



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 10:44 AM EDT

PDB ID : 2SQC / pdb_00002sqc
Title : SQUALENE-HOPENE CYCLASE FROM ALICYCLOBACILLUS ACIDOCALDARIUS
Authors : Wendt, K.U.; Schulz, G.E.
Deposited on : 1998-08-02
Resolution : 2.00 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

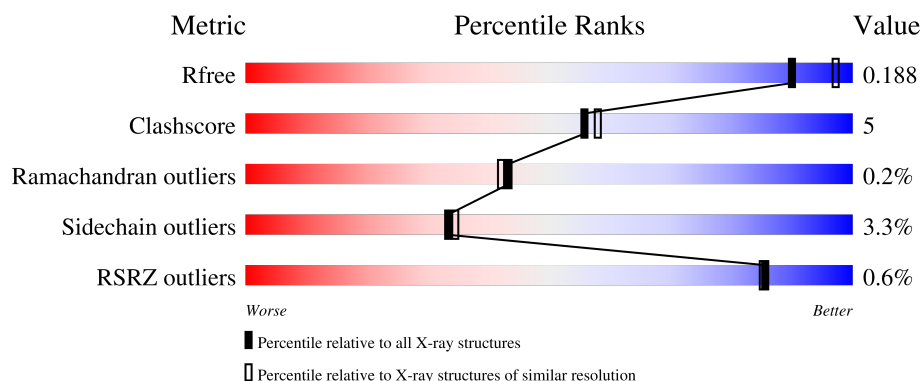
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	 87% 10% ..
1	B	631	 88% 9% ..

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11627 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.

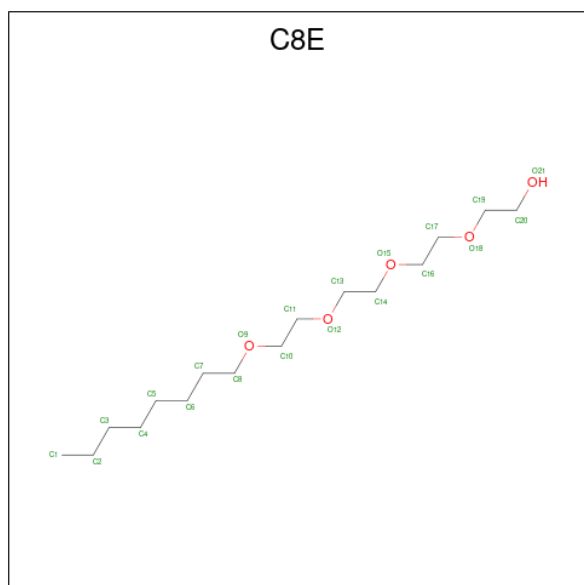
- Molecule 1 is a protein called SQUALENE-HOPENE CYCLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	623	Total	C	N	O	S	0	0	0
			4993	3206	865	902	20			
1	B	623	Total	C	N	O	S	0	0	0
			4993	3206	865	902	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	376	CYS	ASP	engineered mutation	UNP P33247
A	435	SER	CYS	engineered mutation	UNP P33247
B	376	CYS	ASP	engineered mutation	UNP P33247
B	435	SER	CYS	engineered mutation	UNP P33247

- Molecule 2 is (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (CCD ID: C8E) (formula: $C_{16}H_{34}O_5$).



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

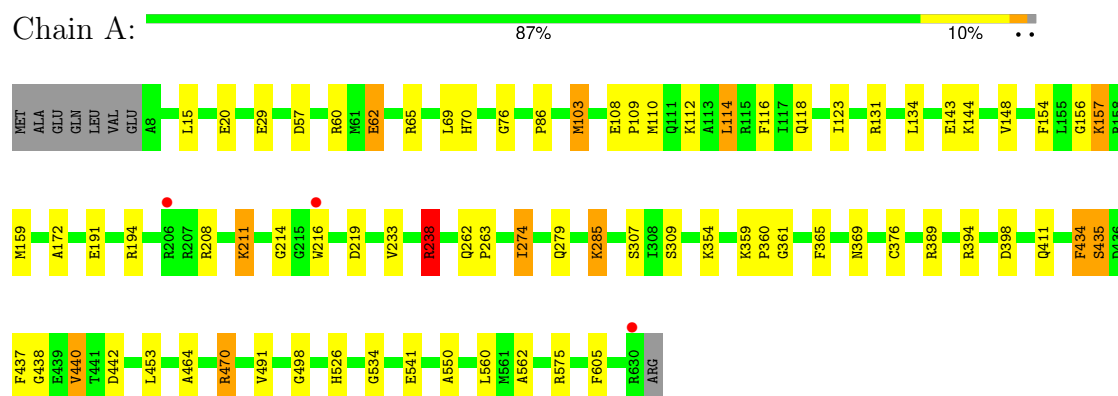
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	730	Total	O	0	0
			730	730		
3	B	785	Total	O	0	0
			785	785		

