Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 01:51 am BST

PDB ID	:	2WVP
Title	:	Synthetically modified OmpG
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Deposited on	:	2009-10-19
Resolution	:	2.40 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 following versions of software and data (see references ⓘ) were used in the production of this report:

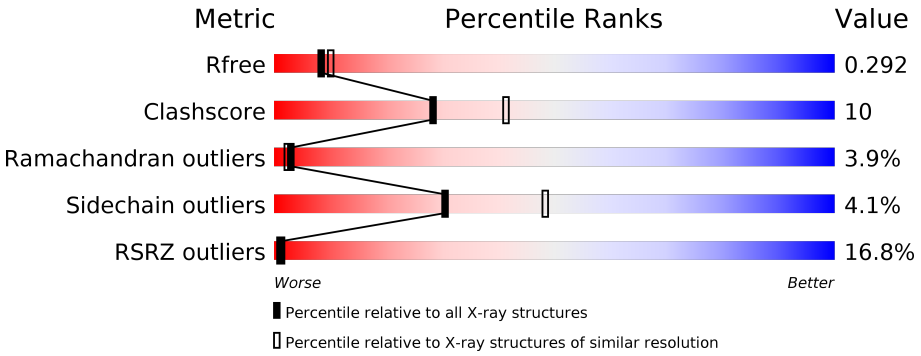
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	286	15% 76% 13% • 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2421 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.

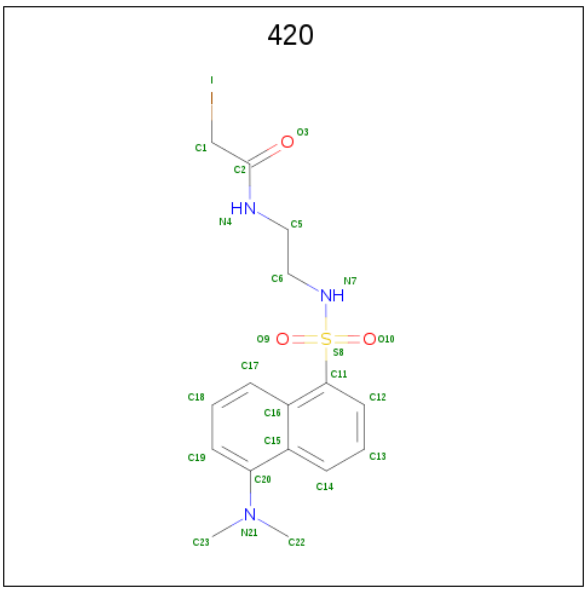
- Molecule 1 is a protein called OUTER MEMBRANE PROTEIN G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	4	0
			2201	1411	368	417	5			

There are 7 discrepancies between the modelled and reference sequences:

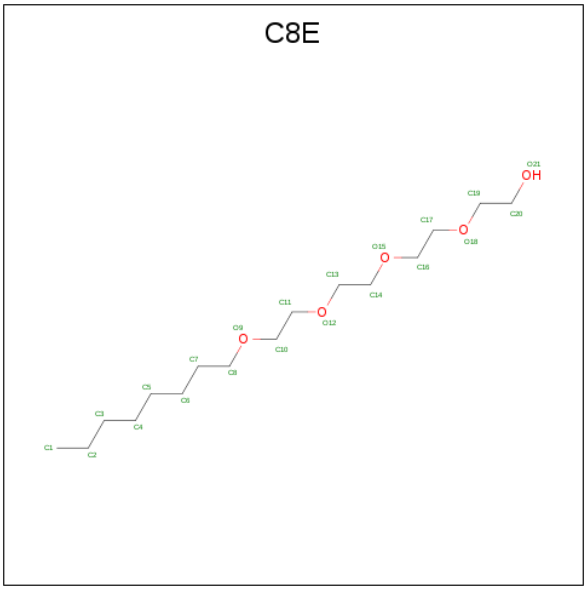
Chain	Residue	Modelled	Actual	Comment	Reference
A	281	HIS	-	expression tag	UNP P76045
A	282	HIS	-	expression tag	UNP P76045
A	283	HIS	-	expression tag	UNP P76045
A	284	HIS	-	expression tag	UNP P76045
A	285	HIS	-	expression tag	UNP P76045
A	286	HIS	-	expression tag	UNP P76045
A	209	CYS	TYR	engineered mutation	UNP P76045

- Molecule 2 is N-[2-({[5-(DIMETHYLAMINO)NAPHTHALEN-1-YL]SULFONYL}AMINO) ETHYL]-2-IODOACETAMIDE (three-letter code: 420) (formula: $C_{16}H_{20}IN_3O_3S$).



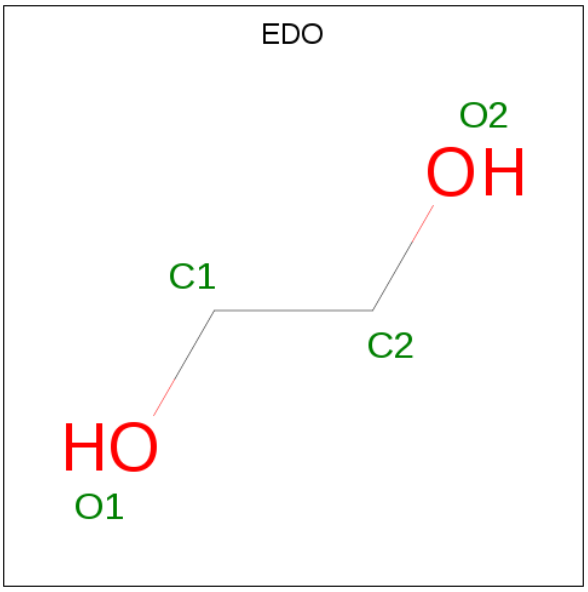
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	1
			46	32	6	6	2		

- Molecule 3 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: $C_{16}H_{34}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	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		0	0
			8	8			
3	A	1	Total	C	O	0	0
			9	8	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

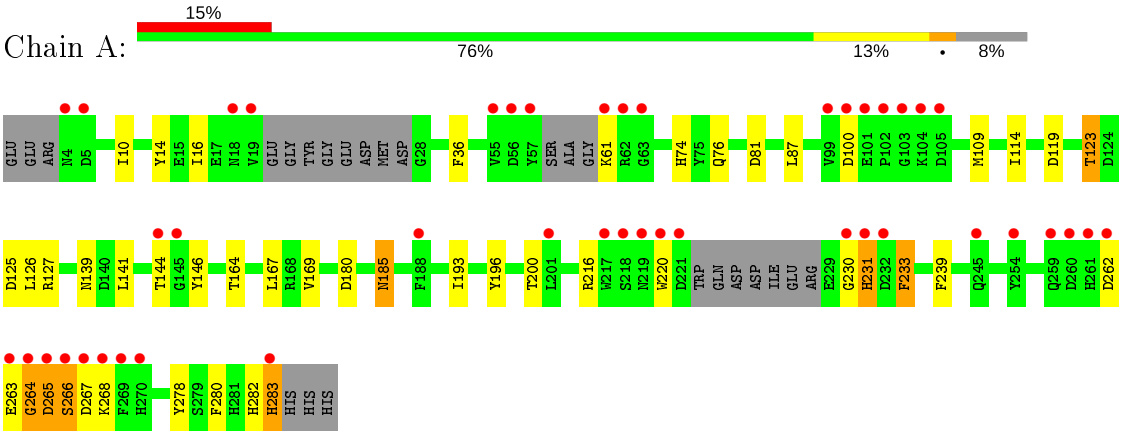
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	77	Total O 77 77	0	0

3 Residue-property plots (i)

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

- Molecule 1: OUTER MEMBRANE PROTEIN G



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	99.56Å 69.81Å 59.13Å 90.00° 103.60° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 29.28 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.5 (30.00-2.40) 98.9 (29.28-2.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	10674.83 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.221 , 0.287 0.233 , 0.292	Depositor DCC
R_{free} test set	761 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	49.3	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 62.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	2421	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.84% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: 420, 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	0.56	0/2282	0.63	0/3101

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	2201	0	1964	31	0
2	A	46	0	36	14	0
3	A	93	0	151	1	0
4	A	4	0	6	0	0
5	A	77	0	0	1	0
All	All	2421	0	2157	44	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 10.

