



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:24 PM UTC

PDB ID : 1O6R / pdb_00001o6r
Title : Structures of human oxidosqualene cyclase inhibitors bound to an homologous enzyme
Authors : Lenhart, A.; Reinert, D.J.; Weihofen, W.A.; Aebi, J.D.; Dehmlow, H.; Morand, O.H.; Schulz, G.E.
Deposited on : 2002-10-13
Resolution : 2.70 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

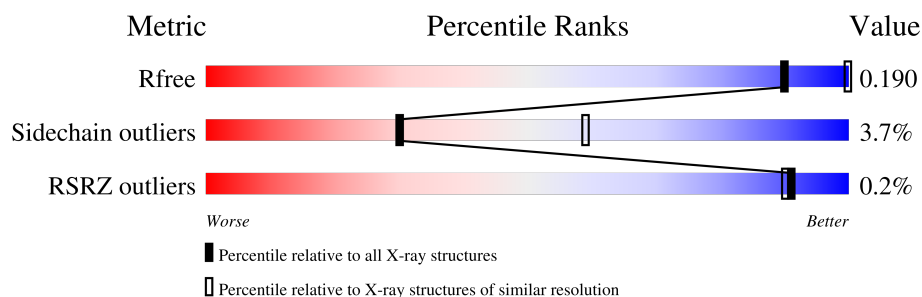
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

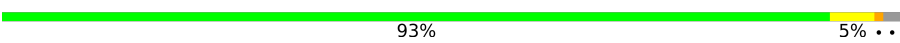
The reported resolution of this entry is 2.70 Å.

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}	180053	3538 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	631	
1	B	631	
1	C	631	

2 Entry composition [i](#)

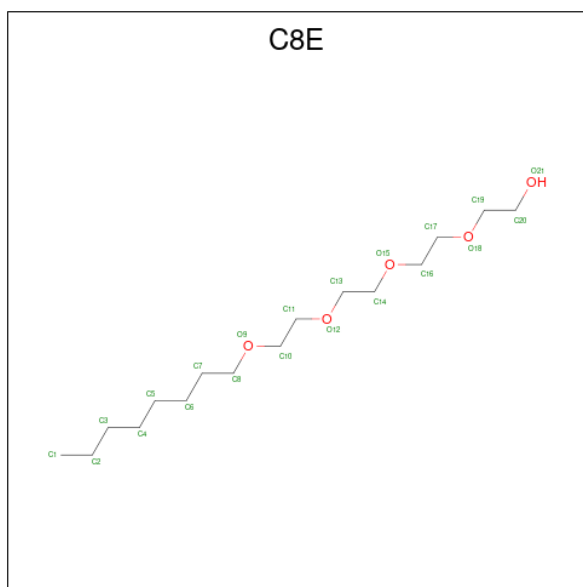
There are 4 unique types of molecules in this entry. The entry contains 15316 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SQUALENE-HOPENE CYCLASE.

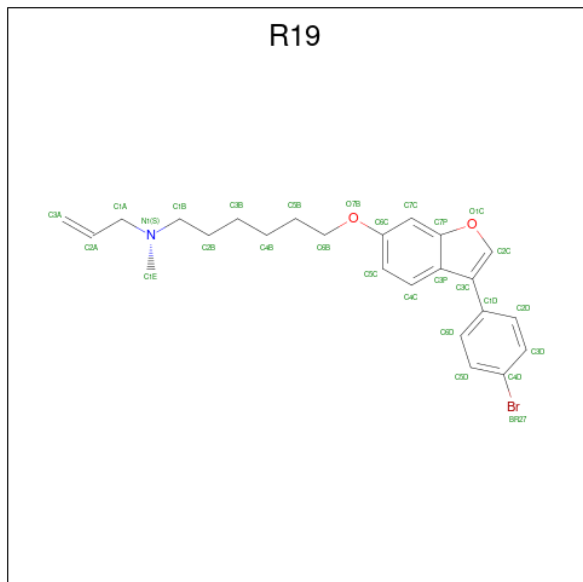
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	620	Total	C	N	O	S	0	0	1
			4964	3188	859	897	20			
1	B	620	Total	C	N	O	S	0	0	1
			4964	3188	859	897	20			
1	C	620	Total	C	N	O	S	0	0	1
			4964	3188	859	897	20			

- Molecule 2 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (CCD ID: C8E) (formula: C₁₆H₃₄O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			21	16	5		
2	B	1	Total	C	O	0	0
			21	16	5		
2	C	1	Total	C	O	0	0
			21	16	5		

- Molecule 3 is ALLYL-{6-[3-(4-BROMO-PHENYL)-BENZOFURAN-6-YLOXY]-HEXYL}-METHYL-AMIN (CCD ID: R19) (formula: $C_{24}H_{28}BrNO_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	Br	C	N	O	0	0
			28	1	24	1	2		
3	B	1	Total	Br	C	N	O	0	0
			28	1	24	1	2		
3	C	1	Total	Br	C	N	O	0	0
			28	1	24	1	2		

- Molecule 4 is water.

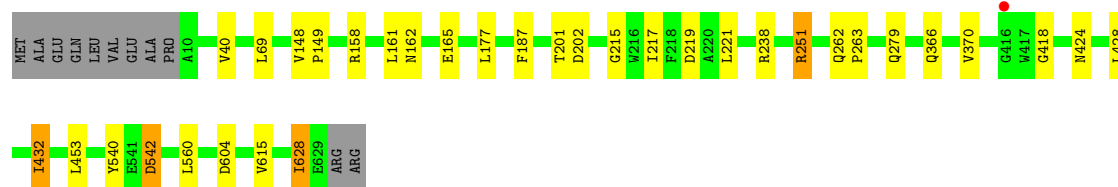
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	80	Total	O	0	0
			80	80		
4	B	105	Total	O	0	0
			105	105		
4	C	92	Total	O	0	0
			92	92		

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.

