wwPDB X-ray Structure Validation Summary Report (i)

Apr 28, 2024 – 05:01 am BST

PDB ID	:	1W96
Title	:	Crystal Structure of Biotin Carboxylase Domain of Acetyl-coenzyme A Carboxylase from Saccharomyces cerevisiae in Complex with Soraphen A
Authors	:	Shen, Y.; Volrath, S.L.; Weatherly, S.C.; Elich, T.D.; Tong, L.
Deposited on	:	2004-10-06
Resolution	:	1.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

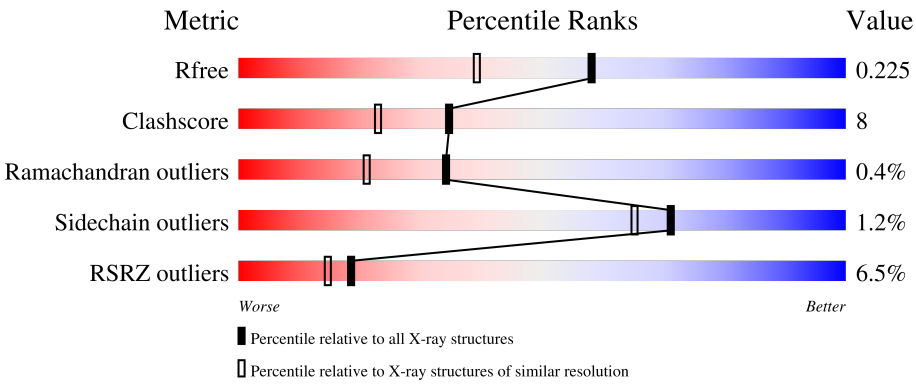
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	554	6% 81% 17% ••
1	B	554	6% 84% 13% ••
1	C	554	7% 80% 16% ••

2 Entry composition (i)

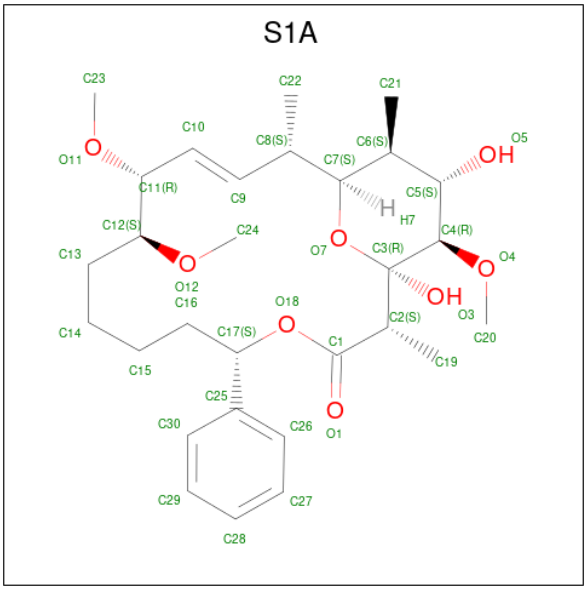
There are 3 unique types of molecules in this entry. The entry contains 14282 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACETYL-COENZYME A CARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	549	4290	2697	751	824	18	0	0	0
1	B	542	4249	2674	746	811	18	0	0	0
1	C	537	4187	2632	740	797	18	0	0	1

- Molecule 2 is SORAPHEN A (three-letter code: S1A) (formula: $C_{29}H_{44}O_8$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	37	29	8	0	0
2	B	1	37	29	8	0	0
2	C	1	37	29	8	0	0

- Molecule 3 is water.

