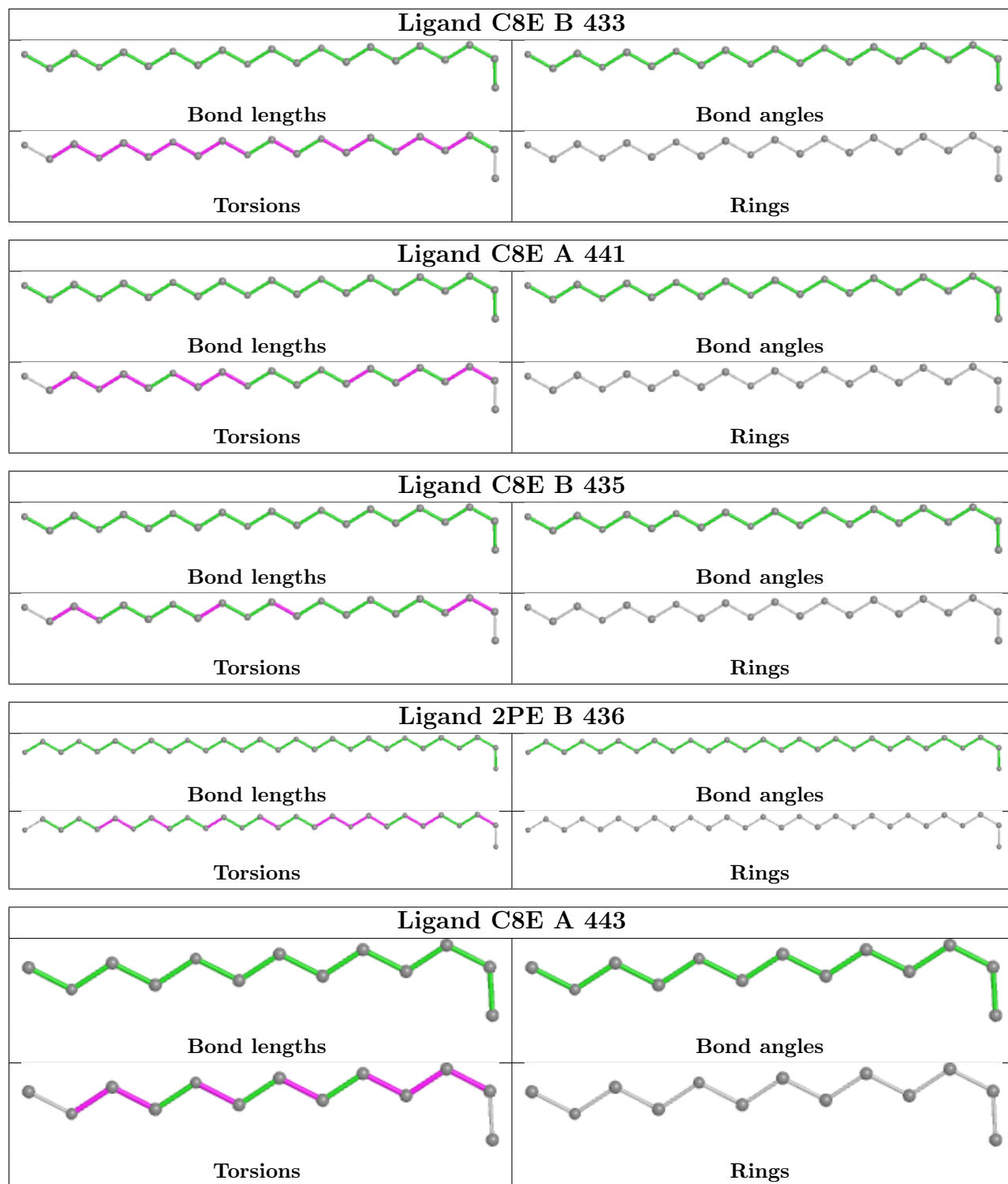
There are no ring outliers.