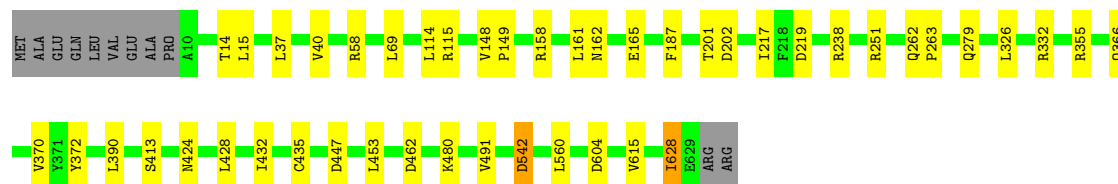
• Molecule 1: SQUALENE-HOPENE CYCLASE

Chain A:  93% 5% ..

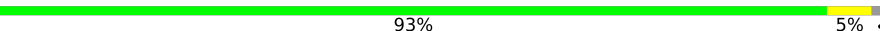


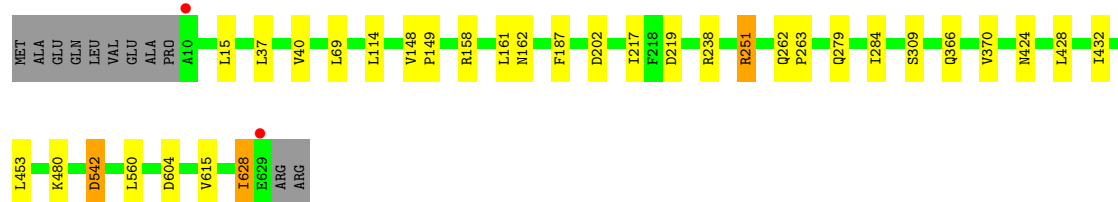
• Molecule 1: SQUALENE-HOPENE CYCLASE

Chain B:  91% 7% .



• Molecule 1: SQUALENE-HOPENE CYCLASE

Chain C:  93% 5% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	140.63Å 140.63Å 244.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.00 – 2.70 25.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	80.3 (25.00-2.70) 80.1 (25.00-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.193 , 0.236 (Not available) , 0.190	Depositor DCC
R_{free} test set	1986 reflections (3.20%)	wwPDB-VP
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 61.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15316	wwPDB-VP
Average B, all atoms (Å ²)	47.0	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 26.27 % 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 2.7156e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: R19, C8E

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.53	1/5117 (0.0%)	1.02	24/6967 (0.3%)
1	B	0.55	1/5117 (0.0%)	1.02	33/6967 (0.5%)
1	C	0.54	1/5117 (0.0%)	0.99	21/6967 (0.3%)
All	All	0.54	3/15351 (0.0%)	1.01	78/20901 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	628	ILE	C-N	-5.47	1.25	1.33
1	B	628	ILE	C-N	-5.34	1.25	1.33
1	C	628	ILE	C-N	-5.12	1.26	1.33

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	PHE	CA-C-N	9.53	129.62	119.90
1	A	187	PHE	C-N-CA	9.53	129.62	119.90
1	B	187	PHE	CA-C-N	8.67	128.74	119.90
1	B	187	PHE	C-N-CA	8.67	128.74	119.90
1	C	187	PHE	CA-C-N	8.32	128.38	119.90
1	C	187	PHE	C-N-CA	8.32	128.38	119.90
1	A	263	PRO	N-CA-C	7.75	120.16	110.70
1	B	263	PRO	N-CA-C	7.75	120.15	110.70
1	A	370	VAL	N-CA-C	7.67	120.63	111.05
1	C	263	PRO	N-CA-C	7.66	120.05	110.70
1	C	370	VAL	N-CA-C	7.53	120.46	111.05
1	B	370	VAL	N-CA-C	7.50	120.42	111.05
1	A	262	GLN	N-CA-C	7.22	122.56	112.75
1	B	262	GLN	N-CA-C	6.99	122.25	112.75
1	B	162	ASN	N-CA-C	-6.87	100.82	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	326	LEU	CA-C-N	6.78	126.75	119.76
1	B	326	LEU	C-N-CA	6.78	126.75	119.76
1	A	418	GLY	N-CA-C	-6.74	102.97	112.60
1	C	162	ASN	N-CA-C	-6.71	101.03	110.50
1	C	262	GLN	N-CA-C	6.60	121.73	112.75
1	A	542	ASP	CA-C-N	6.49	127.95	119.84
1	A	542	ASP	C-N-CA	6.49	127.95	119.84
1	B	615	VAL	N-CA-C	6.46	118.04	111.00
1	C	542	ASP	CA-C-N	6.38	127.82	119.84
1	C	542	ASP	C-N-CA	6.38	127.82	119.84
1	A	251	ARG	N-CA-C	6.33	121.01	113.16
1	A	615	VAL	N-CA-C	6.27	117.83	111.00
1	B	435	CYS	N-CA-C	6.26	119.35	109.39
1	A	162	ASN	N-CA-C	-6.25	101.23	110.48
1	B	542	ASP	CA-C-N	6.23	127.63	119.84
1	B	542	ASP	C-N-CA	6.23	127.63	119.84
1	C	424	ASN	N-CA-C	-6.19	100.34	109.62
1	A	424	ASN	N-CA-C	-6.10	100.47	109.62
1	C	251	ARG	N-CA-C	6.08	120.69	113.16
1	B	424	ASN	N-CA-C	-6.05	100.54	109.62
1	B	355	ARG	CA-C-N	6.05	125.94	119.28
1	B	355	ARG	C-N-CA	6.05	125.94	119.28
1	B	462	ASP	N-CA-C	5.98	116.32	108.07
1	C	149	PRO	N-CA-C	5.96	117.97	110.70
1	C	615	VAL	N-CA-C	5.94	117.48	111.00
1	B	390	LEU	CA-C-N	5.92	125.39	119.24
1	B	390	LEU	C-N-CA	5.92	125.39	119.24
1	B	491	VAL	N-CA-C	5.89	116.16	107.15
1	A	161	LEU	N-CA-C	5.85	119.72	112.58
1	C	148	VAL	CA-C-N	5.83	126.38	120.38
1	C	148	VAL	C-N-CA	5.83	126.38	120.38
1	A	604	ASP	N-CA-C	5.82	121.82	114.31
1	B	604	ASP	N-CA-C	5.78	121.77	114.31
1	B	251	ARG	N-CA-C	5.73	120.39	113.17
1	C	284	ILE	N-CA-C	-5.66	105.33	110.82
1	A	148	VAL	CA-C-N	5.64	126.19	120.38
1	A	148	VAL	C-N-CA	5.64	126.19	120.38
1	C	161	LEU	N-CA-C	5.60	119.70	112.86
1	A	432	ILE	CA-C-N	5.58	125.42	119.28
1	A	432	ILE	C-N-CA	5.58	125.42	119.28
1	B	161	LEU	N-CA-C	5.56	119.64	112.86
1	B	40	VAL	N-CA-C	5.51	120.80	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	215	GLY	N-CA-C	-5.40	105.17	112.14
1	B	148	VAL	CA-C-N	5.33	125.87	120.38
1	B	148	VAL	C-N-CA	5.33	125.87	120.38
1	B	149	PRO	N-CA-C	5.33	117.20	110.70
1	B	165	GLU	N-CA-C	-5.33	106.82	113.38
1	A	40	VAL	N-CA-C	5.32	120.39	109.34
1	A	149	PRO	N-CA-C	5.31	117.18	110.70
1	C	309	SER	N-CA-C	5.29	121.50	109.81
1	C	40	VAL	N-CA-C	5.27	120.29	109.34
1	B	480	LYS	CA-C-N	5.25	125.30	119.32
1	B	480	LYS	C-N-CA	5.25	125.30	119.32
1	B	413	SER	N-CA-C	5.22	116.66	111.07
1	B	372	TYR	N-CA-C	5.21	117.07	109.30
1	A	165	GLU	N-CA-C	-5.21	106.97	113.38
1	C	604	ASP	N-CA-C	5.16	120.97	114.31
1	B	447	ASP	N-CA-C	5.09	116.91	111.36
1	C	480	LYS	CA-C-N	5.06	125.09	119.32
1	C	480	LYS	C-N-CA	5.06	125.09	119.32
1	A	540	TYR	N-CA-C	-5.05	105.42	112.45
1	A	177	LEU	N-CA-C	5.04	117.50	111.71
1	B	14	THR	N-CA-C	-5.02	105.69	111.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	490/513 (96%)	473 (96%)	17 (4%)	32	61
1	B	503/513 (98%)	482 (96%)	21 (4%)	26	55
1	C	503/513 (98%)	485 (96%)	18 (4%)	31	60
All	All	1496/1539 (97%)	1440 (96%)	56 (4%)	30	59