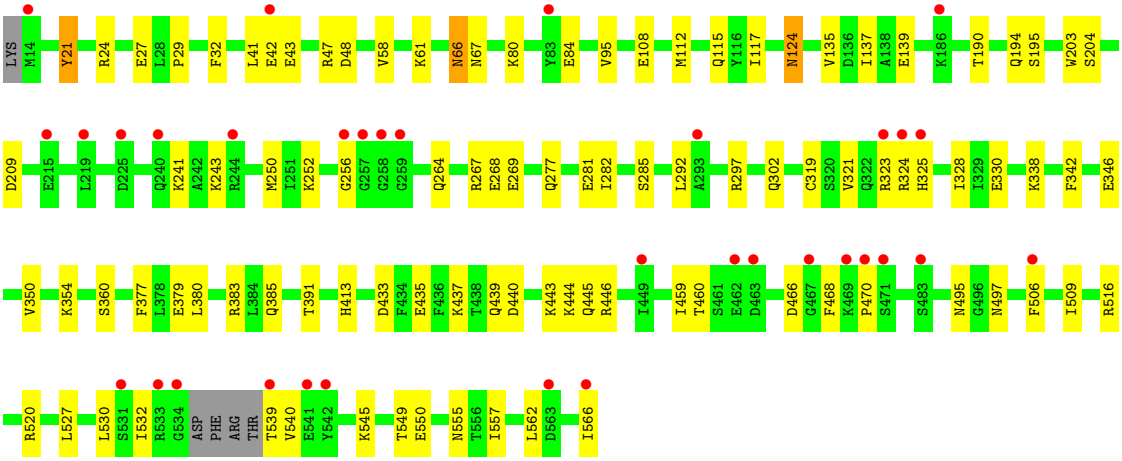
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	454	454	454	0	0
			Total	O		
3	B	510	510	510	0	0
			Total	O		
3	C	481	481	481	0	0

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.

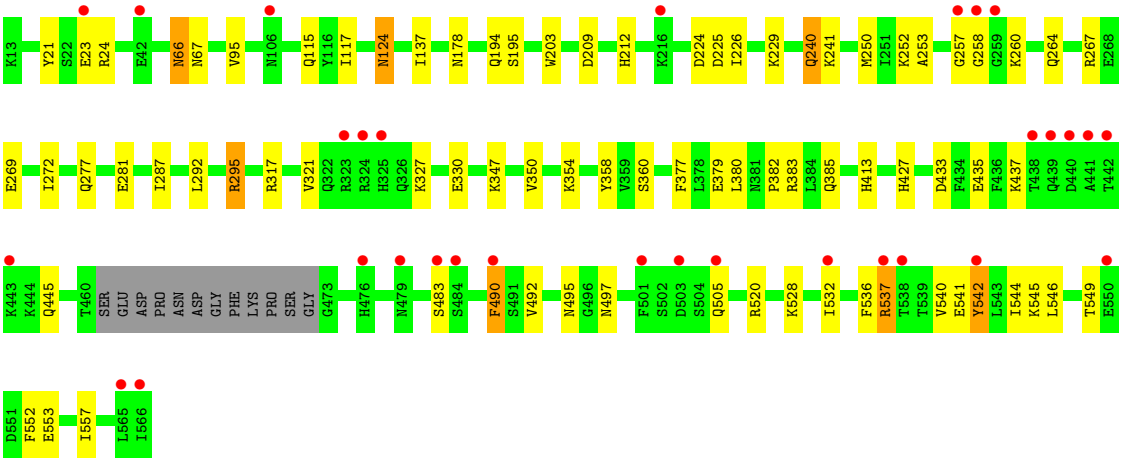
• Molecule 1: ACETYL-COENZYME A CARBOXYLASE

Chain A:



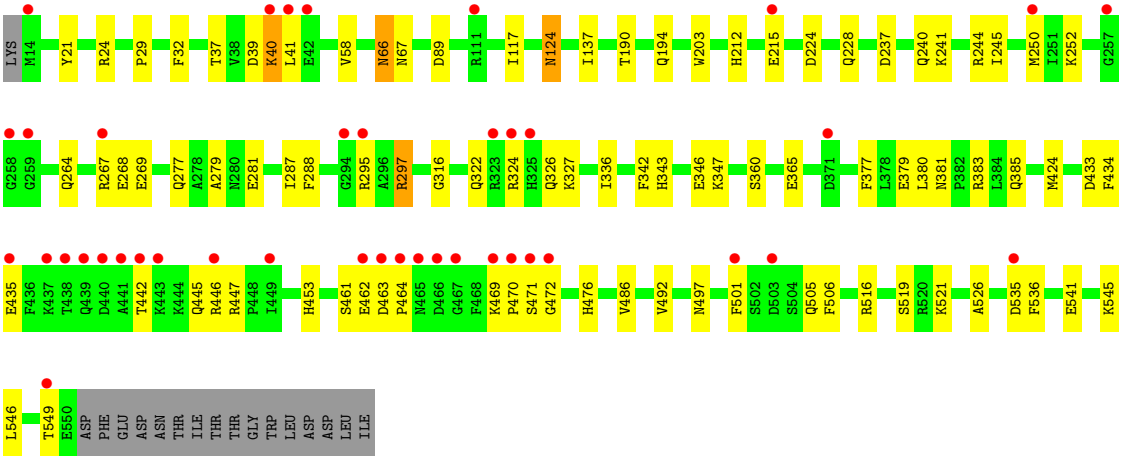
• Molecule 1: ACETYL-COENZYME A CARBOXYLASE