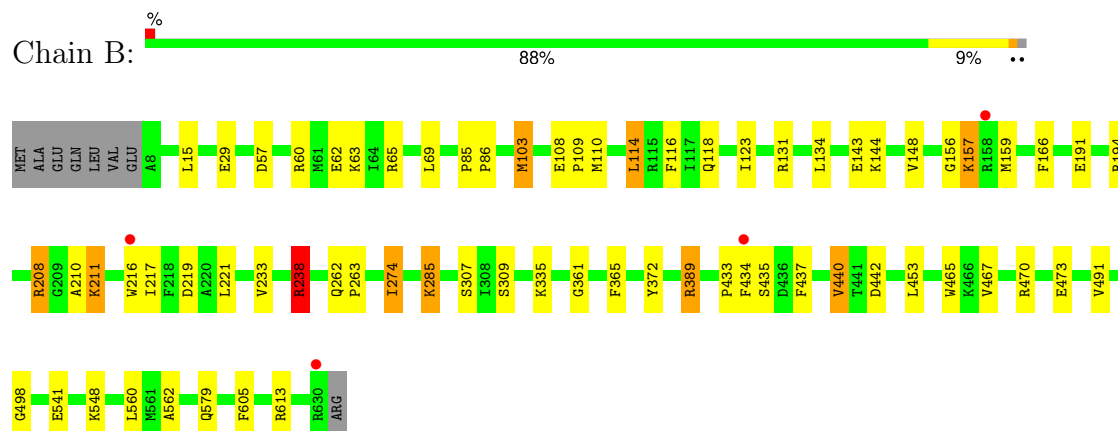
3 Residue-property plots [i](#)

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



• Molecule 1: SQUALENE-HOPENE CYCLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	118.82Å 118.82Å 276.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	90.0 (20.00-2.00) 89.9 (20.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.29 (at 2.00Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.153 , 0.187 0.157 , 0.188	Depositor DCC
R_{free} test set	6063 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	13.4	Xtrriage
Anisotropy	0.389	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 59.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11627	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.53 % 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 3.7662e-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: 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	0.67	0/5147	1.37	25/7007 (0.4%)
1	B	0.68	1/5147 (0.0%)	1.35	22/7007 (0.3%)
All	All	0.67	1/10294 (0.0%)	1.36	47/14014 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	372	TYR	CA-CB	6.11	1.60	1.53

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	440	VAL	N-CA-CB	-13.34	97.54	112.21
1	B	440	VAL	N-CA-CB	-13.20	97.69	112.21
1	A	491	VAL	O-C-N	-13.17	106.43	122.77
1	B	491	VAL	O-C-N	-12.62	107.12	122.77
1	B	440	VAL	CB-CA-C	11.27	124.92	110.84
1	A	440	VAL	CB-CA-C	11.19	124.83	110.84
1	A	365	PHE	CA-CB-CG	10.58	124.38	113.80
1	A	389	ARG	CD-NE-CZ	10.56	139.18	124.40
1	B	389	ARG	CD-NE-CZ	10.51	139.12	124.40
1	B	365	PHE	CA-CB-CG	9.55	123.35	113.80
1	A	62	GLU	CB-CG-CD	9.49	128.73	112.60
1	A	470	ARG	NE-CZ-NH1	9.28	130.78	121.50
1	A	238	ARG	CD-NE-CZ	8.49	136.29	124.40
1	B	238	ARG	CD-NE-CZ	8.44	136.21	124.40
1	B	442	ASP	CA-CB-CG	7.80	120.40	112.60
1	B	62	GLU	CB-CG-CD	7.37	125.13	112.60
1	A	442	ASP	CA-CB-CG	7.07	119.67	112.60
1	A	60	ARG	CD-NE-CZ	7.01	134.22	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	433	PRO	CA-C-O	6.91	130.05	119.55
1	B	579	GLN	OE1-CD-NE2	-6.81	115.79	122.60
1	A	394	ARG	CD-NE-CZ	6.35	133.29	124.40
1	A	434	PHE	CA-CB-CG	-6.25	107.55	113.80
1	B	60	ARG	CD-NE-CZ	5.97	132.75	124.40
1	B	470	ARG	NE-CZ-NH1	5.96	127.46	121.50
1	A	262	GLN	OE1-CD-NE2	-5.93	116.67	122.60
1	A	464	ALA	N-CA-C	-5.91	104.96	111.82
1	A	208	ARG	CA-C-N	-5.85	116.28	122.30
1	A	208	ARG	C-N-CA	-5.85	116.28	122.30
1	B	57	ASP	CA-CB-CG	-5.82	106.78	112.60
1	B	309	SER	N-CA-C	5.71	122.44	109.81
1	A	309	SER	N-CA-C	5.68	122.36	109.81
1	A	148	VAL	N-CA-C	-5.57	102.63	108.15
1	B	434	PHE	CA-CB-CG	-5.56	108.24	113.80
1	A	57	ASP	CA-CB-CG	-5.40	107.20	112.60
1	B	166	PHE	CA-C-O	-5.37	115.29	121.47
1	B	85	PRO	O-C-N	5.34	123.66	121.15
1	B	262	GLN	OE1-CD-NE2	-5.31	117.29	122.60
1	A	208	ARG	CA-C-O	-5.30	114.64	120.69
1	B	440	VAL	N-CA-C	-5.24	107.72	113.43
1	A	307	SER	CA-C-O	-5.21	115.73	121.31
1	A	526	HIS	CA-CB-CG	-5.20	108.60	113.80
1	B	148	VAL	N-CA-C	-5.20	103.00	108.15
1	A	274	ILE	CA-CB-CG2	5.18	119.30	110.50
1	A	470	ARG	NE-CZ-NH2	-5.17	114.55	119.20
1	A	435	SER	N-CA-C	5.08	117.74	110.68
1	B	274	ILE	CA-CB-CG2	5.00	119.00	110.50
1	B	307	SER	CA-C-O	-5.00	115.96	121.31