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LEU
1	A	158	ARG
1	A	201	THR
1	A	202	ASP
1	A	217	ILE
1	A	219	ASP
1	A	221	LEU
1	A	238	ARG
1	A	251	ARG
1	A	279	GLN
1	A	366	GLN
1	A	428	LEU
1	A	432	ILE
1	A	453	LEU
1	A	542	ASP
1	A	560	LEU
1	A	628	ILE
1	B	15	LEU
1	B	37	LEU
1	B	58	ARG
1	B	69	LEU
1	B	114	LEU
1	B	115	ARG
1	B	158	ARG
1	B	201	THR
1	B	202	ASP
1	B	217	ILE
1	B	219	ASP
1	B	238	ARG
1	B	279	GLN
1	B	332	ARG

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Mol	Chain	Res	Type
1	B	366	GLN
1	B	428	LEU
1	B	432	ILE
1	B	453	LEU
1	B	542	ASP
1	B	560	LEU
1	B	628	ILE
1	C	15	LEU
1	C	37	LEU
1	C	69	LEU
1	C	114	LEU
1	C	158	ARG
1	C	202	ASP
1	C	217	ILE
1	C	219	ASP
1	C	238	ARG
1	C	251	ARG
1	C	279	GLN
1	C	366	GLN
1	C	428	LEU
1	C	432	ILE
1	C	453	LEU
1	C	542	ASP
1	C	560	LEU
1	C	628	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	HIS
1	A	279	GLN
1	A	357	ASN
1	A	614	HIS
1	B	70	HIS
1	B	279	GLN
1	B	357	ASN
1	B	414	ASN
1	B	614	HIS
1	C	279	GLN
1	C	357	ASN
1	C	614	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 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	R19	A	800	-	29,30,30	1.93	11 (37%)	36,39,39	1.54	5 (13%)
2	C8E	B	700	-	20,20,20	0.81	0	19,19,19	1.73	5 (26%)
2	C8E	C	700	-	20,20,20	0.79	0	19,19,19	1.75	5 (26%)
3	R19	C	800	-	29,30,30	1.93	13 (44%)	36,39,39	1.61	5 (13%)
3	R19	B	800	-	29,30,30	1.83	11 (37%)	36,39,39	1.64	5 (13%)
2	C8E	A	700	-	20,20,20	0.86	0	19,19,19	1.77	5 (26%)