All (44) 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)
2:A:1284[B]:420:H14	2:A:1284[B]:420:C23	1.75	1.16
2:A:1284[A]:420:C23	2:A:1284[A]:420:H14	1.91	1.00
2:A:1284[B]:420:H14	2:A:1284[B]:420:H233	1.47	0.94
2:A:1284[B]:420:H14	2:A:1284[B]:420:H232	1.47	0.93
1:A:123:THR:HG22	1:A:125:ASP:H	1.33	0.92
2:A:1284[B]:420:C14	2:A:1284[B]:420:C23	2.52	0.86
2:A:1284[A]:420:H232	2:A:1284[A]:420:H14	1.60	0.82
2:A:1284[A]:420:H233	2:A:1284[A]:420:H14	1.62	0.80
1:A:10:ILE:HD12	1:A:10:ILE:O	1.89	0.72
1:A:239:PHE:CE1	2:A:1284[A]:420:H12	2.25	0.70
1:A:119:ASP:OD1	1:A:127:ARG:NH1	2.25	0.70
1:A:164:THR:HG23	1:A:200:THR:O	1.94	0.68
1:A:10:ILE:HD11	1:A:278:TYR:HB3	1.77	0.67
1:A:109:MET:SD	1:A:144:THR:HG21	2.35	0.66
1:A:264:GLY:O	1:A:265:ASP:CB	2.44	0.65
1:A:141:LEU:HA	1:A:144:THR:HG22	1.80	0.64
1:A:265:ASP:O	1:A:266:SER:CB	2.49	0.60
2:A:1284[B]:420:C14	2:A:1284[B]:420:H232	2.25	0.59
2:A:1284[B]:420:C14	2:A:1284[B]:420:H233	2.25	0.58
1:A:87:LEU:HD11	1:A:114:ILE:HD11	1.85	0.58
2:A:1284[B]:420:H222	5:A:2073:HOH:O	2.06	0.55
1:A:193[B]:ILE:HG21	3:A:1288:C8E:H82	1.90	0.54
2:A:1284[A]:420:C14	2:A:1284[A]:420:C23	2.65	0.53
1:A:10:ILE:C	1:A:10:ILE:HD12	2.27	0.53
1:A:10:ILE:HG22	1:A:36:PHE:HD1	1.74	0.53
2:A:1284[A]:420:H232	2:A:1284[A]:420:C14	2.37	0.52
1:A:216:ARG:HG2	1:A:233:PHE:CE1	2.46	0.51
1:A:167:LEU:HD12	1:A:196:TYR:O	2.11	0.51
1:A:87:LEU:HD11	1:A:114:ILE:CD1	2.40	0.51
1:A:14:TYR:CE1	1:A:16:ILE:HD11	2.46	0.50
1:A:10:ILE:CD1	1:A:278:TYR:HB3	2.40	0.50
1:A:233:PHE:CD1	1:A:233:PHE:N	2.79	0.49
1:A:263:GLU:O	1:A:265:ASP:N	2.47	0.48
1:A:10:ILE:CG2	1:A:36:PHE:HD1	2.26	0.47
1:A:169:VAL:CG1	1:A:193[B]:ILE:HD11	2.46	0.46
1:A:81:ASP:O	1:A:127:ARG:NH2	2.46	0.45
1:A:185:ASN:N	1:A:185:ASN:HD22	2.15	0.45
1:A:144:THR:HG23	1:A:146:TYR:H	1.82	0.44
2:A:1284[A]:420:H233	2:A:1284[A]:420:C14	2.37	0.43
1:A:123:THR:HB	1:A:126:LEU:HB3	2.03	0.41
1:A:282:HIS:O	1:A:283:HIS:HB2	2.21	0.41
1:A:74:HIS:HE1	1:A:76:GLN:NE2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:TYR:HE1	1:A:16:ILE:HD11	1.86	0.41
1:A:87:LEU:HD21	1:A:114:ILE:HD11	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	258/286 (90%)	239 (93%)	9 (4%)	10 (4%)	3 2

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	HIS
1	A	264	GLY
1	A	265	ASP
1	A	267	ASP
1	A	262	ASP
1	A	266	SER
1	A	100	ASP
1	A	180	ASP
1	A	139	ASN
1	A	230	GLY

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	225/244 (92%)	216 (96%)	9 (4%)	31 49

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	LYS
1	A	123	THR
1	A	185	ASN
1	A	220	TRP
1	A	231	HIS
1	A	233	PHE
1	A	268	LYS
1	A	280	PHE
1	A	283	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	76	GLN
1	A	184	ASN
1	A	185	ASN
1	A	191	GLN
1	A	259	GLN
1	A	277	ASN
1	A	281	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

9 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	1285	-	12,12,20	0.38	0	11,11,19	0.37	0
2	420	A	1284[A]	1	24,24,25	1.77	4 (16%)	34,34,35	1.45	4 (11%)
3	C8E	A	1290	-	8,8,20	0.35	0	7,7,19	0.36	0
2	420	A	1284[B]	1	24,24,25	1.43	2 (8%)	34,34,35	1.34	2 (5%)
3	C8E	A	1289	-	7,7,20	0.37	0	6,6,19	0.30	0
3	C8E	A	1287	-	20,20,20	0.43	0	19,19,19	0.40	0
3	C8E	A	1288	-	20,20,20	0.41	0	19,19,19	0.30	0
4	EDO	A	1291	-	3,3,3	0.44	0	2,2,2	0.35	0
3	C8E	A	1286	-	20,20,20	0.52	0	19,19,19	0.54	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	1285	-	-	5/10/10/18	-
2	420	A	1284[A]	1	-	8/18/18/20	0/2/2/2
3	C8E	A	1290	-	-	4/6/6/18	-
2	420	A	1284[B]	1	-	16/18/18/20	0/2/2/2
3	C8E	A	1289	-	-	2/5/5/18	-
3	C8E	A	1287	-	-	8/18/18/18	-
3	C8E	A	1288	-	-	7/18/18/18	-
4	EDO	A	1291	-	-	1/1/1/1	-
3	C8E	A	1286	-	-	11/18/18/18	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1284[A]	420	S8-N7	6.06	1.70	1.61
2	A	1284[B]	420	S8-N7	4.60	1.68	1.61
2	A	1284[A]	420	C12-C11	3.24	1.41	1.37
2	A	1284[B]	420	C12-C11	2.70	1.40	1.37
2	A	1284[A]	420	O10-S8	2.15	1.46	1.43
2	A	1284[A]	420	O9-S8	2.10	1.45	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1284[A]	420	C15-C20-N21	4.01	124.00	118.23
2	A	1284[A]	420	C19-C20-N21	-3.44	116.49	121.68
2	A	1284[B]	420	C15-C20-N21	3.37	123.08	118.23
2	A	1284[B]	420	C19-C20-N21	-2.93	117.26	121.68
2	A	1284[A]	420	O10-S8-C11	2.24	112.03	108.08
2	A	1284[A]	420	O9-S8-C11	-2.20	104.19	108.08

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1284[A]	420	C6-N7-S8-O10
2	A	1284[A]	420	C6-N7-S8-C11
2	A	1284[B]	420	C5-C6-N7-S8
2	A	1284[B]	420	C12-C11-S8-O9
2	A	1284[B]	420	C16-C11-S8-O9
2	A	1284[B]	420	C6-C5-N4-C2
2	A	1284[A]	420	C19-C20-N21-C23
2	A	1284[B]	420	C19-C20-N21-C23
2	A	1284[A]	420	C15-C20-N21-C23
2	A	1284[B]	420	C15-C20-N21-C23
2	A	1284[B]	420	C6-N7-S8-O10
3	A	1286	C8E	C5-C6-C7-C8
3	A	1288	C8E	O12-C13-C14-O15
2	A	1284[B]	420	C6-N7-S8-C11
3	A	1286	C8E	O9-C10-C11-O12
3	A	1285	C8E	O15-C16-C17-O18
3	A	1287	C8E	O15-C16-C17-O18
3	A	1287	C8E	O12-C13-C14-O15
3	A	1285	C8E	O18-C19-C20-O21
3	A	1285	C8E	O12-C13-C14-O15
3	A	1286	C8E	O12-C13-C14-O15