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	4993	0	4819	48	0
1	B	4993	0	4819	45	0
2	A	42	0	68	6	0
2	B	84	0	136	9	0
3	A	730	0	0	22	1
3	B	785	0	0	19	1
All	All	11627	0	9842	94	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (94) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:GLY:H	1:A:159:MET:HE3	1.36	0.91
1:B:156:GLY:H	1:B:159:MET:HE3	1.40	0.86
1:A:285:LYS:HE2	1:B:285:LYS:HE2	1.57	0.84
1:A:103:MET:HE2	1:A:110:MET:HG2	1.63	0.79
1:B:103:MET:HE2	1:B:110:MET:HG2	1.67	0.77
1:A:435:SER:HB2	3:A:979:HOH:O	1.97	0.65
1:B:435:SER:HB2	3:B:889:HOH:O	1.96	0.64
1:A:131:ARG:NH2	3:A:738:HOH:O	2.33	0.60
1:B:29:GLU:HG3	3:B:1408:HOH:O	2.03	0.59
1:A:156:GLY:N	1:A:159:MET:HE3	2.13	0.58
1:B:156:GLY:N	1:B:159:MET:HE3	2.15	0.58
2:A:632:C8E:H161	3:A:822:HOH:O	2.04	0.57
1:A:437:PHE:HE1	2:A:632:C8E:H11	1.69	0.57
2:B:632:C8E:H172	3:B:1216:HOH:O	2.05	0.56
1:B:389:ARG:HG2	3:B:1229:HOH:O	2.05	0.56
1:A:154:PHE:HB3	2:A:633:C8E:H62	1.88	0.55
1:B:498:GLY:HA2	1:B:562:ALA:HB2	1.88	0.55
1:A:498:GLY:HA2	1:A:562:ALA:HB2	1.87	0.55
1:B:65:ARG:NH1	3:B:1419:HOH:O	2.23	0.55
1:B:157:LYS:HG2	3:B:786:HOH:O	2.07	0.55
1:B:263:PRO:CG	2:B:633:C8E:H31	2.37	0.54
2:B:633:C8E:H161	3:B:832:HOH:O	2.08	0.54
1:A:605:PHE:CE2	2:A:632:C8E:H41	2.44	0.53
1:A:376:CYS:HG	2:A:632:C8E:HO2	1.57	0.52
1:A:354:LYS:HD3	3:A:959:HOH:O	2.09	0.52
1:B:144:LYS:HD3	3:B:1319:HOH:O	2.09	0.52
1:A:114:LEU:HD22	1:A:118:GLN:HG3	1.92	0.51
1:A:123:ILE:HD13	1:A:134:LEU:CD1	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:437:PHE:HE1	2:B:633:C8E:H11	1.76	0.51
1:B:605:PHE:CE2	2:B:633:C8E:H41	2.45	0.51
1:B:114:LEU:HD22	1:B:118:GLN:HG3	1.93	0.50
1:A:103:MET:HG2	3:A:1336:HOH:O	2.11	0.50
1:A:65:ARG:NH1	3:A:1328:HOH:O	2.40	0.50
1:A:285:LYS:CE	1:B:285:LYS:HE2	2.37	0.50
1:A:157:LYS:HG2	3:A:809:HOH:O	2.10	0.50
1:B:123:ILE:HD13	1:B:134:LEU:CD1	2.42	0.50
1:B:473:GLU:HG3	3:B:1412:HOH:O	2.10	0.50
1:A:191:GLU:HG3	1:A:194:ARG:NH1	2.27	0.50
1:B:191:GLU:HG3	1:B:194:ARG:NH1	2.27	0.48
1:B:238:ARG:HH11	1:B:238:ARG:HG3	1.78	0.48
1:A:123:ILE:HD13	1:A:134:LEU:HD12	1.95	0.48
1:A:29:GLU:HG3	3:A:1344:HOH:O	2.13	0.47
1:B:335:LYS:HE2	3:B:1028:HOH:O	2.13	0.47
1:B:435:SER:HA	3:B:785:HOH:O	2.13	0.47
1:A:144:LYS:HD3	3:A:1356:HOH:O	2.15	0.47
1:A:263:PRO:CG	2:A:632:C8E:H31	2.44	0.47
1:B:238:ARG:HG3	2:B:632:C8E:H42	1.96	0.47
1:A:575:ARG:NH1	3:A:917:HOH:O	2.47	0.47
1:B:123:ILE:HD13	1:B:134:LEU:HD12	1.97	0.47
1:A:369:ASN:HB2	3:A:955:HOH:O	2.15	0.47
1:B:103:MET:HE2	1:B:110:MET:CG	2.40	0.47
1:A:211:LYS:HD3	1:A:438:GLY:O	2.14	0.46
1:B:548:LYS:NZ	3:B:1281:HOH:O	2.44	0.46
1:B:217:ILE:HG22	3:B:1355:HOH:O	2.15	0.46
1:B:221:LEU:HD23	3:B:1332:HOH:O	2.16	0.46
1:A:238:ARG:HG3	1:A:238:ARG:HH11	1.80	0.46
1:B:131:ARG:NH2	3:B:796:HOH:O	2.49	0.46
1:B:156:GLY:H	1:B:159:MET:CE	2.21	0.45
1:B:143:GLU:H	1:B:143:GLU:CD	2.25	0.45
1:A:76:GLY:HA3	1:A:112:LYS:HB3	1.98	0.45
1:A:123:ILE:CD1	1:A:134:LEU:HD12	2.47	0.45
1:B:63:LYS:NZ	3:B:761:HOH:O	2.49	0.45
1:B:211:LYS:HG3	3:B:927:HOH:O	2.18	0.44
1:B:263:PRO:HG2	2:B:633:C8E:H31	2.00	0.44
1:B:108:GLU:HB3	1:B:109:PRO:HD3	2.00	0.44
1:A:62:GLU:HB2	3:A:1350:HOH:O	2.18	0.43
1:A:285:LYS:HE2	1:B:285:LYS:CE	2.38	0.43
1:B:238:ARG:CZ	2:B:632:C8E:H61	2.48	0.43
1:A:534:GLY:HA3	1:A:550:ALA:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ASP:HB3	3:A:1243:HOH:O	2.18	0.42
1:A:359:LYS:HA	1:A:360:PRO:HD3	1.91	0.42
1:B:86:PRO:HB2	1:B:116:PHE:CZ	2.53	0.42
1:B:157:LYS:HG2	1:B:157:LYS:H	1.57	0.42
1:A:143:GLU:H	1:A:143:GLU:CD	2.27	0.42
1:A:411:GLN:OE1	1:A:470:ARG:NH2	2.52	0.42
2:B:634:C8E:O21	2:B:634:C8E:H51	2.19	0.42
1:A:108:GLU:HB3	1:A:109:PRO:HD3	2.00	0.42
1:A:62:GLU:HG2	3:A:1192:HOH:O	2.20	0.42
1:A:434:PHE:HE2	3:A:1292:HOH:O	2.03	0.42
1:B:613:ARG:NH2	3:B:1400:HOH:O	2.45	0.42
1:B:123:ILE:CD1	1:B:134:LEU:HD12	2.50	0.42
1:A:103:MET:HE2	1:A:110:MET:CG	2.40	0.41
1:A:214:GLY:HA3	3:A:1294:HOH:O	2.20	0.41
1:B:208:ARG:HE	1:B:208:ARG:HB2	1.72	0.41
1:B:465:TRP:CE2	1:B:467:VAL:HB	2.55	0.41
1:A:86:PRO:HB2	1:A:116:PHE:CZ	2.55	0.41
1:A:279:GLN:NE2	3:A:1035:HOH:O	2.53	0.41
1:A:172:ALA:HB3	3:A:796:HOH:O	2.21	0.41
1:B:210:ALA:HB1	3:B:889:HOH:O	2.20	0.41
1:B:285:LYS:HD3	1:B:285:LYS:HA	1.81	0.40
1:A:70:HIS:HE1	3:A:1311:HOH:O	2.03	0.40
1:A:434:PHE:HB2	3:A:968:HOH:O	2.21	0.40
1:A:20:GLU:HG2	3:A:1361:HOH:O	2.21	0.40
1:A:285:LYS:HG3	3:A:898:HOH:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1311:HOH:O	3:B:1417:HOH:O[8_665]	2.15	0.05