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	R19	A	800	-	-	8/17/17/17	0/3/3/3
2	C8E	B	700	-	-	12/18/18/18	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	C8E	C	700	-	-	13/18/18/18	-
3	R19	C	800	-	-	7/17/17/17	0/3/3/3
3	R19	B	800	-	-	8/17/17/17	0/3/3/3
2	C8E	A	700	-	-	14/18/18/18	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	800	R19	C3P-C7P	5.06	1.45	1.39
3	C	800	R19	C3P-C7P	4.25	1.44	1.39
3	B	800	R19	C3P-C7P	3.60	1.44	1.39
3	B	800	R19	C4C-C5C	3.20	1.44	1.38
3	A	800	R19	C5D-C4D	3.11	1.44	1.38
3	C	800	R19	C3D-C4D	2.94	1.44	1.38
3	A	800	R19	C5D-C6D	2.89	1.43	1.38
3	B	800	R19	C5D-C4D	2.89	1.43	1.38
3	C	800	R19	C4C-C5C	2.84	1.43	1.38
3	C	800	R19	C2D-C3D	2.78	1.43	1.38
3	B	800	R19	C7C-C7P	2.78	1.43	1.38
3	A	800	R19	C4C-C5C	2.76	1.43	1.38
3	C	800	R19	C5D-C4D	2.75	1.43	1.38
3	A	800	R19	C1D-C3C	2.71	1.53	1.49
3	C	800	R19	C1D-C3C	2.70	1.53	1.49
3	C	800	R19	C6D-C1D	2.66	1.43	1.39
3	A	800	R19	C6D-C1D	2.65	1.43	1.39
3	C	800	R19	C5D-C6D	2.60	1.43	1.38
3	A	800	R19	C3D-C4D	2.59	1.43	1.38
3	B	800	R19	C5D-C6D	2.58	1.43	1.38
3	B	800	R19	C2D-C3D	2.57	1.43	1.38
3	B	800	R19	C2D-C1D	2.55	1.43	1.39
3	C	800	R19	C7C-C7P	2.54	1.43	1.38
3	B	800	R19	C3D-C4D	2.47	1.43	1.38
3	C	800	R19	C7C-C6C	2.40	1.42	1.39
3	A	800	R19	C2D-C3D	2.40	1.42	1.38
3	C	800	R19	C5C-C6C	2.19	1.42	1.38
3	A	800	R19	C2D-C1D	2.17	1.42	1.39
3	A	800	R19	C5C-C6C	2.16	1.42	1.38
3	B	800	R19	C1B-N1	2.15	1.53	1.46
3	C	800	R19	C2D-C1D	2.09	1.42	1.39
3	A	800	R19	C7C-C6C	2.05	1.42	1.39
3	B	800	R19	C7C-C6C	2.02	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	800	R19	C6D-C1D	2.01	1.42	1.39
3	C	800	R19	C1B-N1	2.00	1.52	1.46

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	800	R19	C7P-O1C-C2C	5.07	109.51	105.19
3	C	800	R19	C7P-O1C-C2C	4.59	109.10	105.19
2	A	700	C8E	O15-C14-C13	4.58	131.22	110.35
2	B	700	C8E	O15-C14-C13	4.50	130.87	110.35
2	C	700	C8E	O15-C14-C13	4.49	130.81	110.35
3	B	800	R19	O1C-C7P-C7C	4.29	132.08	125.01
3	C	800	R19	O1C-C7P-C7C	4.24	132.00	125.01
3	A	800	R19	C7P-O1C-C2C	3.95	108.55	105.19
3	A	800	R19	O1C-C7P-C7C	3.94	131.51	125.01
3	B	800	R19	O1C-C7P-C3P	-3.81	106.50	110.53
3	C	800	R19	O1C-C7P-C3P	-3.50	106.84	110.53
3	C	800	R19	C7C-C7P-C3P	-3.10	121.16	124.70
3	A	800	R19	O1C-C7P-C3P	-3.09	107.26	110.53
3	A	800	R19	C7C-C7P-C3P	-3.04	121.22	124.70
2	A	700	C8E	O15-C16-C17	2.89	123.54	110.35
3	B	800	R19	C7C-C7P-C3P	-2.88	121.42	124.70
2	C	700	C8E	O15-C16-C17	2.83	123.27	110.35
3	A	800	R19	C7P-C3P-C3C	2.81	107.48	105.83
3	B	800	R19	C7P-C3P-C3C	2.79	107.48	105.83
2	C	700	C8E	C19-O18-C17	-2.79	101.03	113.26
2	A	700	C8E	O18-C19-C20	2.77	122.32	110.11
2	B	700	C8E	O15-C16-C17	2.77	122.97	110.35
3	C	800	R19	C7P-C3P-C3C	2.75	107.45	105.83
2	B	700	C8E	O18-C19-C20	2.72	122.11	110.11
2	C	700	C8E	O18-C19-C20	2.68	121.92	110.11
2	B	700	C8E	C19-O18-C17	-2.64	101.72	113.26
2	A	700	C8E	C19-O18-C17	-2.57	101.99	113.26
2	B	700	C8E	C16-O15-C14	-2.09	104.12	113.26
2	C	700	C8E	C16-O15-C14	-2.07	104.20	113.26
2	A	700	C8E	C7-C6-C5	-2.03	104.13	114.37

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	700	C8E	O12-C13-C14-O15

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Mol	Chain	Res	Type	Atoms
2	A	700	C8E	O9-C10-C11-O12
3	A	800	R19	C5C-C6C-O7B-C6B
3	A	800	R19	C7C-C6C-O7B-C6B
3	C	800	R19	C5C-C6C-O7B-C6B
3	B	800	R19	C7C-C6C-O7B-C6B
3	C	800	R19	C7C-C6C-O7B-C6B
3	B	800	R19	C5C-C6C-O7B-C6B
2	A	700	C8E	O18-C19-C20-O21
3	A	800	R19	C4B-C5B-C6B-O7B
3	B	800	R19	C4B-C5B-C6B-O7B
3	C	800	R19	C4B-C5B-C6B-O7B
3	A	800	R19	N1-C1B-C2B-C3B
3	C	800	R19	N1-C1B-C2B-C3B
2	A	700	C8E	C5-C6-C7-C8
3	A	800	R19	C2B-C3B-C4B-C5B
2	B	700	C8E	O12-C13-C14-O15
3	B	800	R19	N1-C1B-C2B-C3B
2	B	700	C8E	C5-C6-C7-C8
2	C	700	C8E	C5-C6-C7-C8
2	A	700	C8E	C3-C4-C5-C6
2	C	700	C8E	C3-C4-C5-C6
3	B	800	R19	C2B-C3B-C4B-C5B
3	C	800	R19	C2B-C3B-C4B-C5B
2	A	700	C8E	C4-C5-C6-C7
2	B	700	C8E	C4-C5-C6-C7
3	A	800	R19	C1B-C2B-C3B-C4B
3	B	800	R19	C1B-C2B-C3B-C4B
3	C	800	R19	C1B-C2B-C3B-C4B
2	A	700	C8E	C1-C2-C3-C4
2	B	700	C8E	C1-C2-C3-C4
2	C	700	C8E	C1-C2-C3-C4
3	A	800	R19	C3B-C4B-C5B-C6B
2	B	700	C8E	O18-C19-C20-O21
2	B	700	C8E	O9-C10-C11-O12
2	A	700	C8E	C2-C3-C4-C5
2	A	700	C8E	C13-C14-O15-C16
3	B	800	R19	C3B-C4B-C5B-C6B
2	C	700	C8E	C14-C13-O12-C11
2	A	700	C8E	C11-C10-O9-C8
2	B	700	C8E	O15-C16-C17-O18
2	A	700	C8E	C14-C13-O12-C11
2	B	700	C8E	C3-C4-C5-C6