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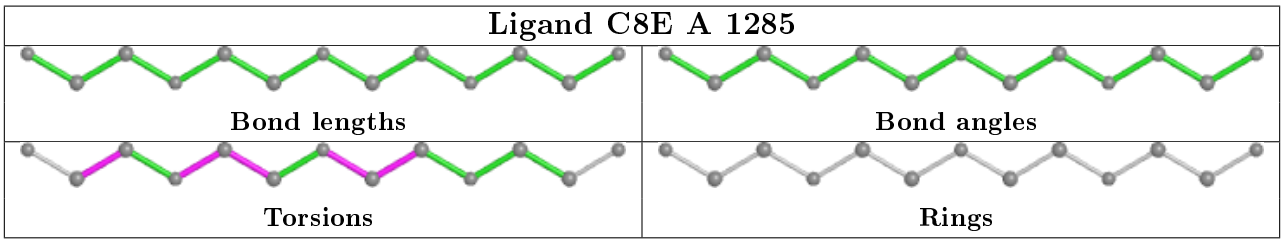
Mol	Chain	Res	Type	Atoms
2	A	1284[B]	420	C1-C2-N4-C5
2	A	1284[B]	420	N4-C5-C6-N7
3	A	1288	C8E	O18-C19-C20-O21
2	A	1284[B]	420	O3-C2-N4-C5
2	A	1284[B]	420	C19-C20-N21-C22
2	A	1284[B]	420	C16-C11-S8-N7
2	A	1284[A]	420	C19-C20-N21-C22
3	A	1288	C8E	C2-C3-C4-C5
3	A	1290	C8E	C5-C6-C7-C8
2	A	1284[A]	420	C6-N7-S8-O9
3	A	1289	C8E	C5-C6-C7-C8
3	A	1287	C8E	C1-C2-C3-C4
3	A	1286	C8E	O18-C19-C20-O21
2	A	1284[A]	420	C15-C20-N21-C22
3	A	1287	C8E	C16-C17-O18-C19
2	A	1284[B]	420	C15-C20-N21-C22
2	A	1284[A]	420	N4-C5-C6-N7
3	A	1286	C8E	O15-C16-C17-O18
3	A	1287	C8E	C5-C6-C7-C8
3	A	1289	C8E	C4-C5-C6-C7
2	A	1284[B]	420	C6-N7-S8-O9
3	A	1286	C8E	C3-C4-C5-C6
3	A	1285	C8E	C13-C14-O15-C16
3	A	1290	C8E	C3-C4-C5-C6
2	A	1284[B]	420	C12-C11-S8-N7
3	A	1288	C8E	C3-C4-C5-C6
3	A	1290	C8E	C1-C2-C3-C4
3	A	1287	C8E	C20-C19-O18-C17
3	A	1288	C8E	O9-C10-C11-O12
3	A	1286	C8E	C17-C16-O15-C14
3	A	1287	C8E	O9-C10-C11-O12
3	A	1287	C8E	C11-C10-O9-C8
3	A	1286	C8E	C14-C13-O12-C11
3	A	1290	C8E	C2-C3-C4-C5
3	A	1285	C8E	C16-C17-O18-C19
3	A	1286	C8E	C7-C8-O9-C10
3	A	1288	C8E	C4-C5-C6-C7
3	A	1288	C8E	O15-C16-C17-O18
3	A	1286	C8E	C6-C7-C8-O9
3	A	1286	C8E	C10-C11-O12-C13
4	A	1291	EDO	O1-C1-C2-O2

There are no ring outliers.

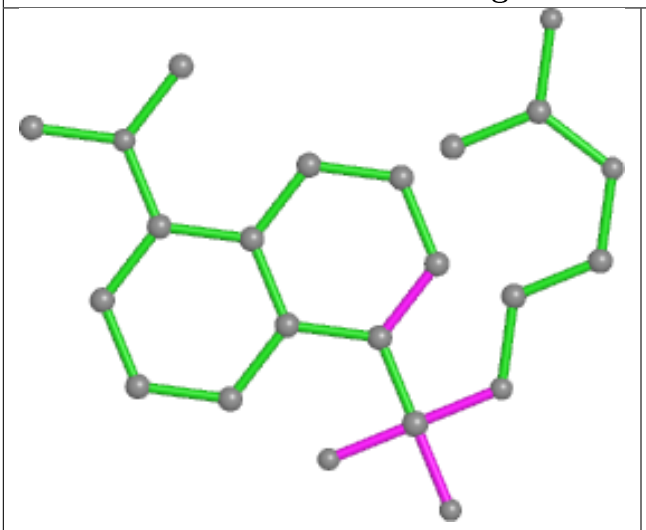
3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1284[A]	420	7	0
2	A	1284[B]	420	7	0
3	A	1288	C8E	1	0

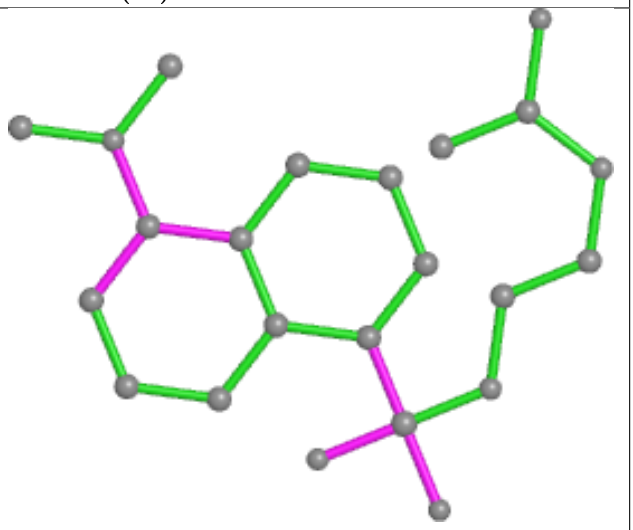
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



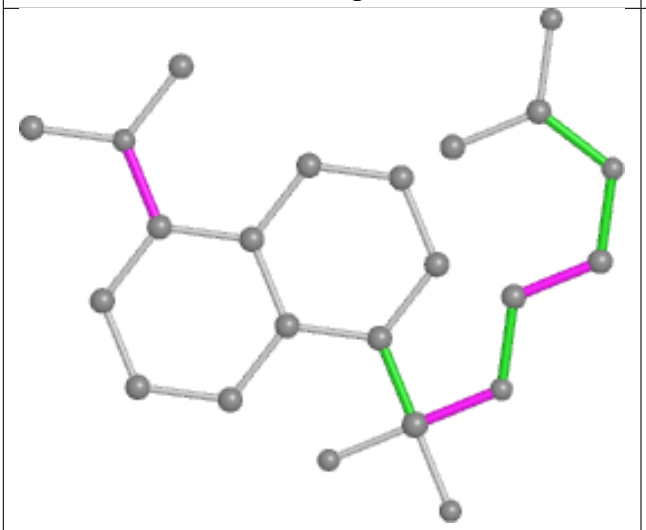
Ligand 420 A 1284 (A)