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	621/631 (98%)	606 (98%)	14 (2%)	1 (0%)	43	42
1	B	621/631 (98%)	607 (98%)	13 (2%)	1 (0%)	43	42
All	All	1242/1262 (98%)	1213 (98%)	27 (2%)	2 (0%)	43	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	361	GLY
1	B	361	GLY

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	506/513 (99%)	490 (97%)	16 (3%)	34	35
1	B	506/513 (99%)	489 (97%)	17 (3%)	32	33
All	All	1012/1026 (99%)	979 (97%)	33 (3%)	33	34

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	69	LEU
1	A	103	MET
1	A	114	LEU
1	A	157	LYS
1	A	211	LYS
1	A	216	TRP
1	A	219	ASP
1	A	233	VAL
1	A	238	ARG
1	A	274	ILE

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Mol	Chain	Res	Type
1	A	285	LYS
1	A	440	VAL
1	A	453	LEU
1	A	541	GLU
1	A	560	LEU
1	B	15	LEU
1	B	69	LEU
1	B	103	MET
1	B	114	LEU
1	B	157	LYS
1	B	208	ARG
1	B	211	LYS
1	B	216	TRP
1	B	219	ASP
1	B	233	VAL
1	B	238	ARG
1	B	274	ILE
1	B	285	LYS
1	B	440	VAL
1	B	453	LEU
1	B	541	GLU
1	B	560	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	GLN
1	A	279	GLN
1	A	357	ASN
1	A	369	ASN
1	A	451	HIS
1	B	369	ASN
1	B	451	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
2	C8E	A	633	-	20,20,20	0.86	0	19,19,19	2.32	8 (42%)
2	C8E	B	634	-	20,20,20	0.81	0	19,19,19	2.15	5 (26%)
2	C8E	A	632	-	20,20,20	0.91	0	19,19,19	2.20	5 (26%)
2	C8E	B	635	-	20,20,20	0.83	0	19,19,19	2.14	7 (36%)
2	C8E	B	632	-	20,20,20	0.86	0	19,19,19	1.80	6 (31%)
2	C8E	B	633	-	20,20,20	0.94	0	19,19,19	2.27	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
2	C8E	A	633	-	-	13/18/18/18	-
2	C8E	B	634	-	-	11/18/18/18	-
2	C8E	A	632	-	-	14/18/18/18	-
2	C8E	B	635	-	-	13/18/18/18	-
2	C8E	B	632	-	-	12/18/18/18	-
2	C8E	B	633	-	-	13/18/18/18	-