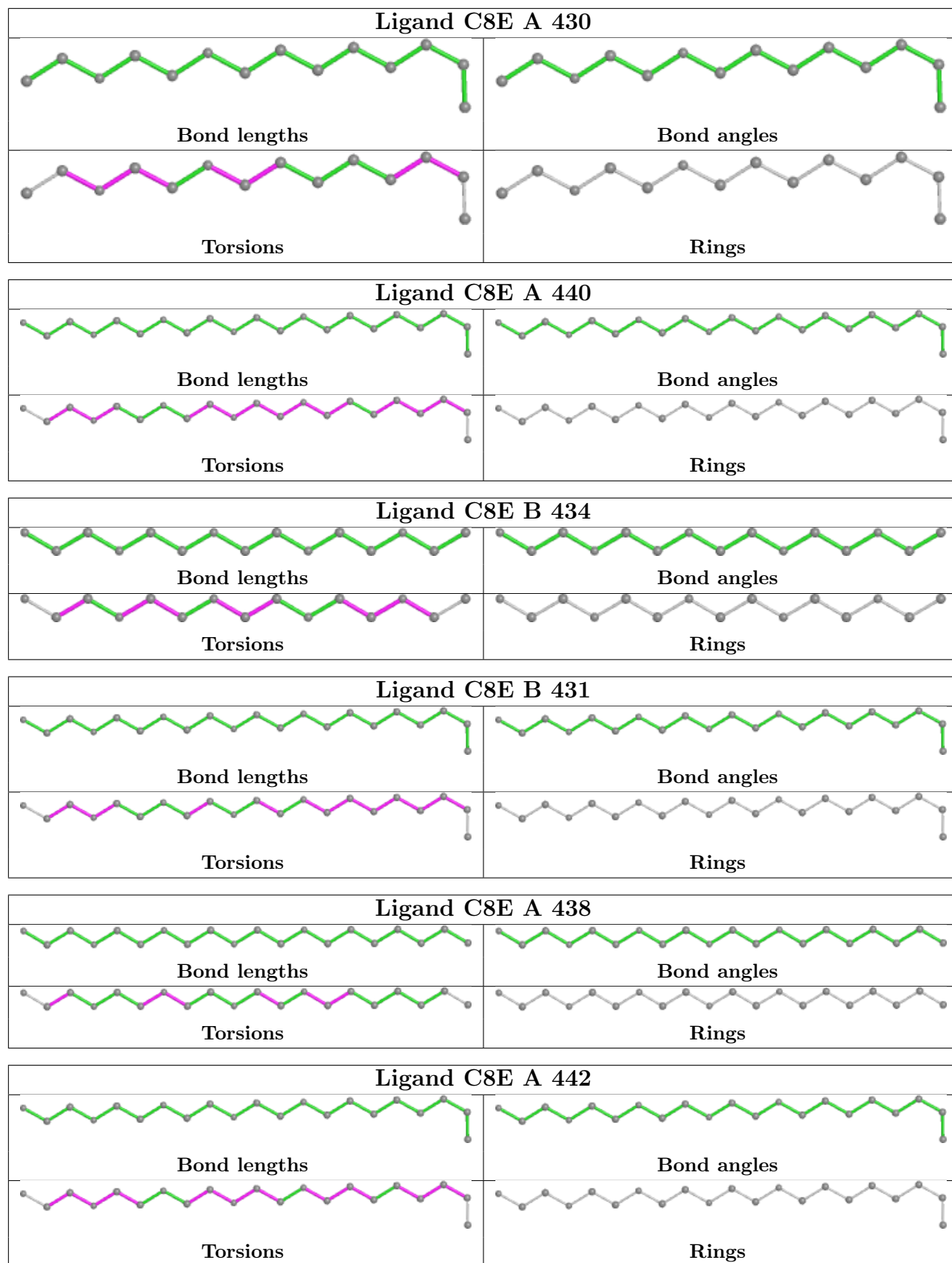
19 monomers are involved in 47 short contacts:

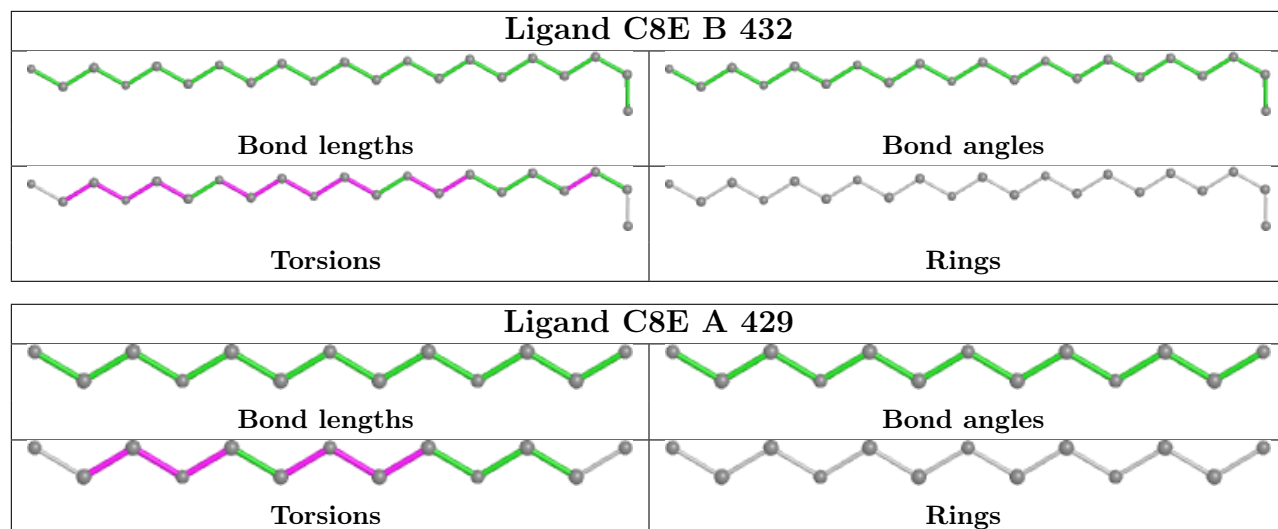
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	439	C8E	1	0
4	A	432	LDA	1	0
3	B	433	C8E	3	0
3	A	441	C8E	2	0
4	B	430	LDA	2	0
4	A	434	LDA	1	0
3	B	435	C8E	4	0
6	B	436	2PE	2	0
3	A	443	C8E	4	0
3	A	430	C8E	2	0
4	B	429	LDA	1	0
3	A	440	C8E	6	0
4	A	433	LDA	3	0
3	B	434	C8E	3	0
3	B	431	C8E	5	0
3	A	438	C8E	3	0
3	A	442	C8E	5	0
3	B	432	C8E	2	0
5	A	1428	ACT	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	427/427 (100%)	-0.41	7 (1%) 72 74	17, 28, 47, 67	0
1	B	426/427 (99%)	-0.28	13 (3%) 49 51	17, 29, 49, 110	1 (0%)
All	All	853/854 (99%)	-0.35	20 (2%) 60 63	17, 29, 49, 110	1 (0%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	426	HIS	10.2
1	B	423	HIS	7.5
1	B	424	HIS	4.4
1	B	419	TYR	4.3
1	B	422	HIS	3.9
1	B	425	HIS	3.6
1	B	335	TYR	3.4
1	B	421	PHE	2.8
1	A	417[A]	PHE	2.7
1	A	425	HIS	2.7
1	A	426	HIS	2.7
1	A	427	HIS	2.6
1	B	287	TRP	2.6
1	B	393	GLN	2.6
1	B	391[A]	HIS	2.5
1	A	367[A]	PHE	2.4
1	B	138[A]	ASN	2.4
1	A	422	HIS	2.3
1	B	333	TYR	2.2
1	A	219	LYS	2.1