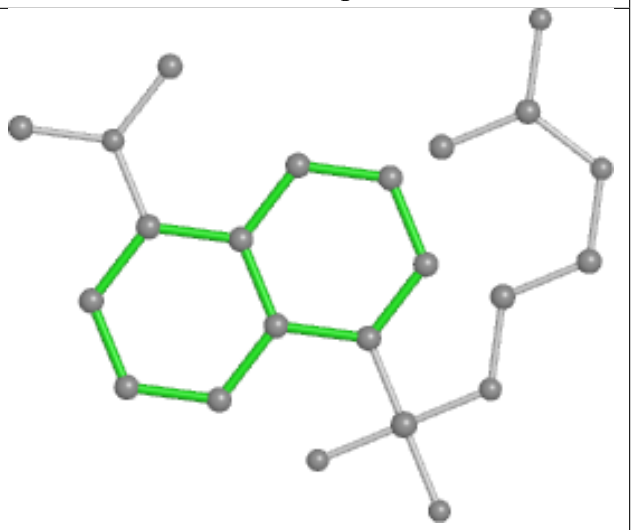
Bond lengths



Bond angles

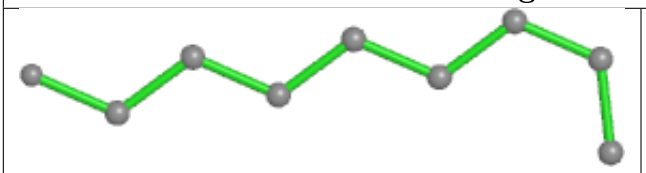


Torsions

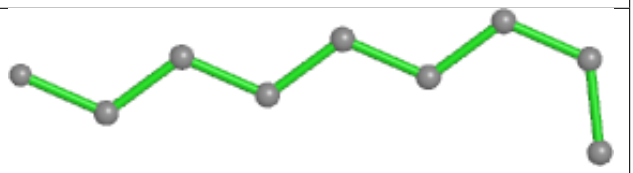


Rings

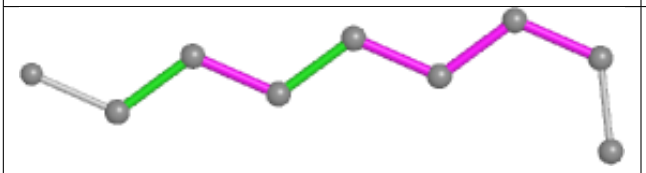
Ligand C8E A 1290



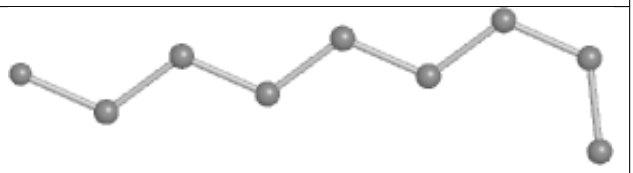
Bond lengths



Bond angles

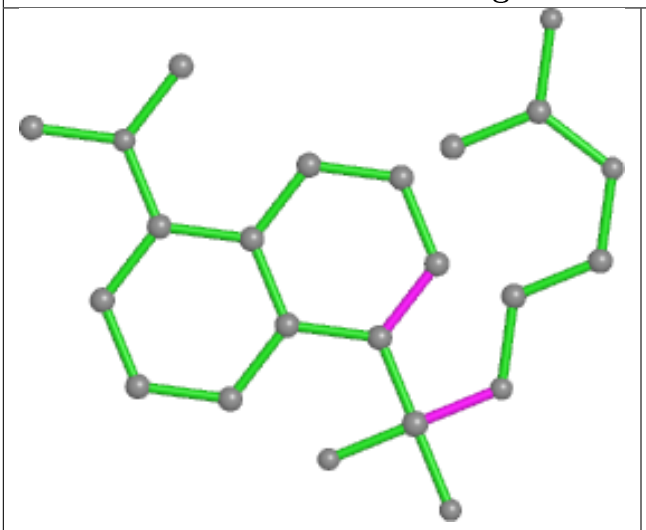


Torsions

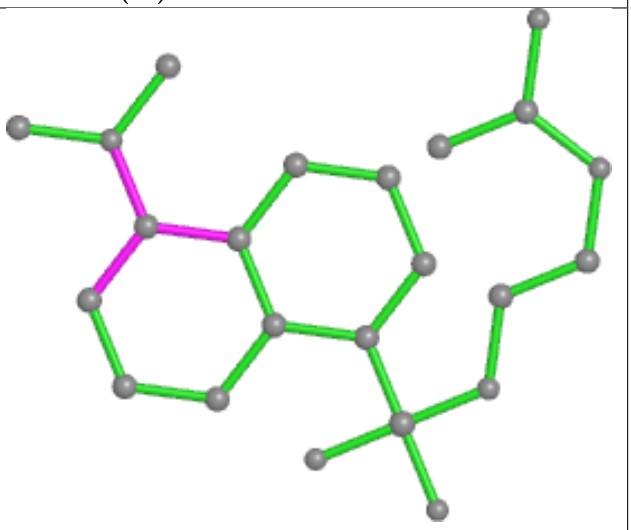


Rings

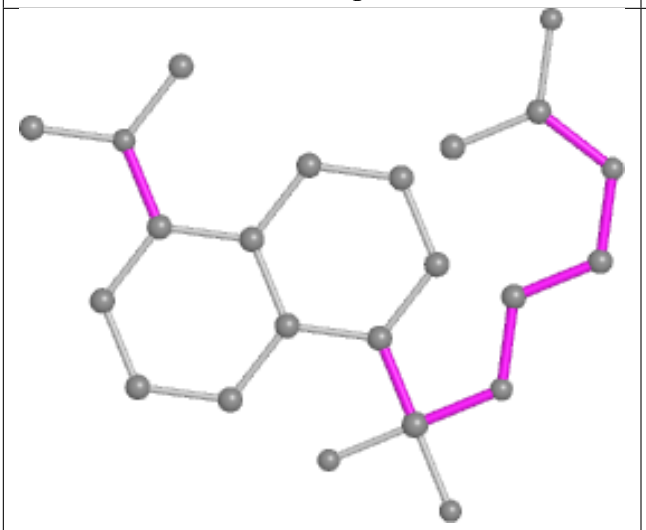
Ligand 420 A 1284 (B)