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	633	C8E	O18-C17-C16	6.09	138.13	110.35
2	B	633	C8E	O15-C14-C13	5.78	136.68	110.35
2	A	632	C8E	O15-C14-C13	5.73	136.46	110.35
2	B	634	C8E	O18-C19-C20	4.81	131.30	110.11
2	B	633	C8E	O15-C16-C17	4.69	131.74	110.35
2	B	632	C8E	O15-C14-C13	4.58	131.22	110.35
2	B	635	C8E	O18-C17-C16	4.57	131.16	110.35
2	B	634	C8E	O15-C14-C13	4.07	128.89	110.35
2	B	635	C8E	O18-C19-C20	4.03	127.89	110.11
2	A	632	C8E	O15-C16-C17	3.96	128.41	110.35
2	B	635	C8E	O15-C14-C13	3.96	128.38	110.35
2	A	633	C8E	O15-C14-C13	3.84	127.87	110.35
2	B	634	C8E	O15-C16-C17	3.80	127.67	110.35
2	B	633	C8E	O18-C19-C20	3.53	125.67	110.11
2	A	632	C8E	O18-C19-C20	3.39	125.06	110.11
2	B	633	C8E	O18-C17-C16	3.24	125.12	110.35
2	A	633	C8E	C5-C4-C3	-3.03	99.03	114.37
2	B	634	C8E	C16-O15-C14	-3.01	100.07	113.26
2	B	634	C8E	C7-C6-C5	-2.99	99.25	114.37
2	B	632	C8E	O15-C16-C17	2.91	123.61	110.35
2	A	633	C8E	C7-C6-C5	-2.89	99.75	114.37
2	A	632	C8E	O18-C17-C16	2.85	123.34	110.35
2	B	635	C8E	C5-C4-C3	-2.82	100.12	114.37
2	A	633	C8E	O9-C8-C7	2.78	124.91	110.32
2	B	632	C8E	O18-C19-C20	2.75	122.21	110.11
2	A	632	C8E	C7-C6-C5	-2.71	100.67	114.37
2	B	632	C8E	C19-O18-C17	-2.65	101.67	113.26
2	A	633	C8E	O15-C16-C17	2.54	121.93	110.35
2	B	633	C8E	C7-C6-C5	-2.49	101.78	114.37
2	B	635	C8E	O12-C13-C14	2.40	121.29	110.35
2	A	633	C8E	C10-O9-C8	2.39	123.70	113.26
2	A	633	C8E	O18-C19-C20	2.37	120.54	110.11
2	B	635	C8E	C7-C6-C5	-2.33	102.59	114.37
2	B	635	C8E	O9-C8-C7	2.17	121.72	110.32
2	B	632	C8E	C7-C6-C5	-2.14	103.53	114.37
2	B	632	C8E	C16-O15-C14	-2.10	104.07	113.26

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	633	C8E	C16-C17-O18-C19
2	B	633	C8E	C17-C16-O15-C14
2	A	632	C8E	C17-C16-O15-C14
2	A	632	C8E	O15-C16-C17-O18
2	B	633	C8E	O15-C16-C17-O18
2	A	633	C8E	C7-C8-O9-C10
2	A	633	C8E	O15-C16-C17-O18
2	A	633	C8E	O12-C13-C14-O15
2	A	633	C8E	C6-C7-C8-O9
2	B	635	C8E	C6-C7-C8-O9
2	B	632	C8E	O15-C16-C17-O18
2	B	634	C8E	O15-C16-C17-O18
2	B	635	C8E	O12-C13-C14-O15
2	A	632	C8E	O18-C19-C20-O21
2	B	635	C8E	C5-C6-C7-C8
2	B	634	C8E	C3-C4-C5-C6
2	B	632	C8E	C2-C3-C4-C5
2	B	632	C8E	C3-C4-C5-C6
2	B	632	C8E	C5-C6-C7-C8
2	B	634	C8E	C2-C3-C4-C5
2	B	633	C8E	C3-C4-C5-C6
2	A	632	C8E	O12-C13-C14-O15
2	A	632	C8E	C3-C4-C5-C6
2	A	633	C8E	C3-C4-C5-C6
2	B	635	C8E	C7-C8-O9-C10
2	B	632	C8E	C4-C5-C6-C7
2	A	633	C8E	C4-C5-C6-C7
2	B	633	C8E	C2-C3-C4-C5
2	A	632	C8E	C2-C3-C4-C5
2	B	633	C8E	C6-C7-C8-O9
2	A	632	C8E	C4-C5-C6-C7
2	B	633	C8E	C4-C5-C6-C7
2	B	635	C8E	O18-C19-C20-O21
2	B	633	C8E	O9-C10-C11-O12
2	B	632	C8E	C6-C7-C8-O9
2	B	635	C8E	C4-C5-C6-C7
2	B	635	C8E	C3-C4-C5-C6
2	B	633	C8E	O12-C13-C14-O15
2	A	632	C8E	O9-C10-C11-O12
2	A	632	C8E	C1-C2-C3-C4
2	B	635	C8E	C20-C19-O18-C17
2	B	634	C8E	C10-C11-O12-C13
2	A	632	C8E	C6-C7-C8-O9

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Mol	Chain	Res	Type	Atoms
2	A	633	C8E	C13-C14-O15-C16
2	B	633	C8E	C20-C19-O18-C17
2	B	634	C8E	C1-C2-C3-C4
2	B	633	C8E	O18-C19-C20-O21
2	A	632	C8E	C20-C19-O18-C17
2	B	635	C8E	C16-C17-O18-C19
2	B	634	C8E	C5-C6-C7-C8
2	A	633	C8E	C11-C10-O9-C8
2	B	634	C8E	C20-C19-O18-C17
2	B	634	C8E	C17-C16-O15-C14
2	B	634	C8E	C4-C5-C6-C7
2	B	635	C8E	C2-C3-C4-C5
2	A	632	C8E	C14-C13-O12-C11
2	B	635	C8E	C13-C14-O15-C16
2	B	633	C8E	C11-C10-O9-C8
2	A	633	C8E	C10-C11-O12-C13
2	B	632	C8E	C13-C14-O15-C16
2	B	632	C8E	C20-C19-O18-C17
2	A	632	C8E	C11-C10-O9-C8
2	B	633	C8E	C1-C2-C3-C4
2	B	634	C8E	C6-C7-C8-O9
2	B	632	C8E	C1-C2-C3-C4
2	A	633	C8E	O9-C10-C11-O12
2	B	635	C8E	C1-C2-C3-C4
2	B	635	C8E	O15-C16-C17-O18
2	B	634	C8E	C13-C14-O15-C16
2	A	633	C8E	C2-C3-C4-C5
2	B	632	C8E	C10-C11-O12-C13
2	A	633	C8E	C14-C13-O12-C11
2	B	632	C8E	C17-C16-O15-C14
2	B	632	C8E	O12-C13-C14-O15
2	B	633	C8E	C5-C6-C7-C8
2	A	632	C8E	C13-C14-O15-C16

There are no ring outliers.