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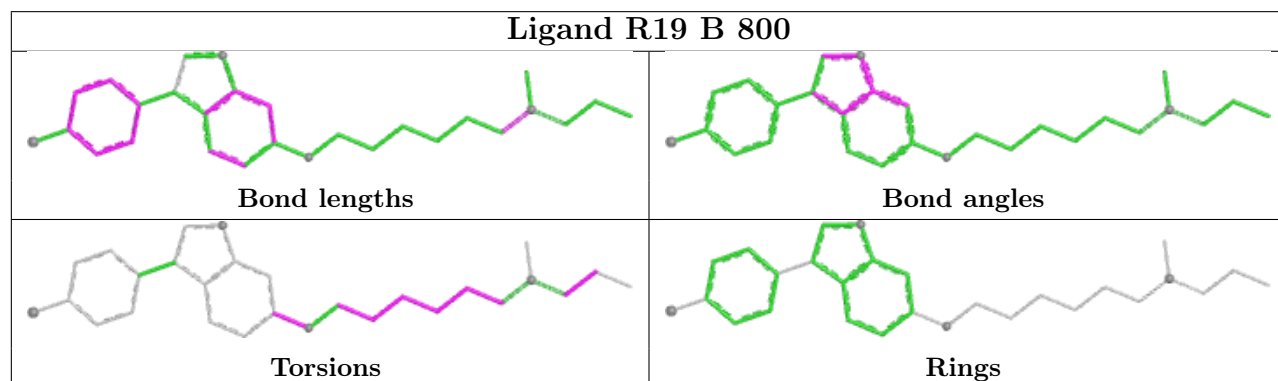
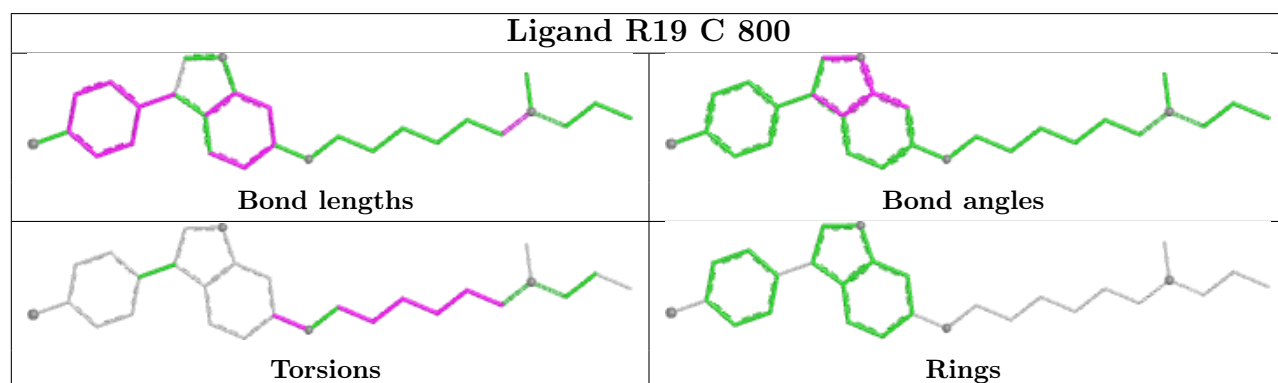
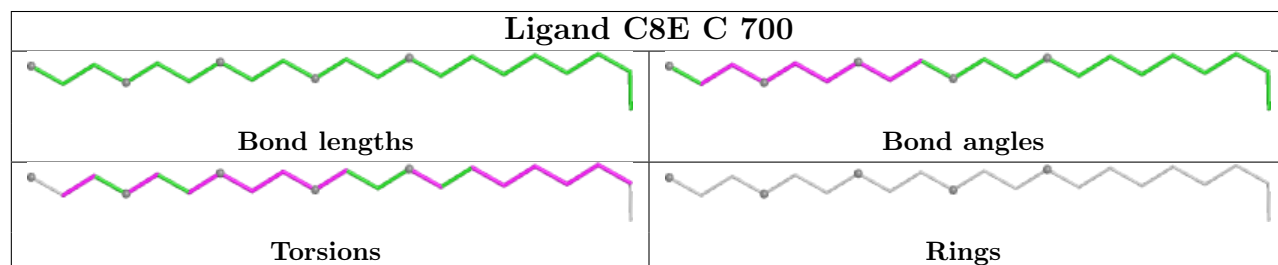
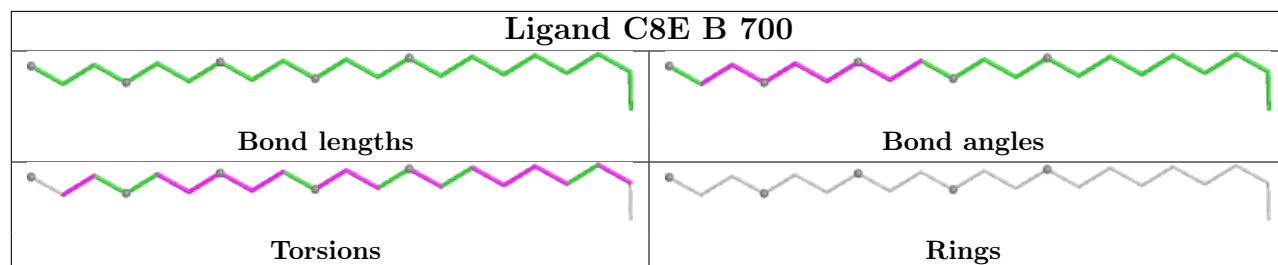
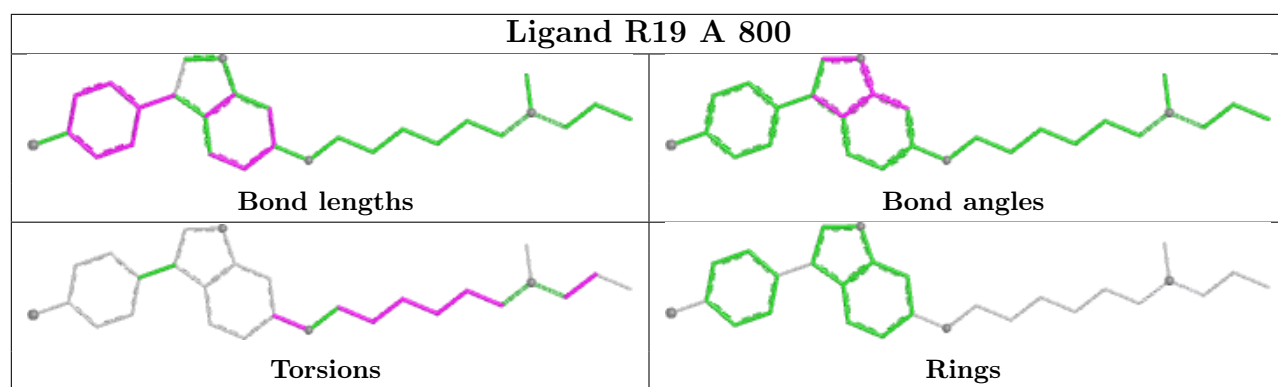
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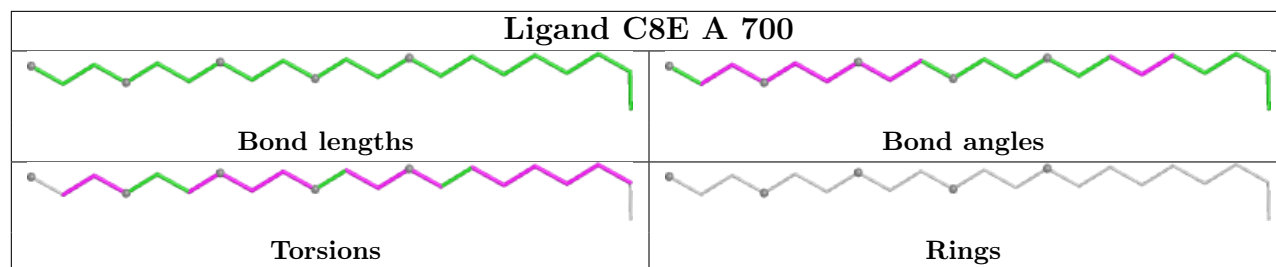
Mol	Chain	Res	Type	Atoms
2	B	700	C8E	C17-C16-O15-C14
3	C	800	R19	C3B-C4B-C5B-C6B
2	C	700	C8E	C13-C14-O15-C16
3	A	800	R19	N1-C1A-C2A-C3A
2	C	700	C8E	C10-C11-O12-C13
3	B	800	R19	N1-C1A-C2A-C3A
2	C	700	C8E	C4-C5-C6-C7
2	C	700	C8E	C17-C16-O15-C14
2	C	700	C8E	O18-C19-C20-O21
2	C	700	C8E	C7-C8-O9-C10
2	A	700	C8E	C17-C16-O15-C14
2	A	700	C8E	C20-C19-O18-C17
2	C	700	C8E	C16-C17-O18-C19
2	C	700	C8E	C2-C3-C4-C5
2	B	700	C8E	C7-C8-O9-C10
2	B	700	C8E	C10-C11-O12-C13
2	A	700	C8E	O12-C13-C14-O15
2	A	700	C8E	C7-C8-O9-C10
2	B	700	C8E	C13-C14-O15-C16