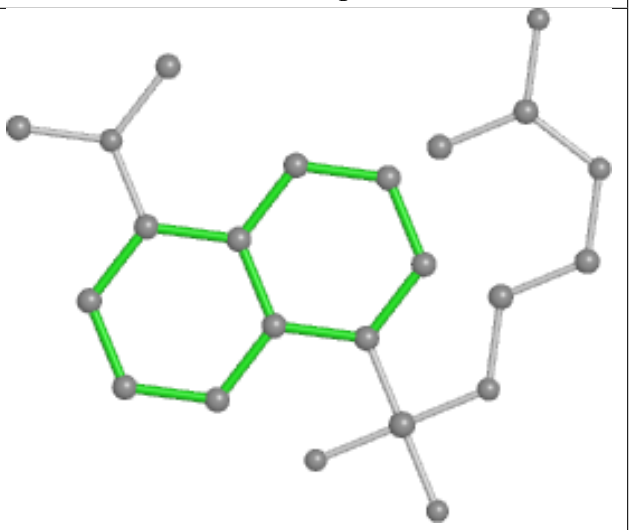
Bond lengths



Bond angles

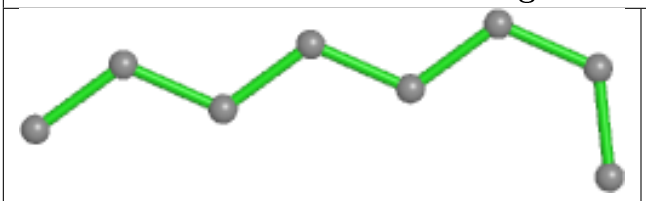


Torsions

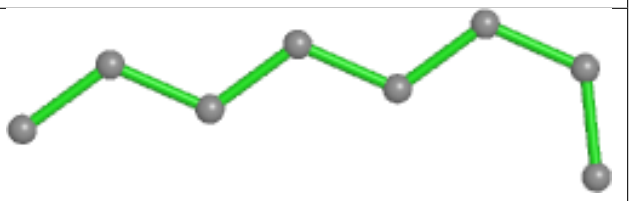


Rings

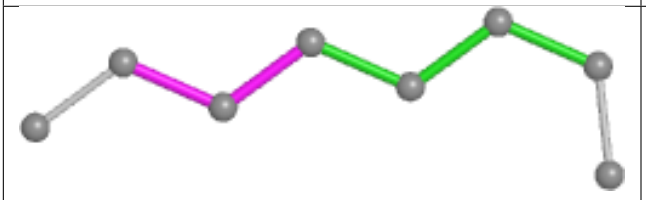
Ligand C8E A 1289



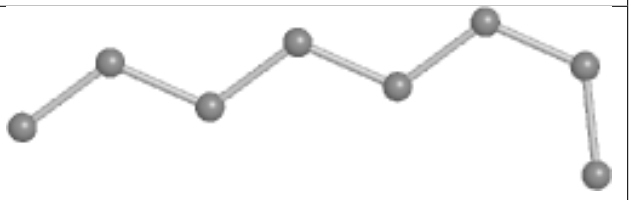
Bond lengths



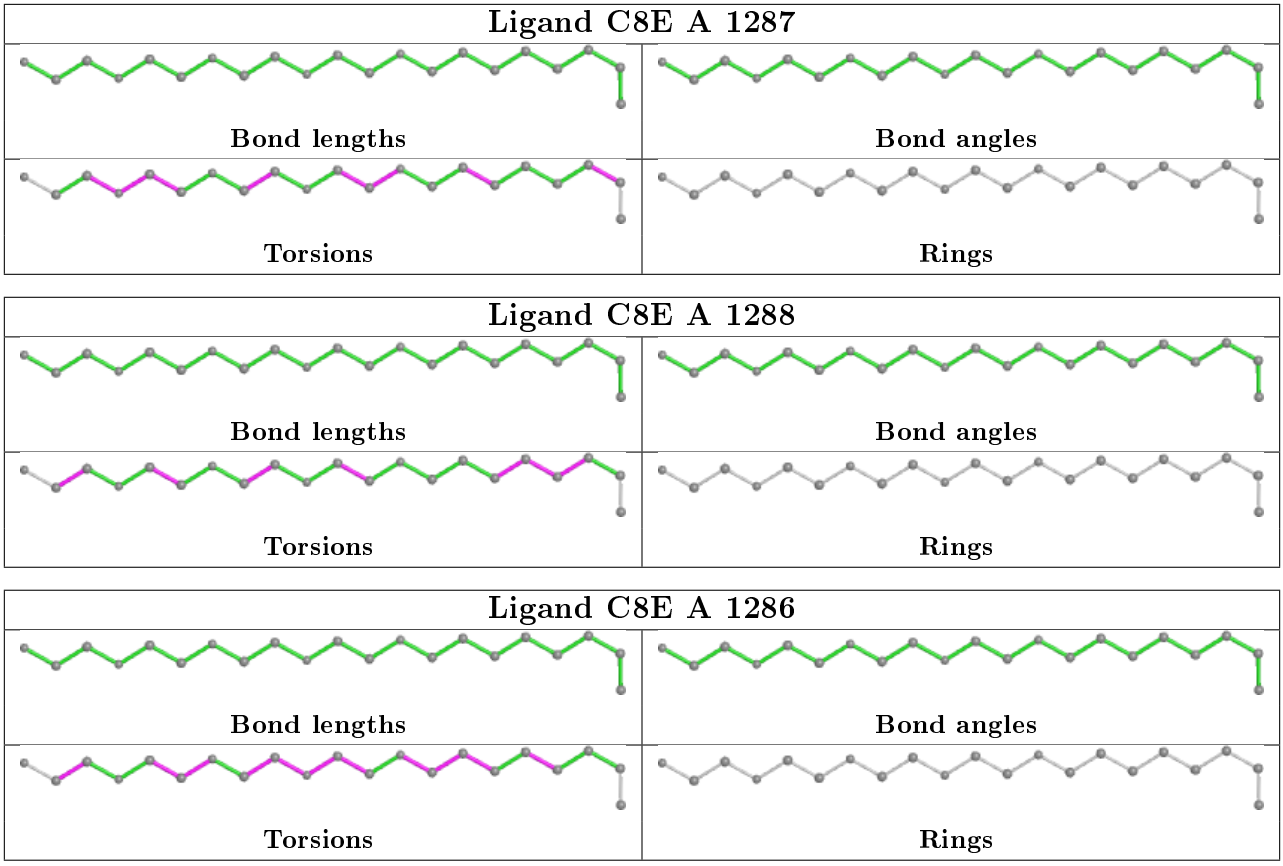
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	262/286 (91%)	1.07	44 (16%) 1 1	38, 54, 102, 125	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	103	GLY	11.2
1	A	102	PRO	10.0
1	A	57	TYR	7.7
1	A	219	ASN	6.3
1	A	100	ASP	6.2
1	A	61	LYS	6.0
1	A	261	HIS	5.9
1	A	221	ASP	5.6
1	A	230	GLY	5.5
1	A	220	TRP	5.3
1	A	62	ARG	5.3
1	A	266	SER	5.2
1	A	231	HIS	4.9
1	A	263	GLU	4.7
1	A	267	ASP	4.7
1	A	269[A]	PHE	4.7
1	A	105	ASP	4.4
1	A	217	TRP	4.3
1	A	218	SER	4.1
1	A	101	GLU	3.9
1	A	262	ASP	3.8
1	A	4	ASN	3.7
1	A	19	VAL	3.4
1	A	104	LYS	3.4
1	A	56	ASP	3.2
1	A	254[A]	TYR	3.1
1	A	201	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	18	ASN	3.0
1	A	55	VAL	2.9
1	A	270	HIS	2.9
1	A	265	ASP	2.8
1	A	145	GLY	2.7
1	A	260	ASP	2.7
1	A	259	GLN	2.4
1	A	232	ASP	2.4
1	A	63	GLY	2.4
1	A	144	THR	2.4
1	A	264	GLY	2.3
1	A	5	ASP	2.2
1	A	283	HIS	2.2
1	A	268	LYS	2.1
1	A	99	VAL	2.1
1	A	245	GLN	2.0
1	A	188	PHE	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^{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	C8E	A	1288	21/21	0.44	0.37	69,79,91,92	0
3	C8E	A	1290	9/21	0.73	0.27	53,60,67,68	0
3	C8E	A	1287	21/21	0.76	0.33	66,78,82,82	0
2	420	A	1284[A]	23/24	0.77	0.39	54,89,94,94	23
2	420	A	1284[B]	23/24	0.77	0.39	47,55,56,57	23
3	C8E	A	1286	21/21	0.77	0.29	69,78,79,80	0