5 monomers are involved in 15 short contacts:

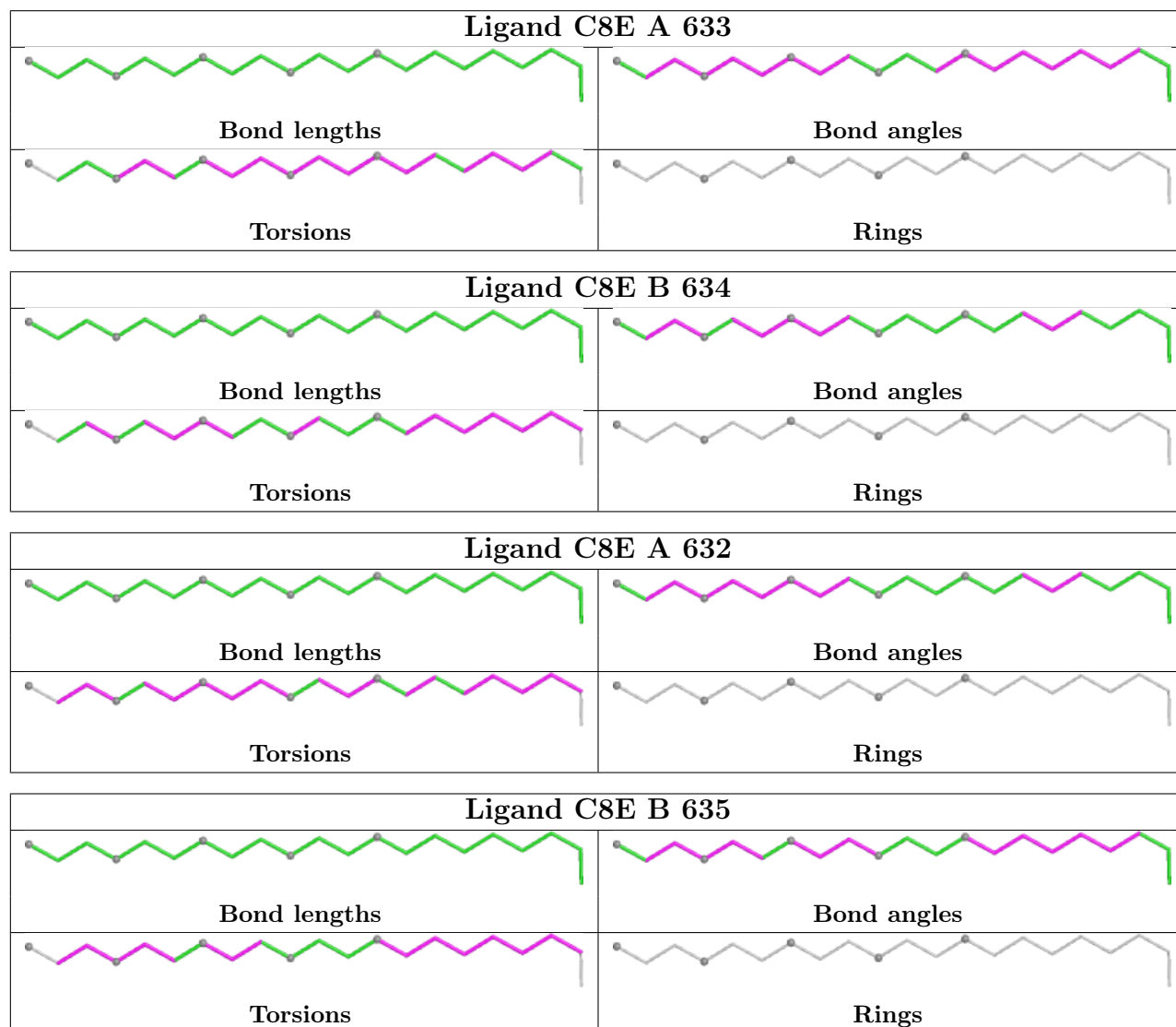
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	633	C8E	1	0
2	B	634	C8E	1	0
2	A	632	C8E	5	0
2	B	632	C8E	3	0

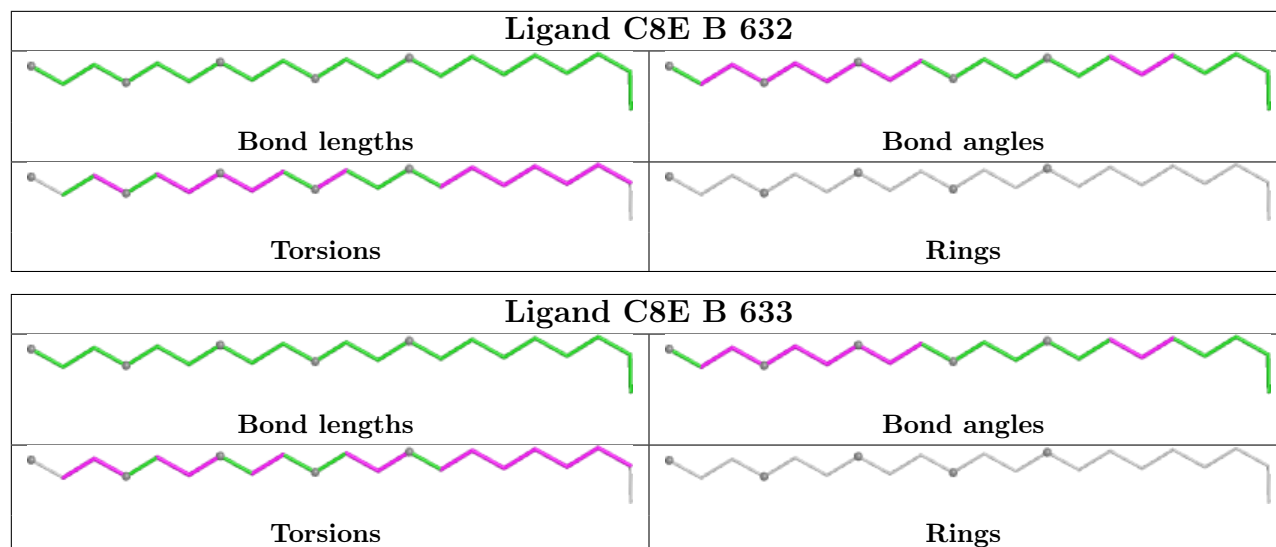
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	633	C8E	5	0