Chain B:



• Molecule 1: ACETYL-COENZYME A CARBOXYLASE

Chain C:


LYS M14 Y21 R24 P29 F32 T37 V38 D39 K40 L41 E42 V58 N66 N67 D89 R111 I117 N124 I137 T190 Q194 W203 H212 E215 D224 Q228 D237 Q240 K241 R244 I245 M250 I251 K252 G257
G258 G259 Q264 R267 E268 E269 Q277 A278 A279 N280 E281 I287 F288 G294 R295 A296 R297 G316 Q322 R323 R324 H325 Q326 K327 I336 F342 H343 E346 K347 S360 E365 D371 F377 L378 E379 L380 N381 P382 R383 L384 Q385 M424 D433 F434
E435 F436 K437 T438 Q439 D440 A441 T442 K443 K444 Q445 R446 R447 P448 I449 H453 S461 E462 D463 P464 N465 D466 G467 F468 K469 P470 S471 G472 H476 V486 V492 N497 F501 S502 D503 S504 Q505 F506 R516 S519 R520 K521 A526 D535 F536 E541 K545
L546 T549 E550 ASP PHE GLU ASP ASN THR ILE THR THR GLY TRP LEU ASP ASP LEU ILE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.83Å 96.52Å 139.95Å 90.00° 96.82° 90.00°	Depositor
Resolution (Å)	29.20 – 1.80 29.20 – 1.79	Depositor EDS
% Data completeness (in resolution range)	96.3 (29.20-1.80) 95.8 (29.20-1.79)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 1.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.195 , 0.230 0.190 , 0.225	Depositor DCC
R_{free} test set	11694 reflections (7.49%)	wwPDB-VP
Wilson B-factor (Å^2)	19.2	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 55.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14282	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: S1A

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	0.30	0/4381	0.56	0/5927
1	B	0.32	0/4338	0.56	0/5867
1	C	0.31	0/4277	0.56	0/5786
All	All	0.31	0/12996	0.56	0/17580

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	4290	0	4199	74	0
1	B	4249	0	4173	63	0
1	C	4187	0	4112	78	0
2	A	37	0	44	0	0
2	B	37	0	44	0	0
2	C	37	0	44	0	0
3	A	454	0	0	9	0
3	B	510	0	0	12	0
3	C	481	0	0	11	0
All	All	14282	0	12616	210	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.

The worst 5 of 210 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:C:66:ASN:HD22	1:C:67:ASN:H	1.18	0.91
1:A:433:ASP:H	1:A:445:GLN:HE22	1.14	0.90
1:B:66:ASN:HD22	1:B:67:ASN:H	1.16	0.88
1:A:66:ASN:HD22	1:A:67:ASN:H	1.17	0.87
1:B:433:ASP:H	1:B:445:GLN:HE22	1.23	0.86

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	545/554 (98%)	523 (96%)	21 (4%)	1 (0%)	47	33
1	B	538/554 (97%)	519 (96%)	16 (3%)	3 (1%)	25	12
1	C	535/554 (97%)	516 (96%)	17 (3%)	2 (0%)	34	21
All	All	1618/1662 (97%)	1558 (96%)	54 (3%)	6 (0%)	34	21

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	258	GLY
1	A	360	SER
1	B	360	SER
1	C	360	SER
1	C	434	PHE

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	462/467 (99%)	459 (99%)	3 (1%)	86	84
1	B	457/467 (98%)	450 (98%)	7 (2%)	65	56
1	C	450/467 (96%)	444 (99%)	6 (1%)	69	62
All	All	1369/1401 (98%)	1353 (99%)	16 (1%)	71	65