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	620/631 (98%)	-0.30	1 (0%) 91 90	11, 51, 92, 99	0
1	B	620/631 (98%)	-0.72	0 100 100	10, 37, 79, 99	0
1	C	620/631 (98%)	-0.60	2 (0%) 90 89	10, 43, 85, 99	0
All	All	1860/1893 (98%)	-0.54	3 (0%) 91 90	10, 44, 87, 99	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	629	GLU	2.9
1	C	10	ALA	2.9
1	A	416	GLY	2.5

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 oligosaccharides 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(Å ²)	Q<0.9
2	C8E	C	700	21/21	0.90	0.17	83,83,83,83	0

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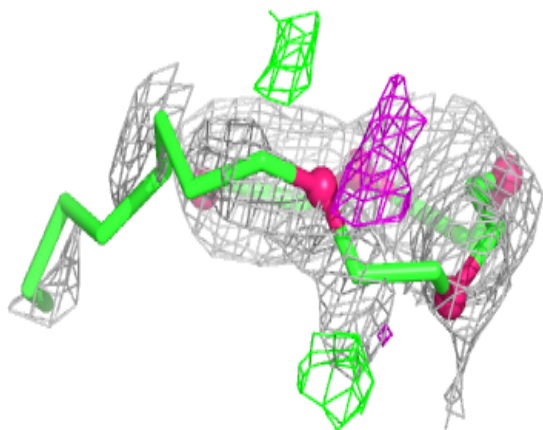
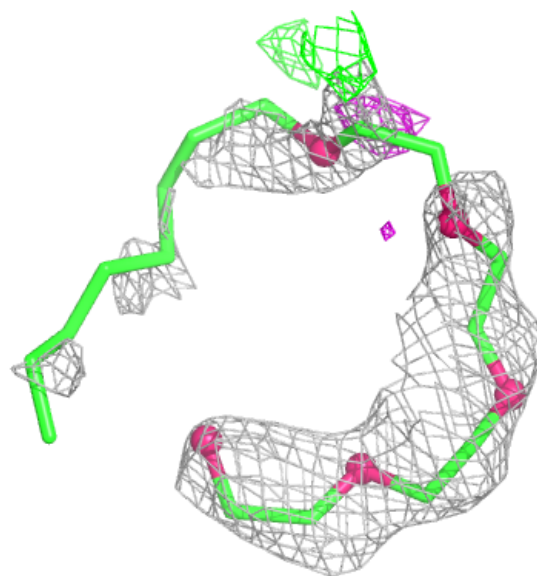
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	C8E	B	700	21/21	0.91	0.17	89,89,89,89	0
2	C8E	A	700	21/21	0.92	0.17	99,99,99,99	0
3	R19	A	800	28/28	0.95	0.11	33,36,69,69	0
3	R19	B	800	28/28	0.97	0.08	29,30,62,62	0
3	R19	C	800	28/28	0.97	0.09	35,35,61,61	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.

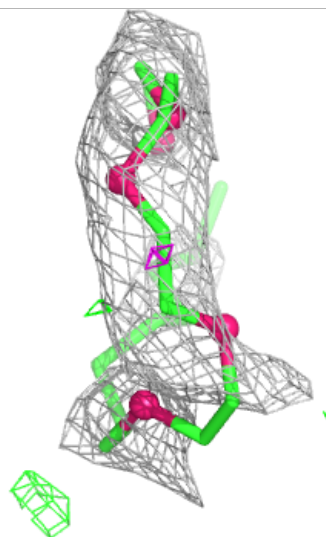
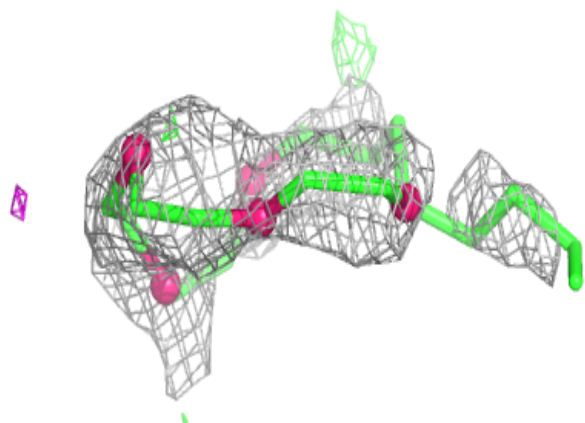
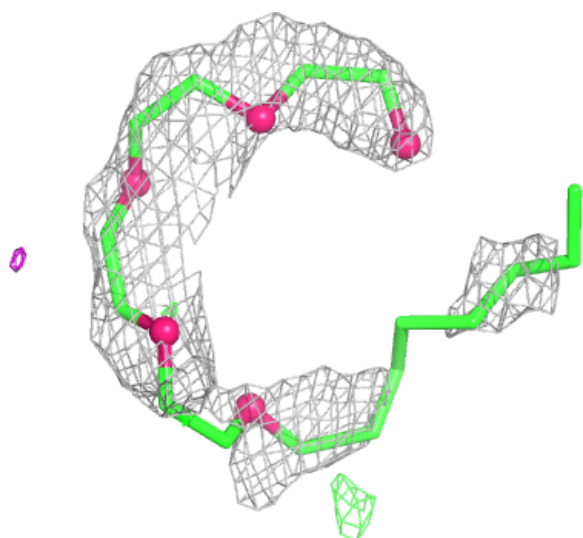
Electron density around C8E C 700:

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



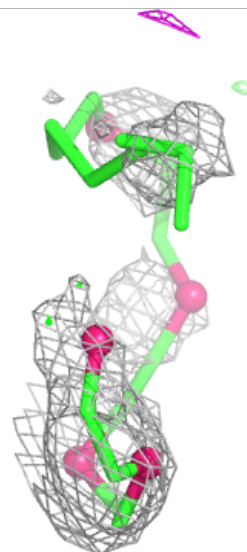
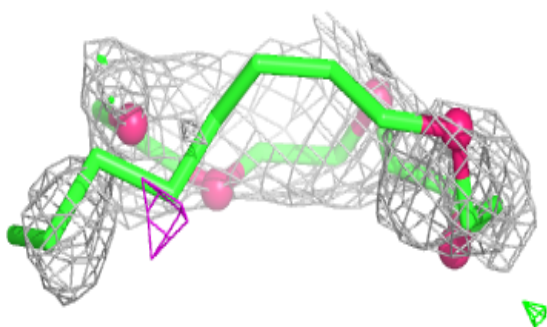
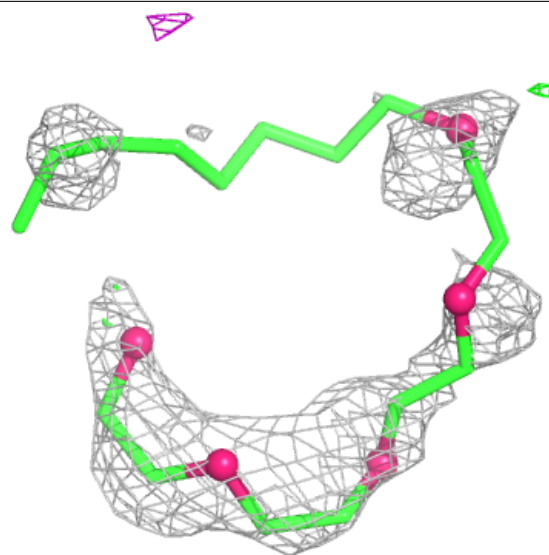
Electron density around C8E B 700:

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



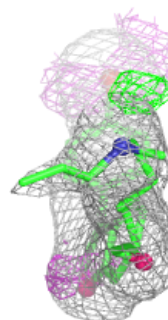
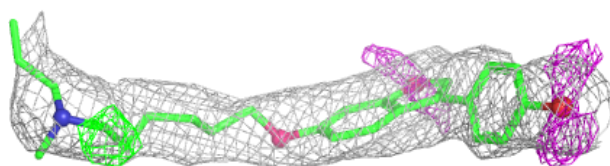
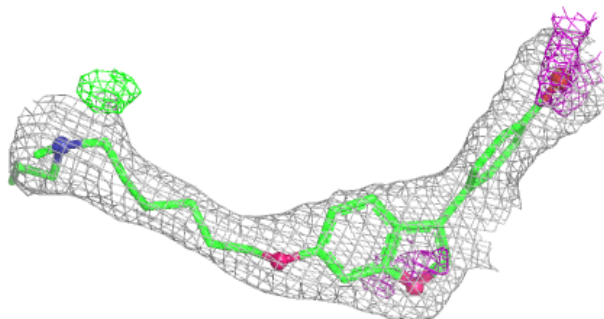
Electron density around C8E A 700:

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

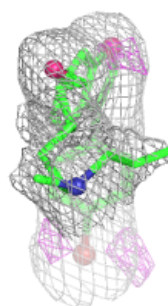
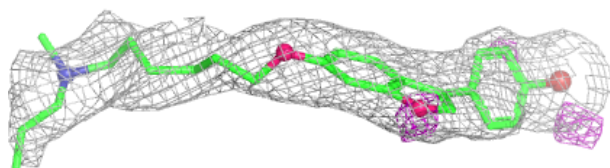
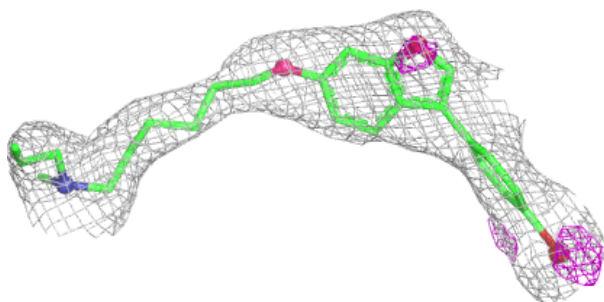


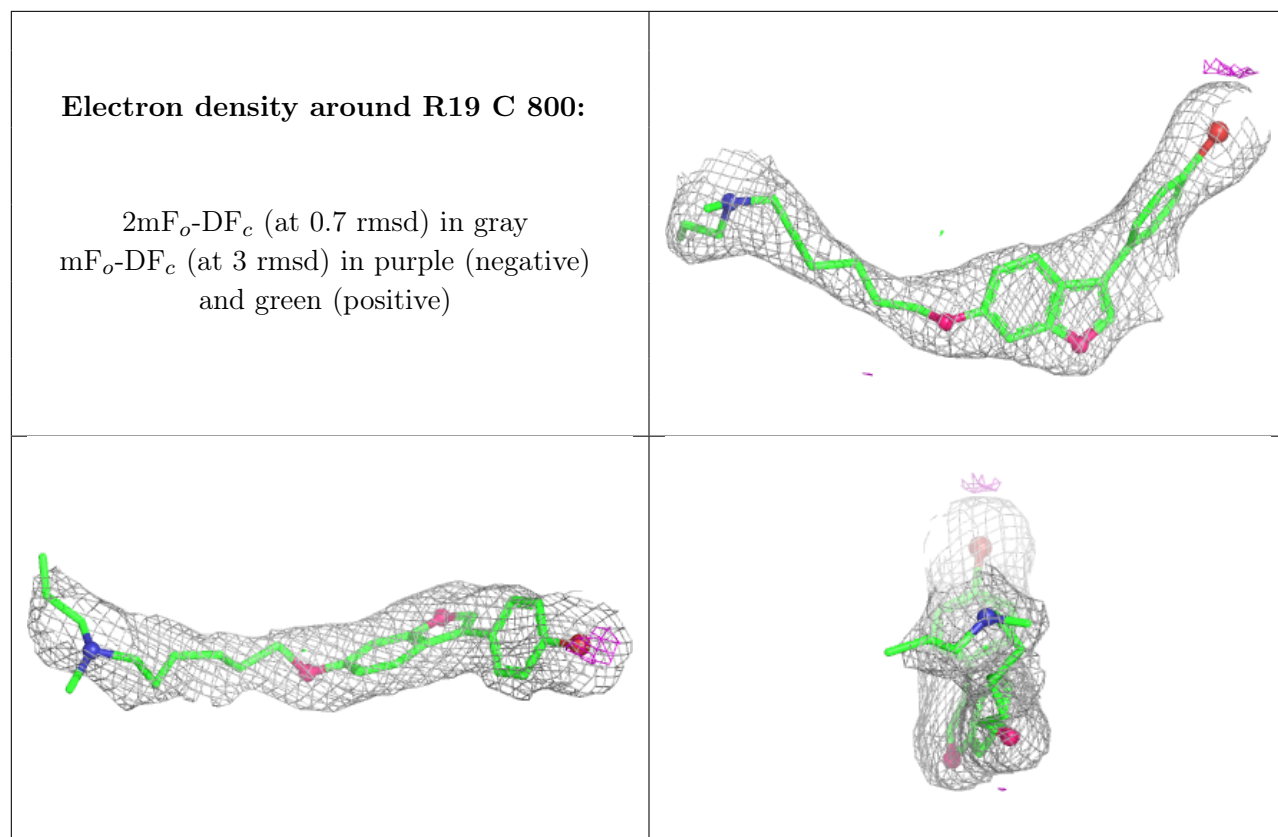
Electron density around R19 A 800:

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

**Electron density around R19 B 800:**

$2mF_o-DF_c$ (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.