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 [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	623/631 (98%)	-0.81	3 (0%) 87 87	6, 13, 32, 60	0
1	B	623/631 (98%)	-0.74	4 (0%) 85 85	6, 13, 32, 59	0
All	All	1246/1262 (98%)	-0.78	7 (0%) 85 85	6, 13, 32, 60	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	216	TRP	3.7
1	B	630	ARG	3.5
1	A	630	ARG	3.4
1	A	216	TRP	3.1
1	A	206	ARG	2.3
1	B	434	PHE	2.1
1	B	158	ARG	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

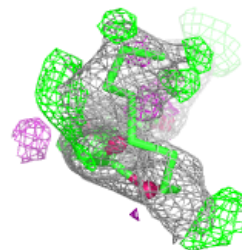
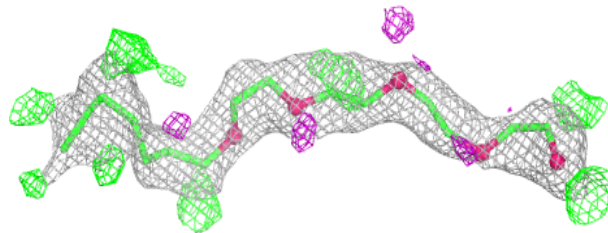
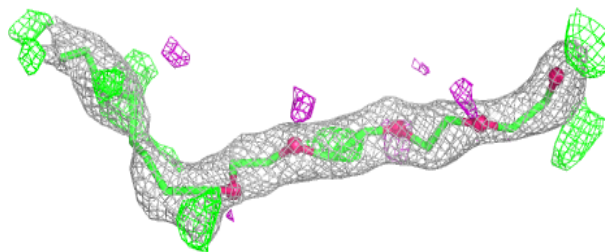
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	C8E	B	635	21/21	0.73	0.20	46,50,56,57	0
2	C8E	A	633	21/21	0.74	0.20	50,54,64,64	0
2	C8E	A	632	21/21	0.83	0.15	24,34,43,44	0
2	C8E	B	633	21/21	0.84	0.15	29,34,44,44	0
2	C8E	B	634	21/21	0.90	0.14	24,33,40,41	0
2	C8E	B	632	21/21	0.90	0.13	20,33,41,41	0

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

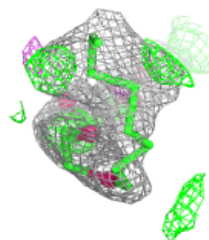
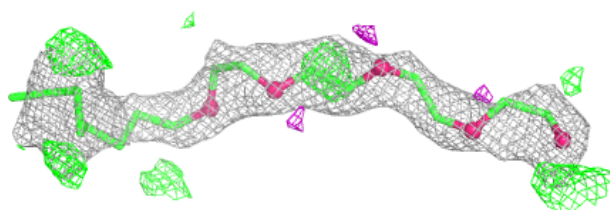
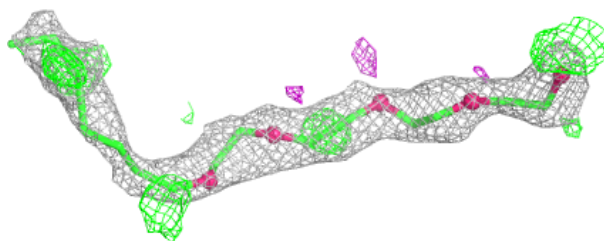
Electron density around C8E B 635:

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

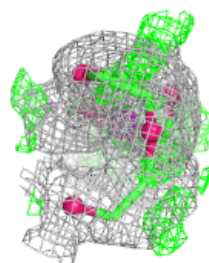
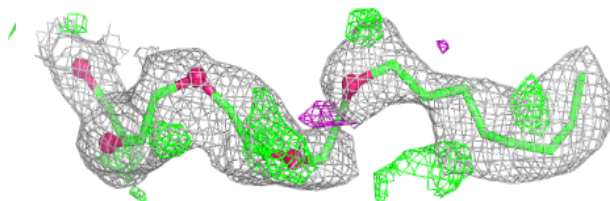
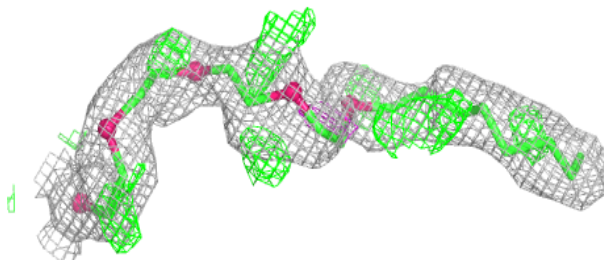