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	297	ARG
1	C	124	ASN
1	B	537	ARG
1	C	89	ASP
1	B	490	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	453	HIS
1	C	66	ASN
1	C	476	HIS
1	B	476	HIS
1	B	497	ASN

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 (i)

3 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	S1A	A	1567	-	39,39,39	1.02	3 (7%)	45,55,55	1.33	8 (17%)
2	S1A	C	1550	-	39,39,39	1.04	2 (5%)	45,55,55	1.34	9 (20%)
2	S1A	B	1567	-	39,39,39	1.09	4 (10%)	45,55,55	1.27	6 (13%)

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	S1A	A	1567	-	-	3/44/67/67	0/2/3/3
2	S1A	C	1550	-	-	5/44/67/67	0/2/3/3
2	S1A	B	1567	-	-	3/44/67/67	0/2/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1550	S1A	C10-C9	2.57	1.39	1.32
2	B	1567	S1A	C25-C17	2.55	1.55	1.51
2	A	1567	S1A	C10-C9	2.46	1.39	1.32
2	B	1567	S1A	C3-C4	2.45	1.57	1.53
2	B	1567	S1A	C5-C4	2.32	1.58	1.53

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1550	S1A	O18-C1-O1	-4.08	116.31	123.94
2	A	1567	S1A	O18-C1-O1	-3.99	116.49	123.94
2	B	1567	S1A	O18-C1-O1	-3.84	116.77	123.94
2	A	1567	S1A	C8-C7-C6	-3.07	110.51	115.55
2	C	1550	S1A	C8-C7-C6	-2.87	110.83	115.55

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

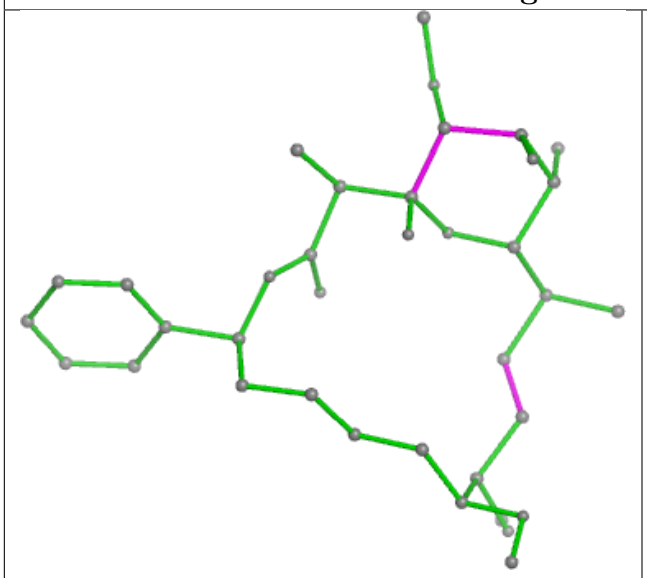
Mol	Chain	Res	Type	Atoms
2	C	1550	S1A	C10-C11-O11-C23
2	C	1550	S1A	C12-C11-O11-C23
2	A	1567	S1A	O1-C1-C2-C19
2	B	1567	S1A	O1-C1-C2-C19
2	C	1550	S1A	O1-C1-C2-C19

There are no ring outliers.

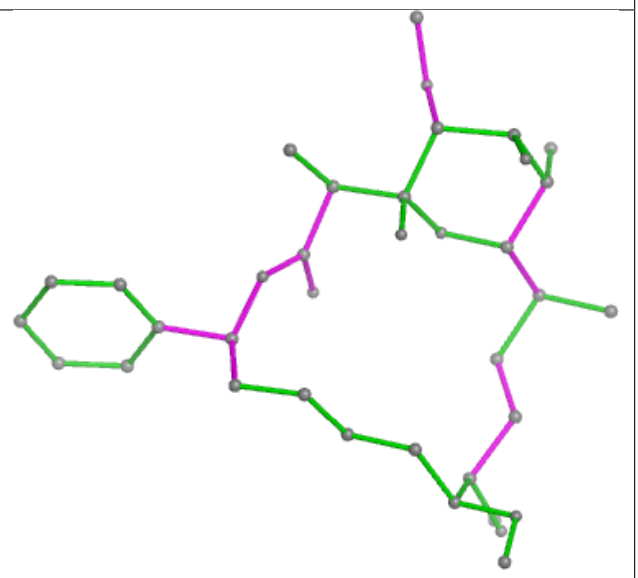
No monomer is involved in short contacts.