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

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

6.3 Carbohydrates [i](#)

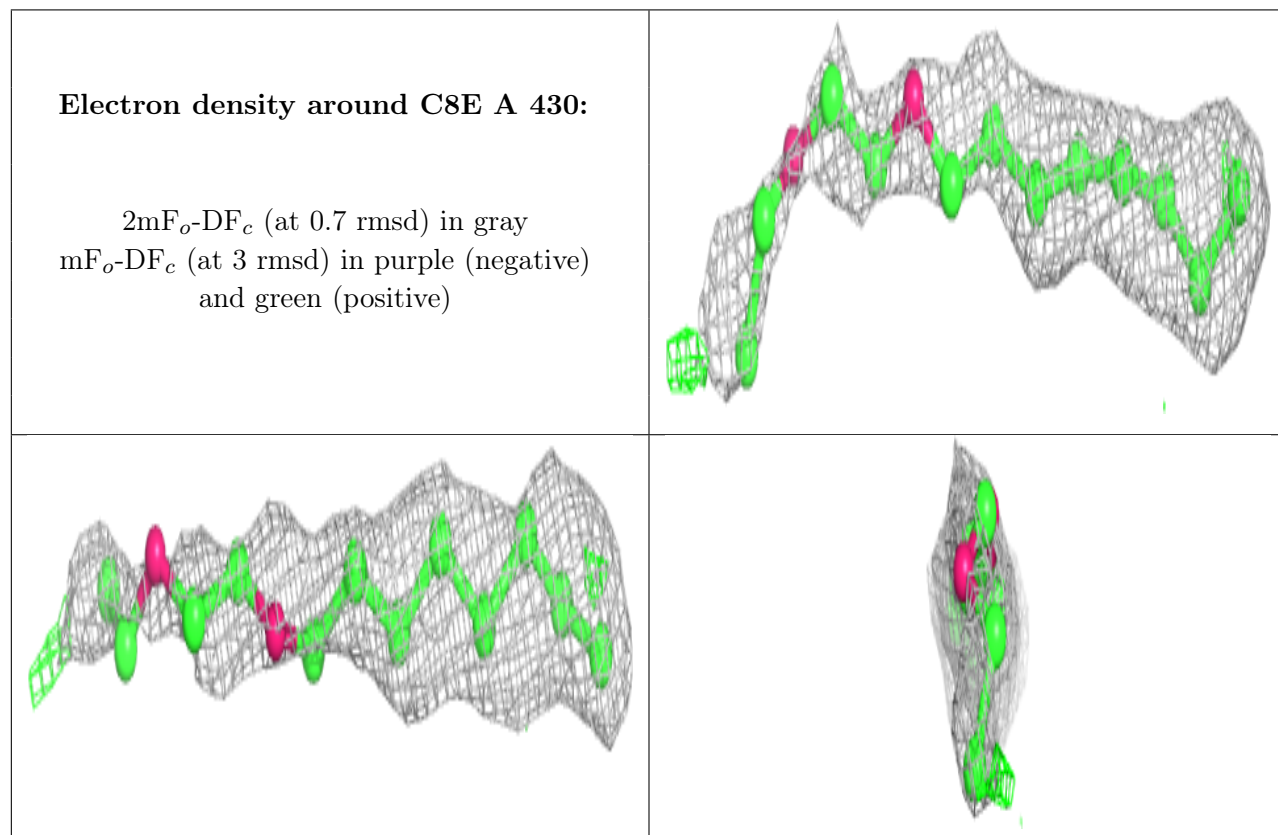
There are no monosaccharides in this entry.