Electron density around C8E A 633:

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

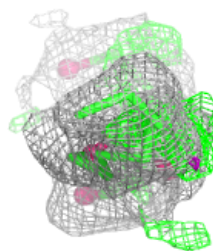
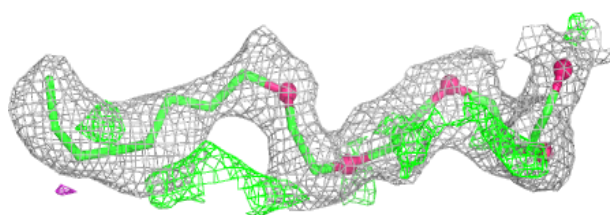
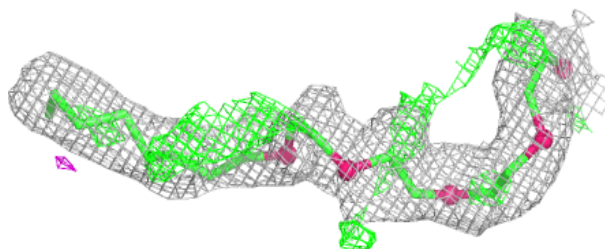
**Electron density around C8E A 632:**

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



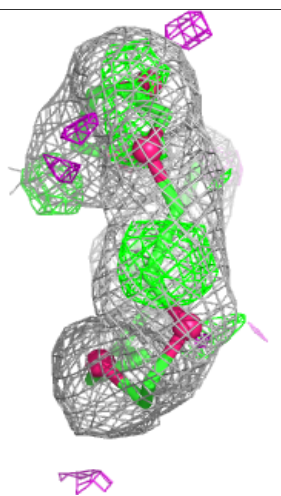
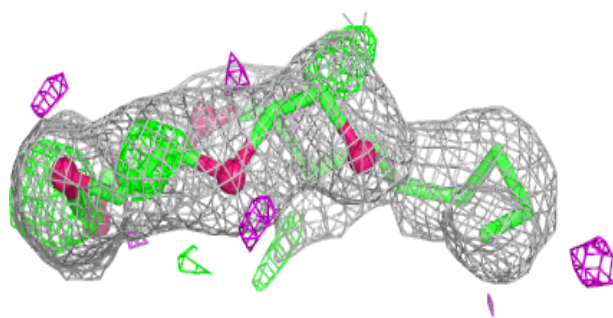
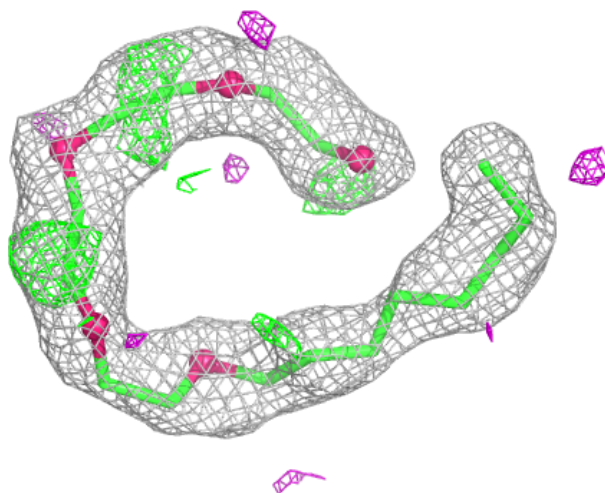
Electron density around C8E B 633:

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



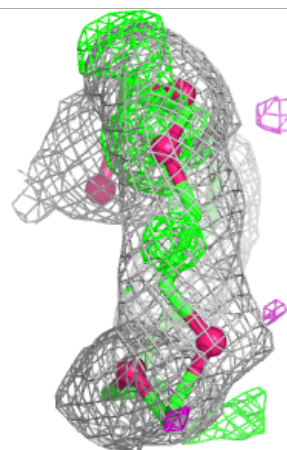
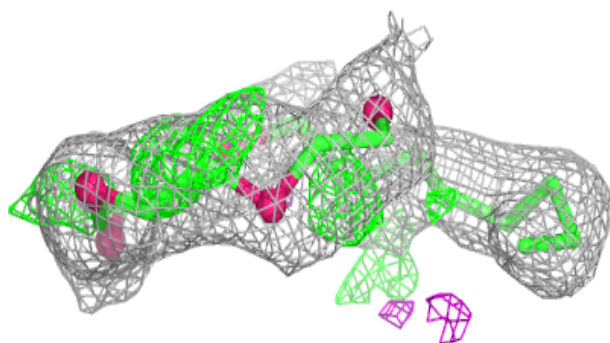
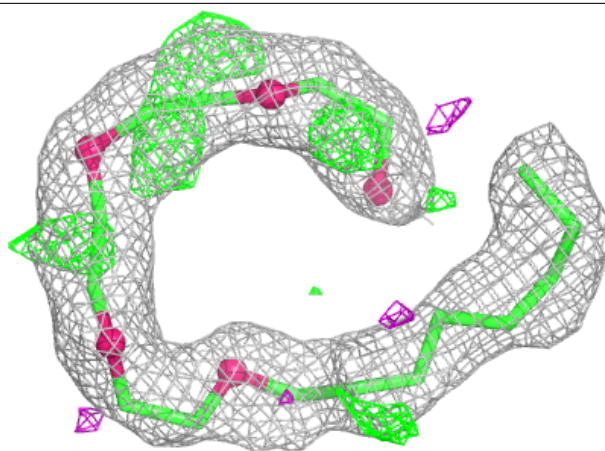
Electron density around C8E B 634:

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



Electron density around C8E B 632:

$2mF_o-DF_c$ (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.