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 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.

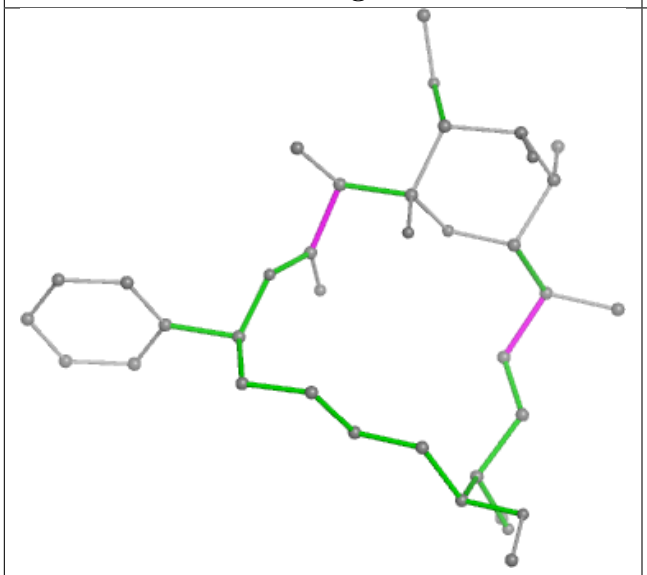
Ligand S1A A 1567



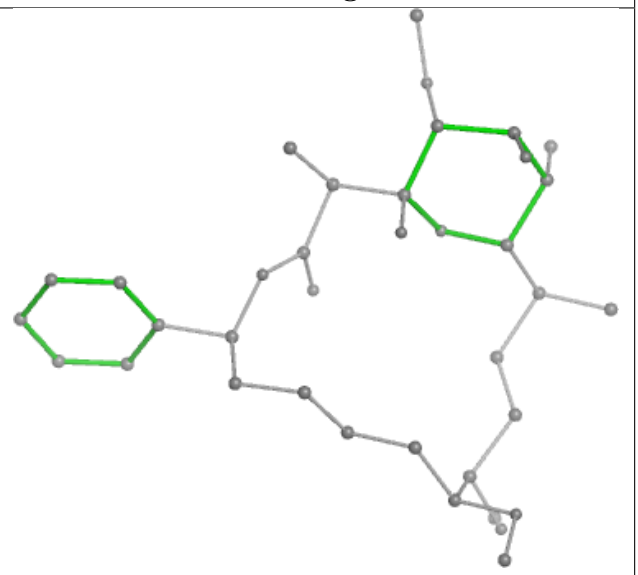
Bond lengths



Bond angles

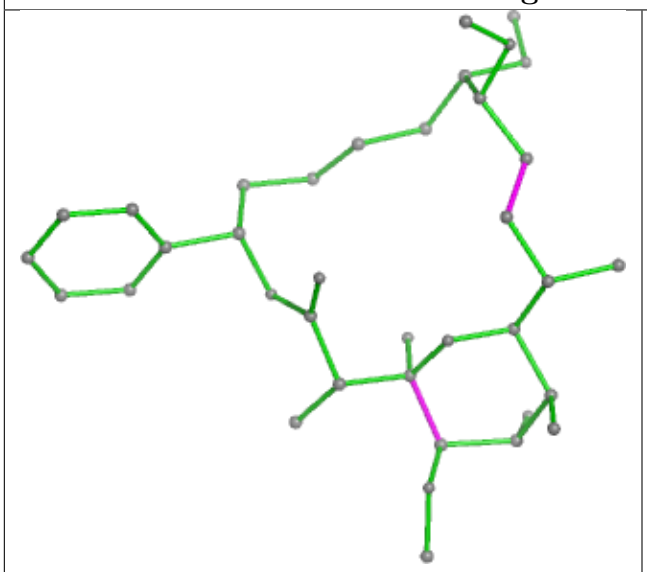


Torsions

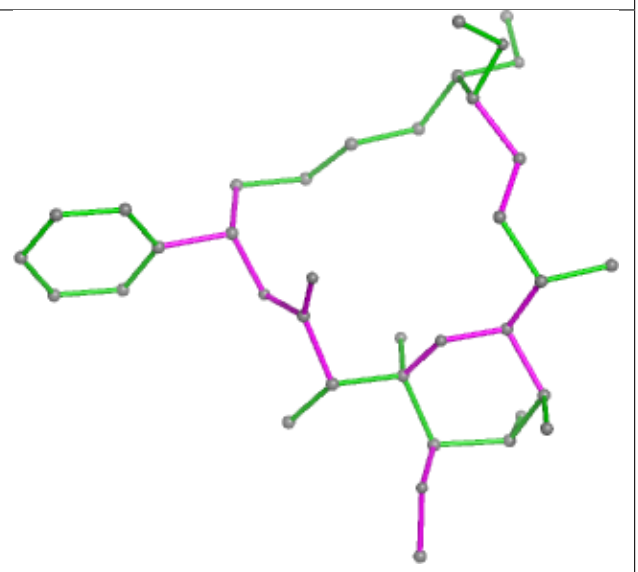