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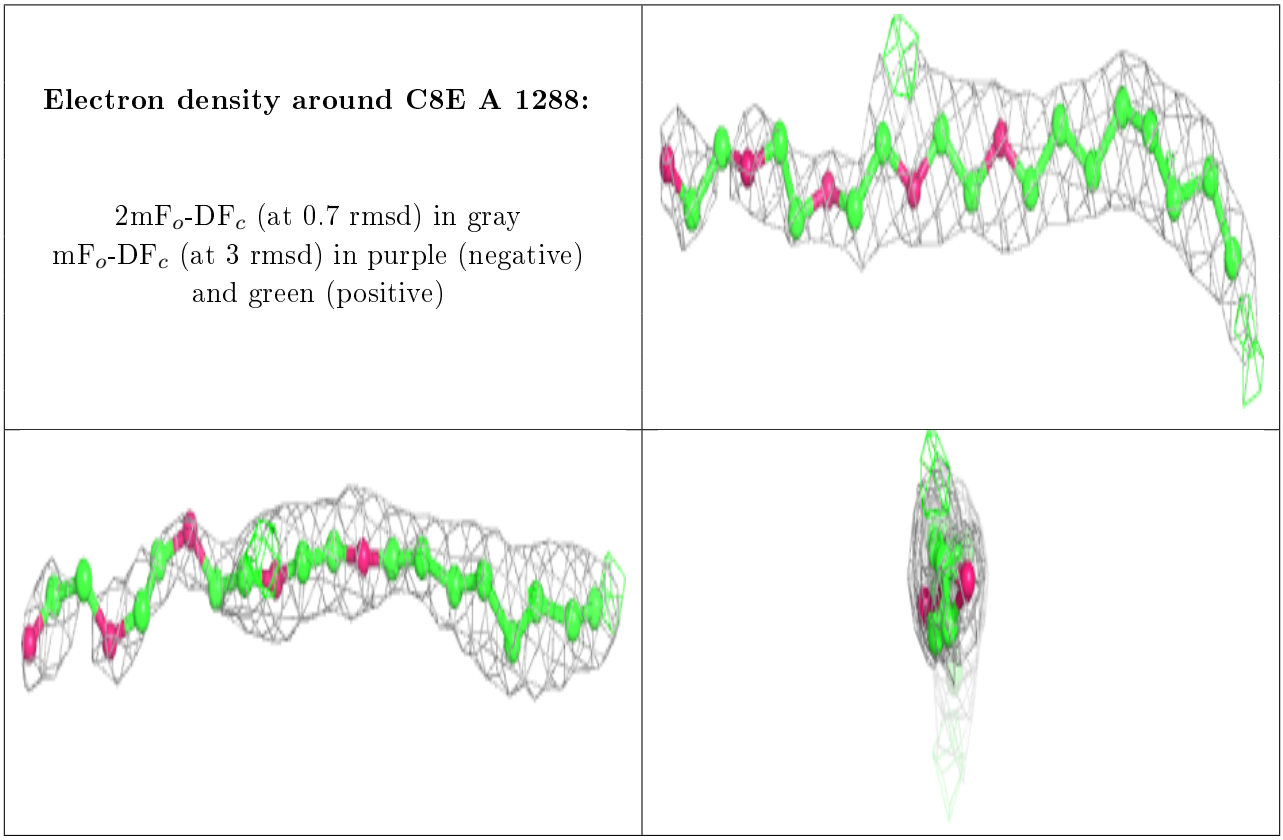
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	C8E	A	1289	8/21	0.88	0.23	67,68,68,68	0
4	EDO	A	1291	4/4	0.90	0.15	68,69,70,71	0
3	C8E	A	1285	13/21	0.90	0.29	65,66,73,74	0

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.

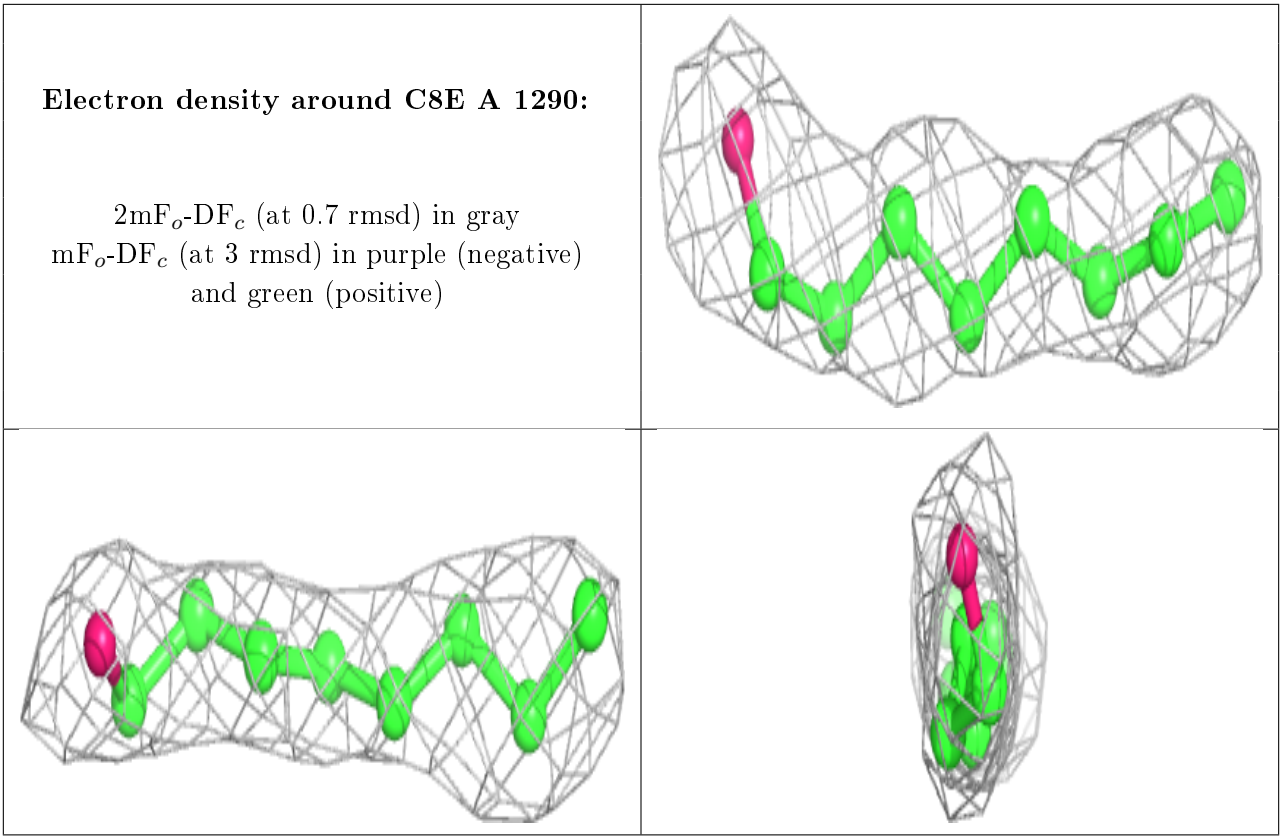
Electron density around C8E A 1288:

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



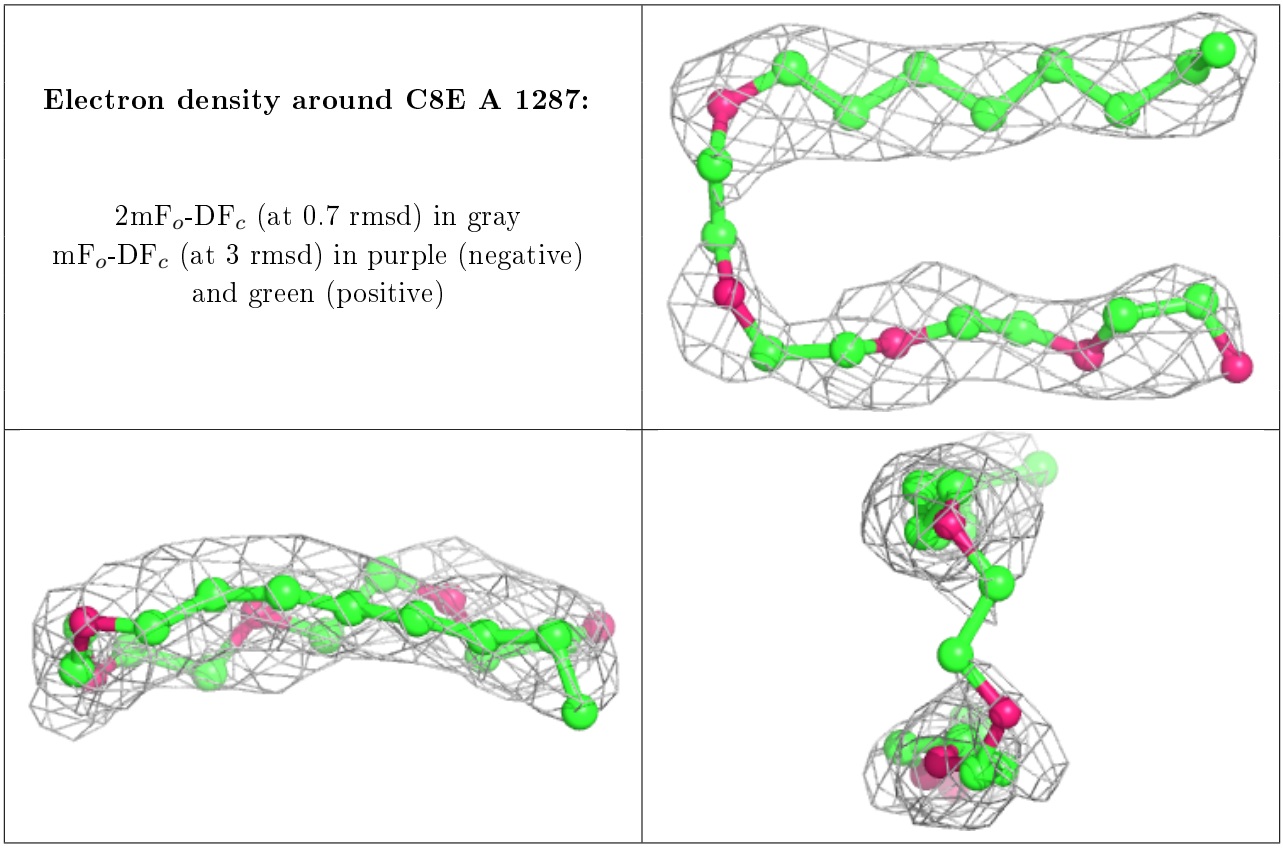
Electron density around C8E A 1290:

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



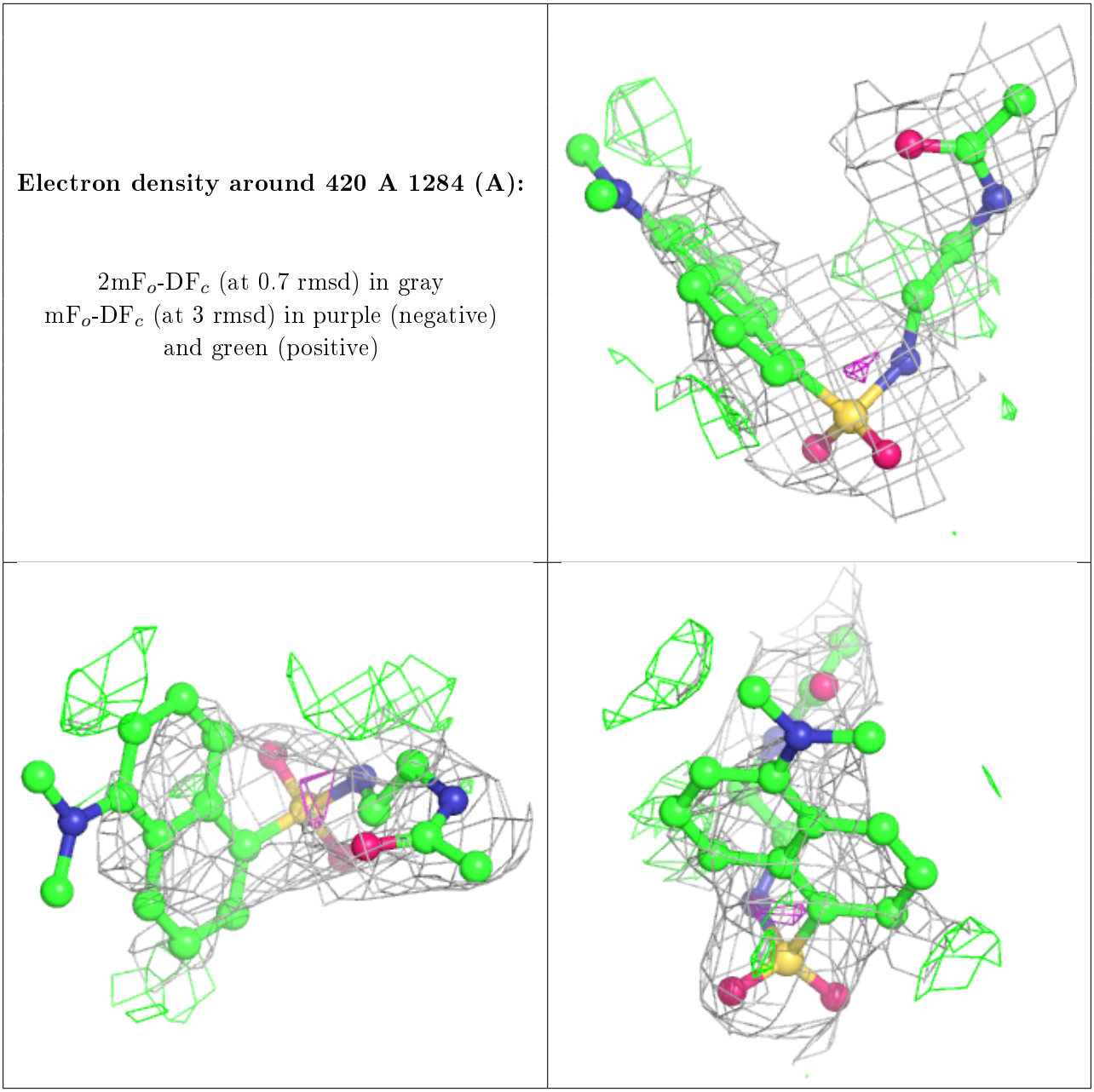
Electron density around C8E A 1287:

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



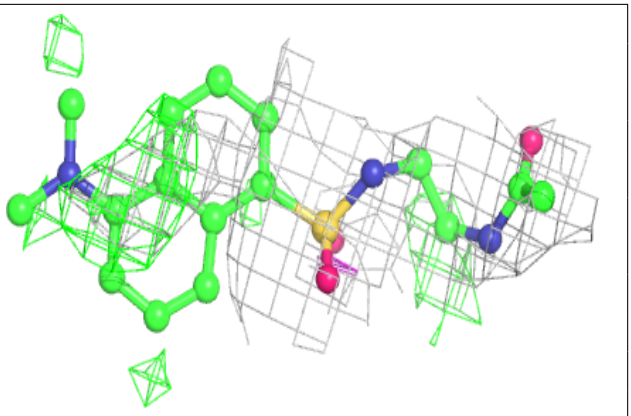
Electron density around 420 A 1284 (A):

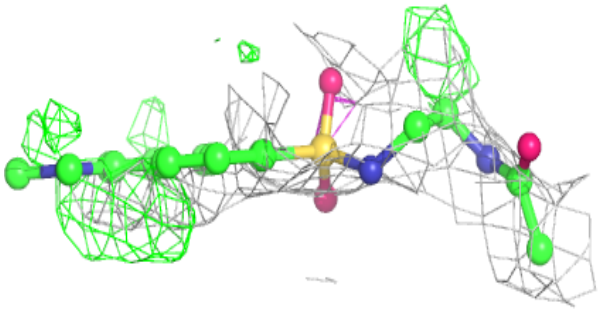
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

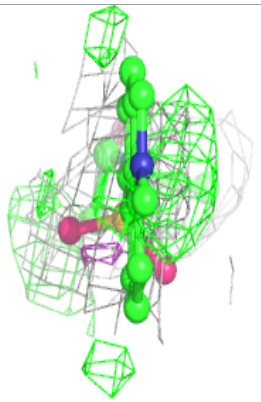


Electron density around 420 A 1284 (B):