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

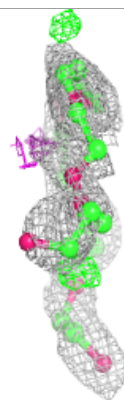
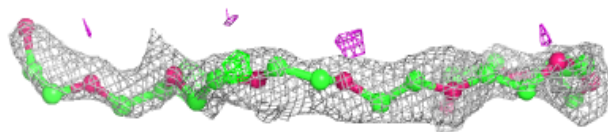
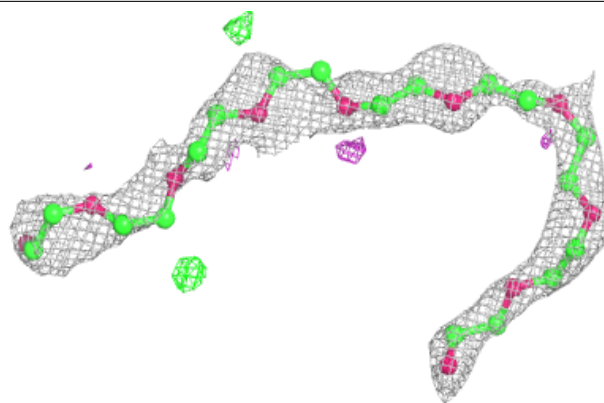
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	C8E	A	430	14/21	0.67	0.24	64,72,88,89	0
4	LDA	A	437	10/16	0.75	0.18	50,57,58,59	0
6	2PE	B	436	28/28	0.75	0.28	75,88,96,97	0
3	C8E	A	441	21/21	0.76	0.23	54,77,89,95	0
3	C8E	A	443	13/21	0.76	0.23	32,49,57,59	0
3	C8E	B	432	21/21	0.77	0.22	51,72,83,86	0
3	C8E	A	442	21/21	0.79	0.25	37,69,78,79	0
4	LDA	A	432	10/16	0.82	0.23	44,60,63,66	0
4	LDA	A	433	12/16	0.82	0.17	41,49,53,54	0
5	ACT	B	1428	4/4	0.84	0.14	39,42,45,48	0
4	LDA	B	429	10/16	0.85	0.28	40,49,53,54	0
3	C8E	B	434	15/21	0.85	0.21	39,48,73,76	0
3	C8E	A	439	21/21	0.85	0.22	56,67,74,77	0
4	LDA	B	430	10/16	0.86	0.13	36,53,70,70	0
3	C8E	B	433	21/21	0.86	0.19	38,52,62,78	0
4	LDA	A	434	10/16	0.86	0.27	58,65,72,74	0
4	LDA	A	431	11/16	0.88	0.18	36,47,52,54	0
3	C8E	B	431	21/21	0.89	0.19	37,50,57,59	0
3	C8E	A	429	13/21	0.90	0.12	31,42,51,64	0
3	C8E	B	435	21/21	0.91	0.20	22,45,93,94	0
3	C8E	A	438	20/21	0.91	0.14	27,44,62,62	0
3	C8E	A	440	21/21	0.92	0.24	35,53,96,102	0
4	LDA	A	436	7/16	0.93	0.15	43,49,54,55	0
5	ACT	A	1428	4/4	0.93	0.15	45,47,48,49	0
4	LDA	A	435	7/16	0.94	0.18	50,56,60,64	0
2	CA	A	428	1/1	0.98	0.04	30,30,30,30	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.

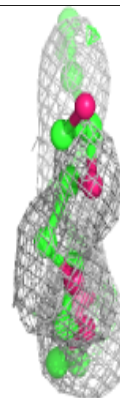
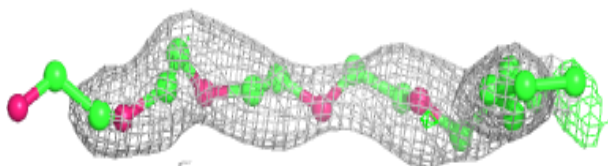
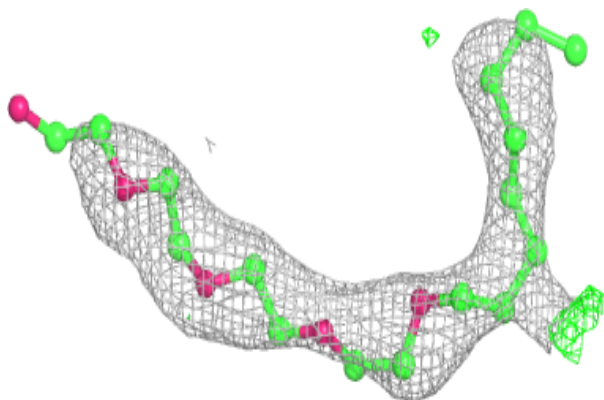


Electron density around 2PE B 436:

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

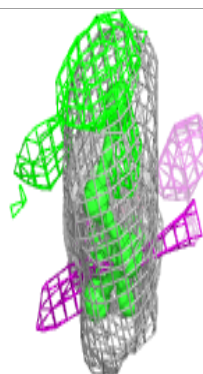
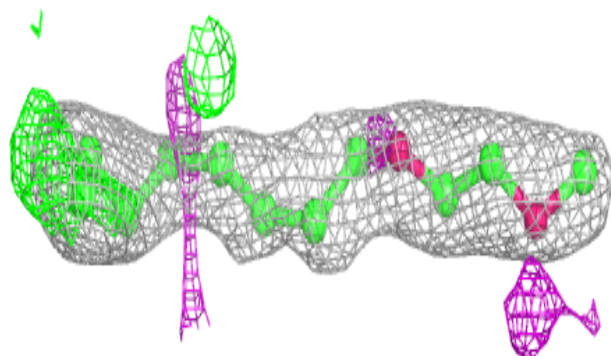
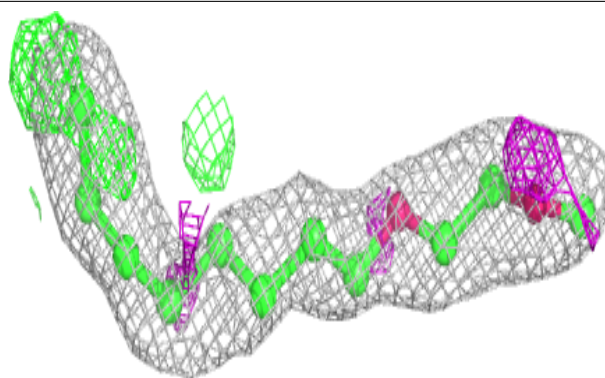
**Electron density around C8E A 441:**

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

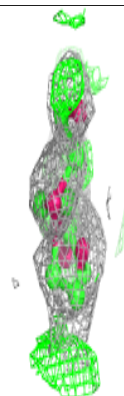
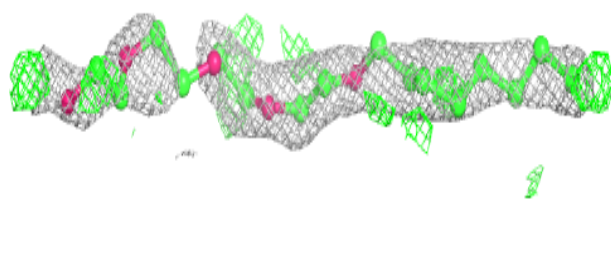
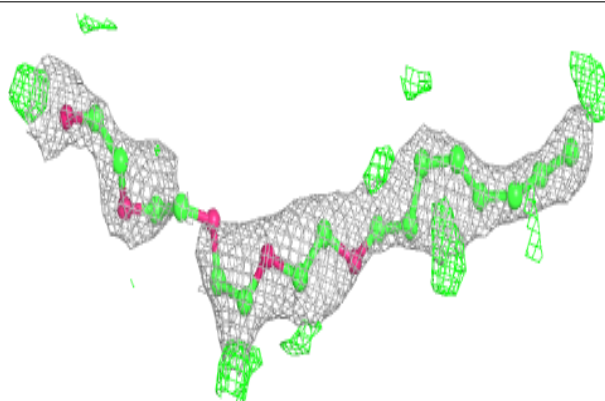


Electron density around C8E A 443:

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

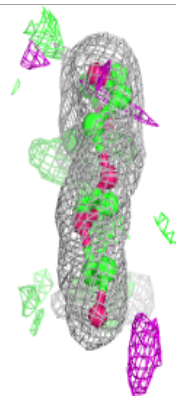
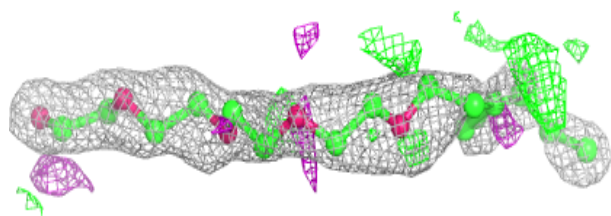
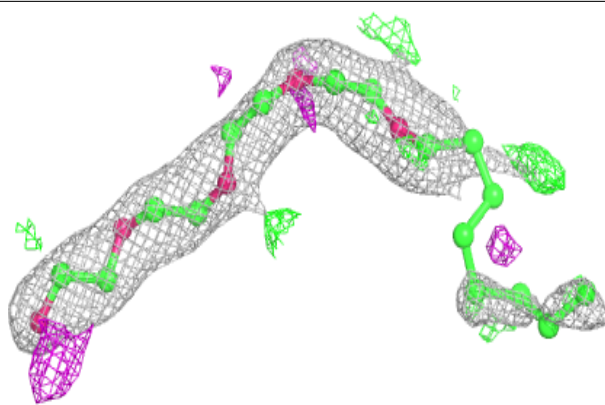
**Electron density around C8E B 432:**