Rings

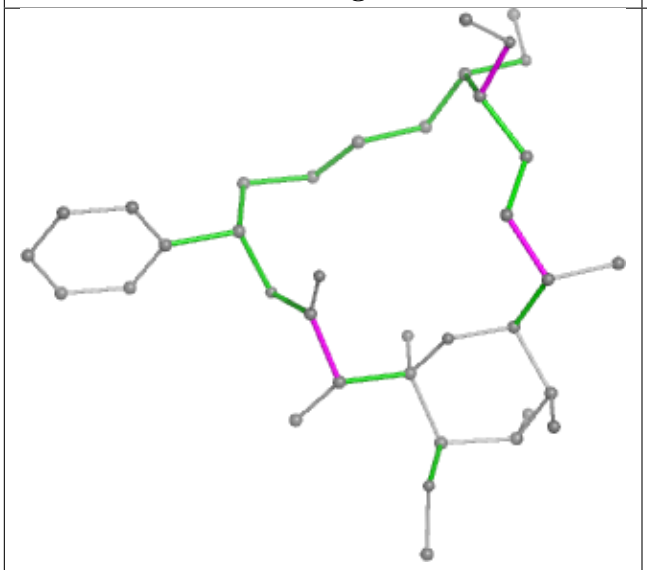
Ligand S1A C 1550



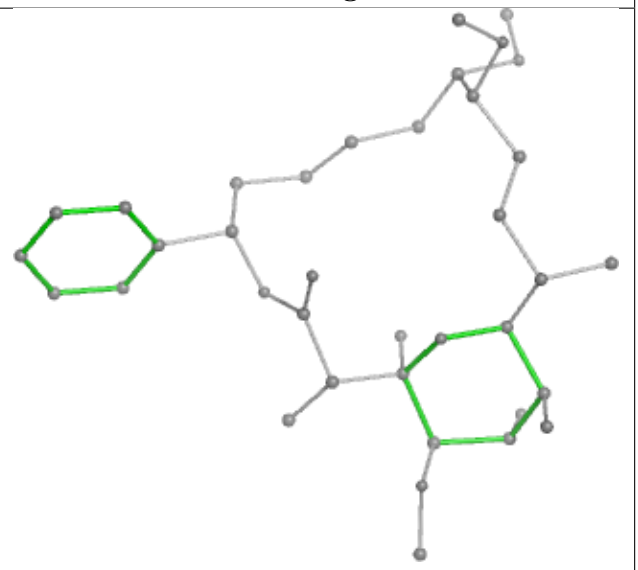
Bond lengths



Bond angles

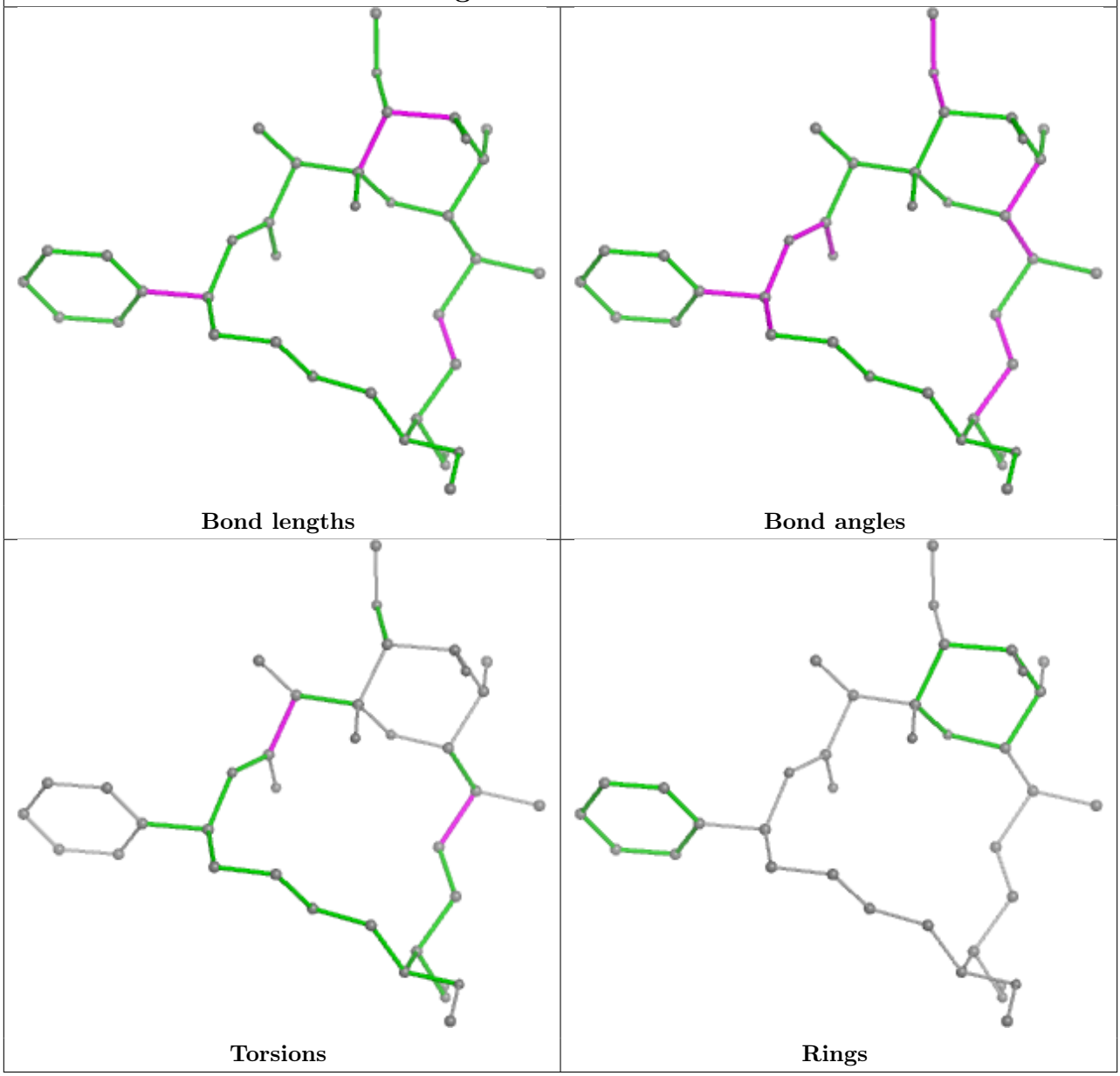


Torsions



Rings

Ligand S1A B 1567



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	549/554 (99%)	0.18	34 (6%)	20	16	10, 24, 47, 57	0
1	B	542/554 (97%)	0.19	31 (5%)	23	19	9, 21, 45, 55	0
1	C	537/554 (96%)	0.25	41 (7%)	13	10	12, 23, 48, 60	0
All	All	1628/1662 (97%)	0.21	106 (6%)	18	15	9, 23, 47, 60	0

The worst 5 of 106 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	325	HIS	7.9
1	B	257	GLY	7.7
1	B	566	ILE	7.3
1	C	258	GLY	6.9
1	C	323	ARG	6.1