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

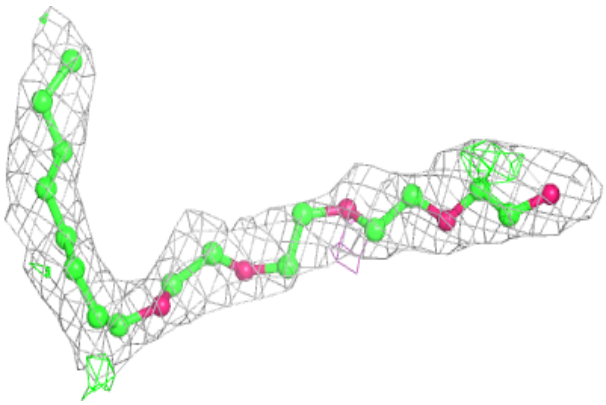


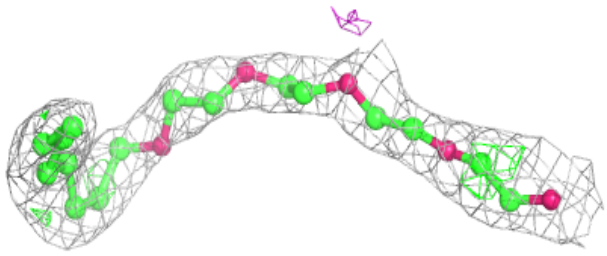


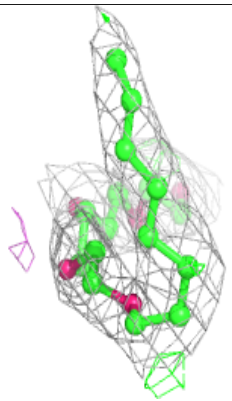


Electron density around C8E A 1286:

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

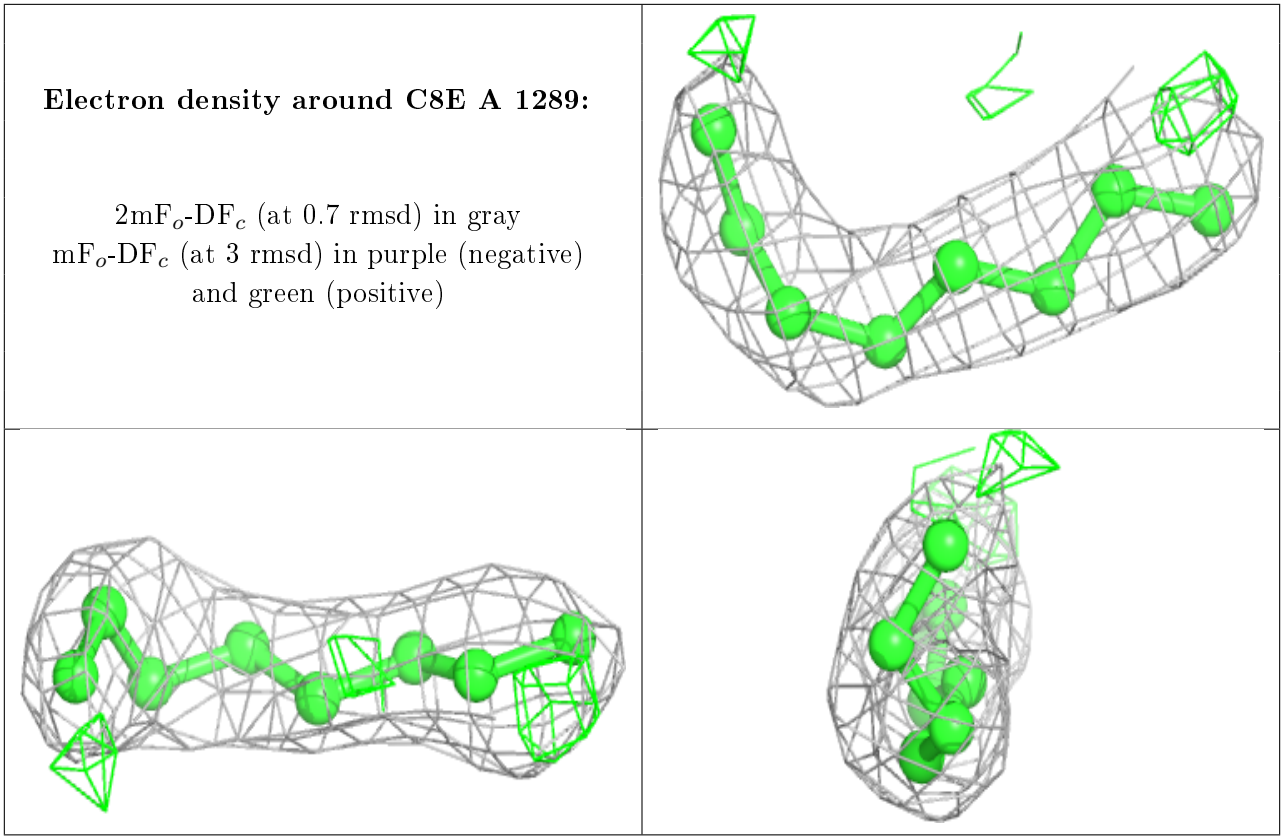






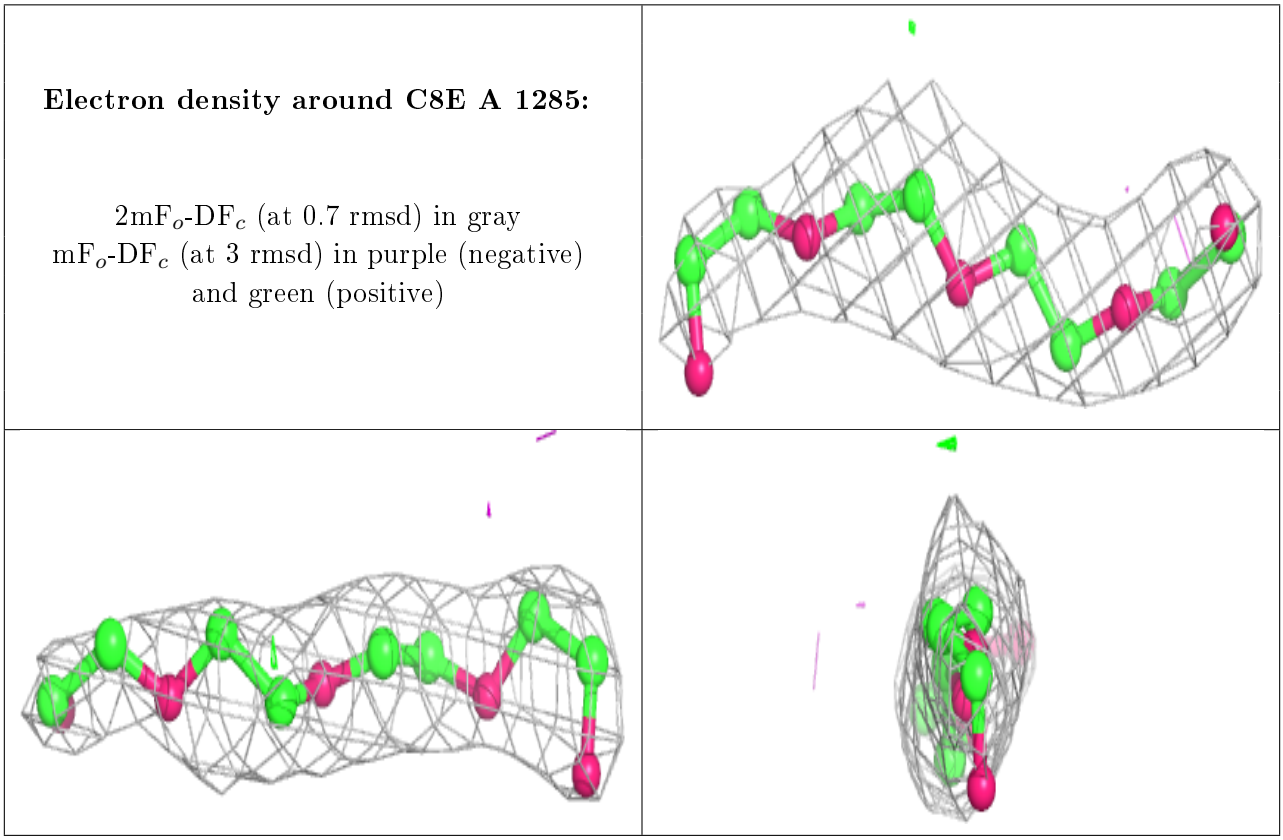
Electron density around C8E A 1289:

$2mF_o$-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 1285:

$2mF_o$-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.