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

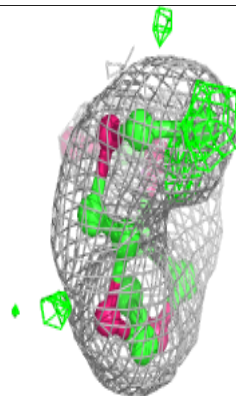
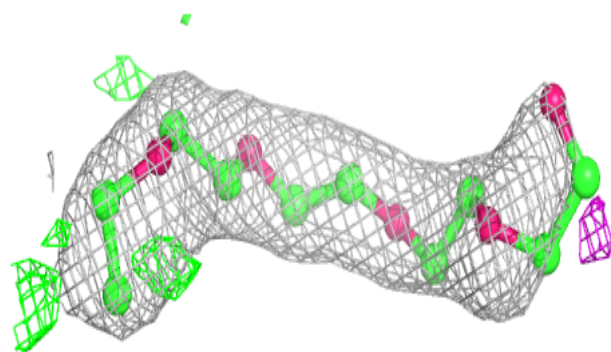
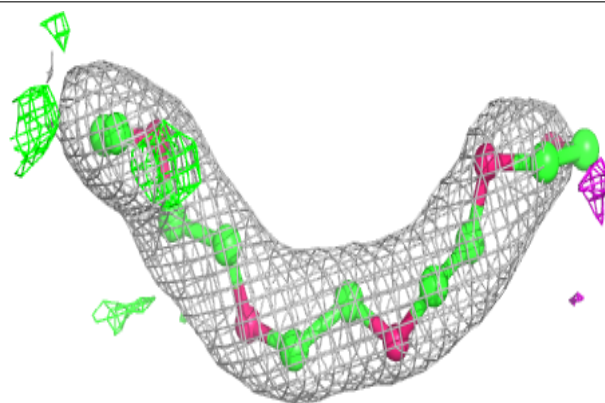


Electron density around C8E A 442:

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

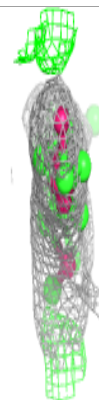
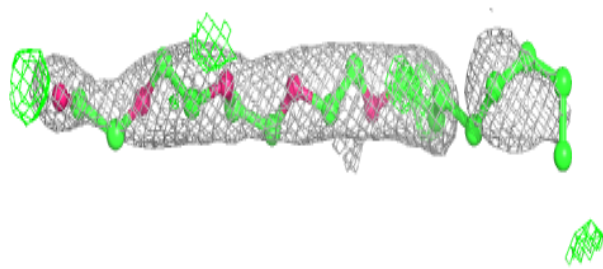
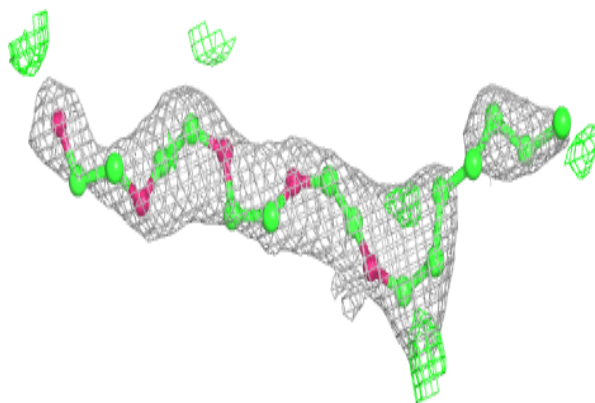
**Electron density around C8E B 434:**

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

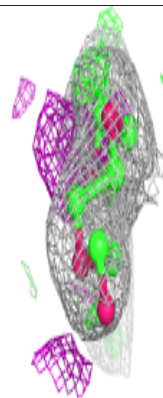
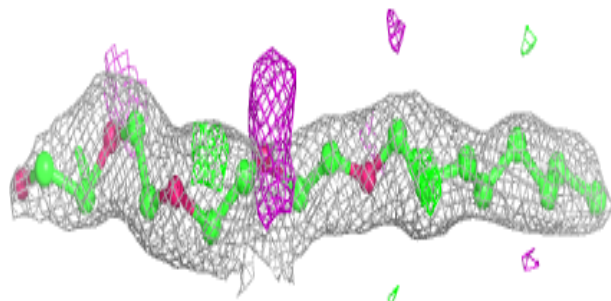
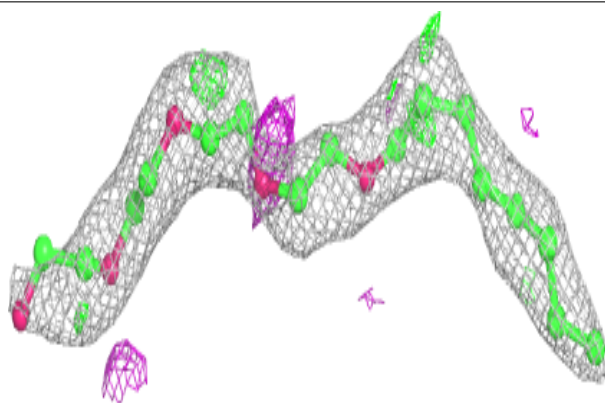


Electron density around C8E A 439:

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

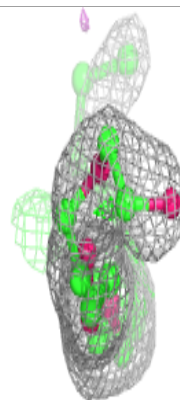
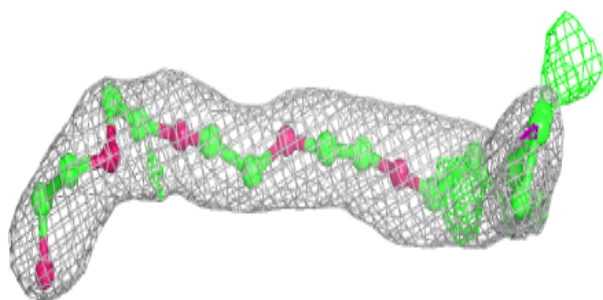
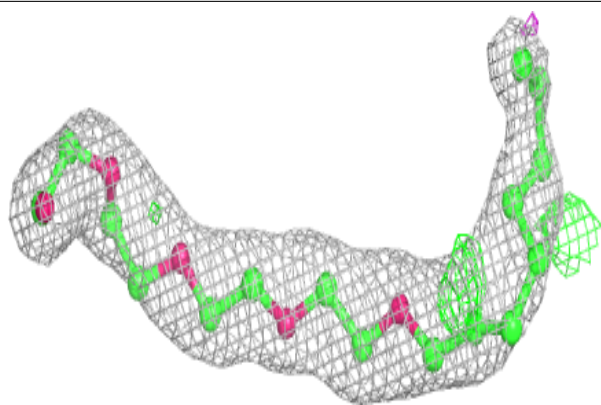
**Electron density around C8E B 433:**

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

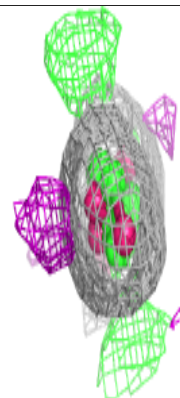
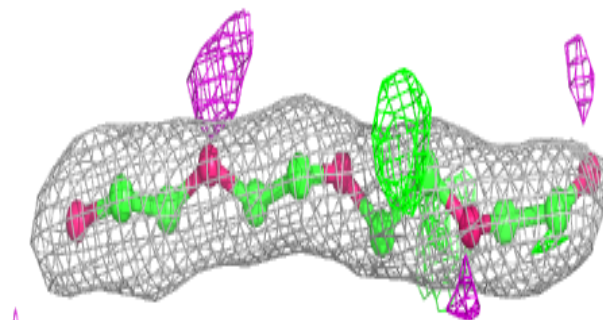
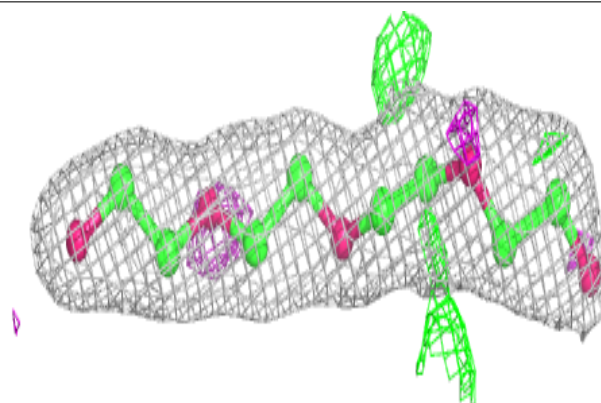


Electron density around C8E B 431:

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

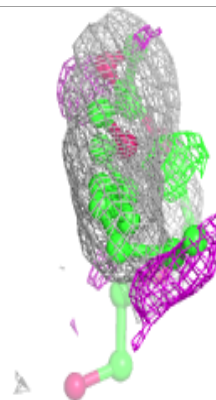
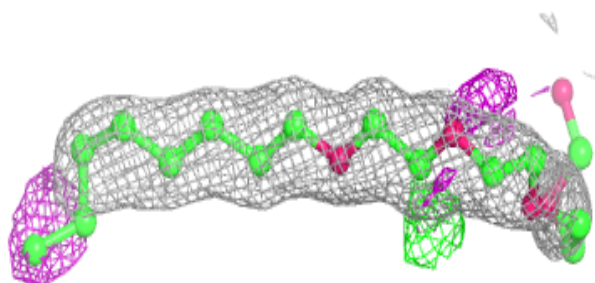
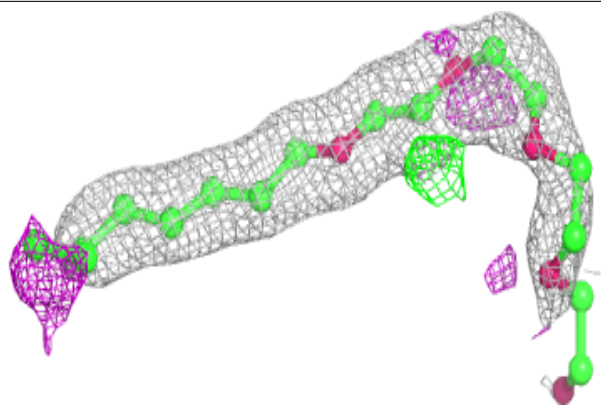
**Electron density around C8E A 429:**

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

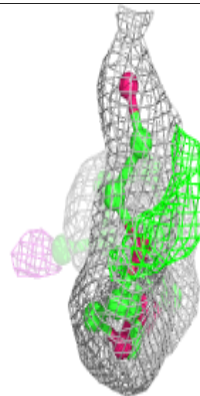
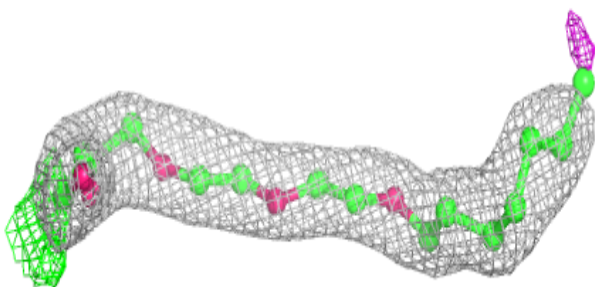
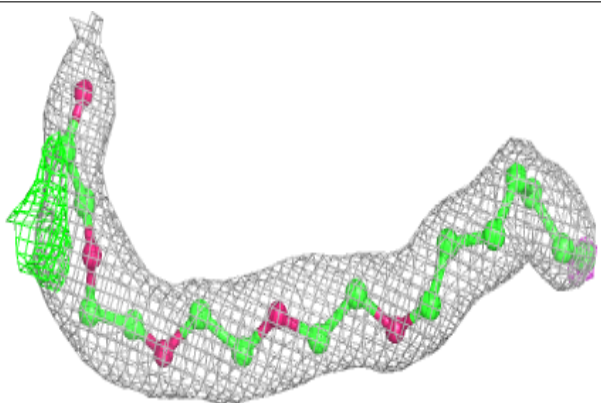


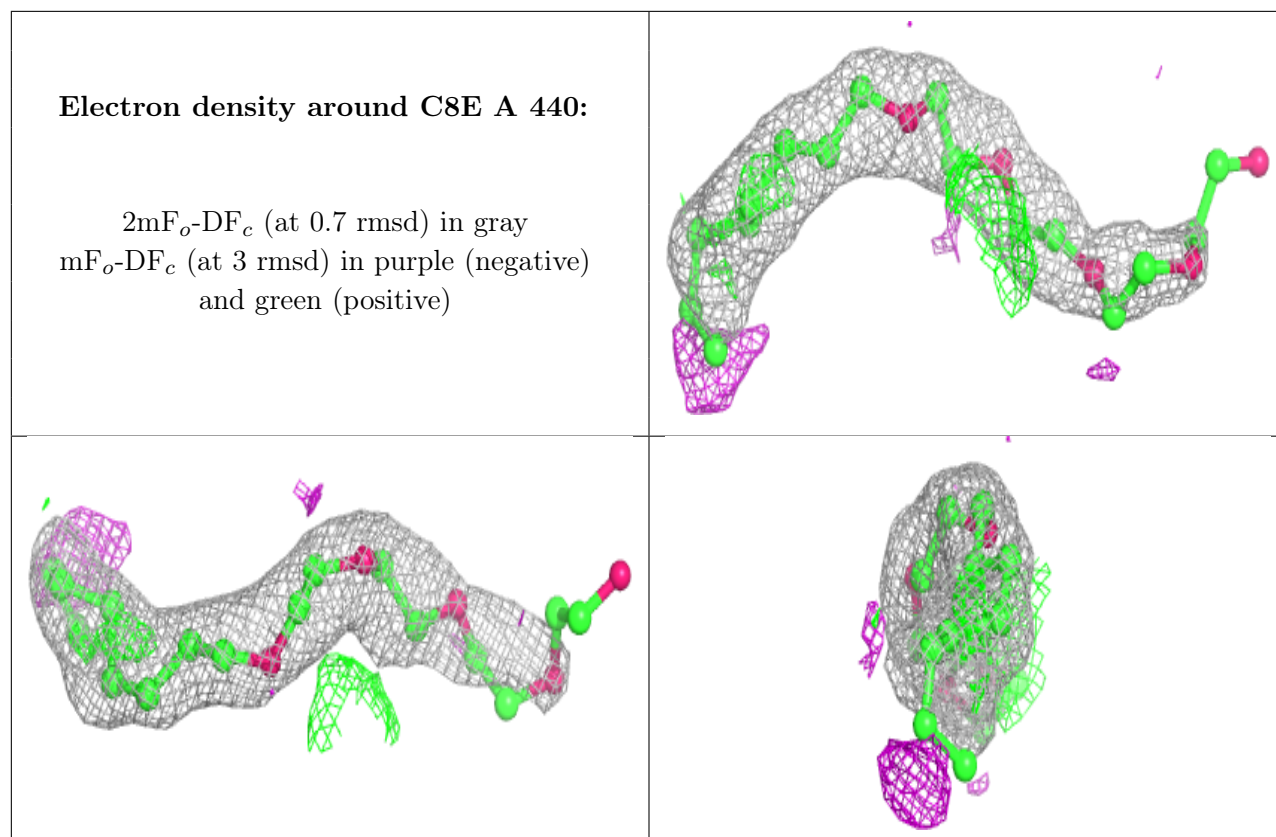
Electron density around C8E B 435:

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

**Electron density around C8E A 438:**

$2mF_o-DF_c$ (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.