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)

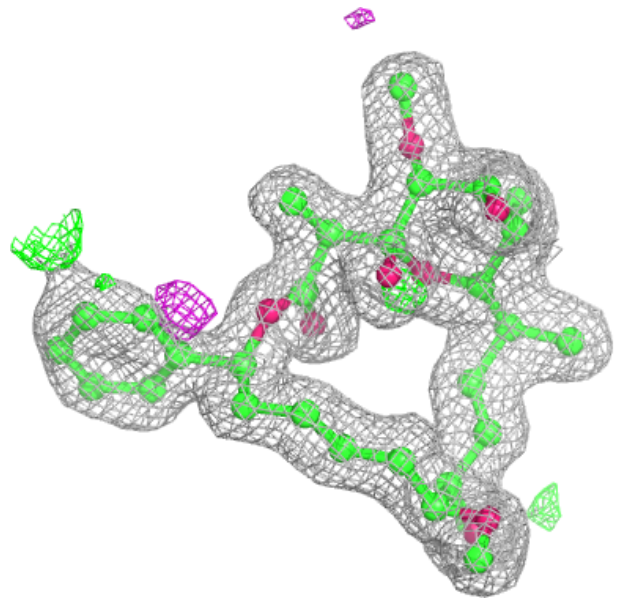
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

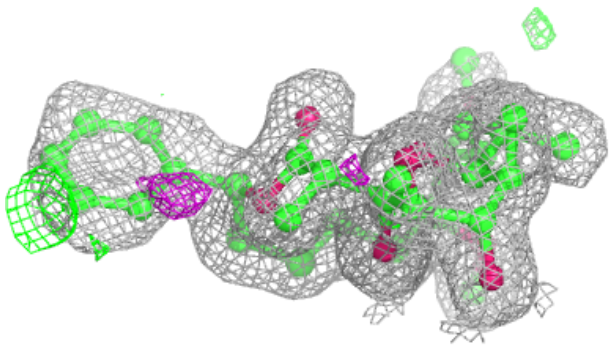
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	S1A	A	1567	37/37	0.93	0.14	13,17,24,26	0
2	S1A	C	1550	37/37	0.94	0.12	14,18,24,24	0
2	S1A	B	1567	37/37	0.95	0.12	9,13,22,23	0

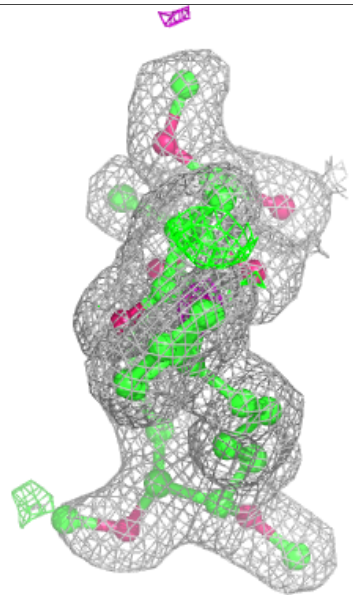
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around S1A A 1567:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

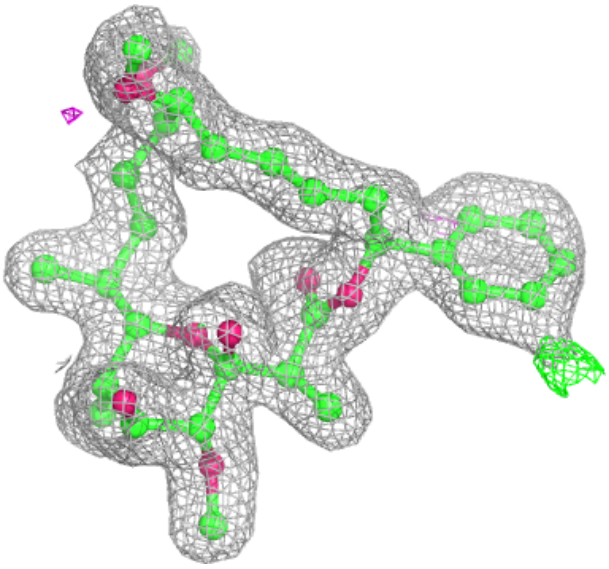


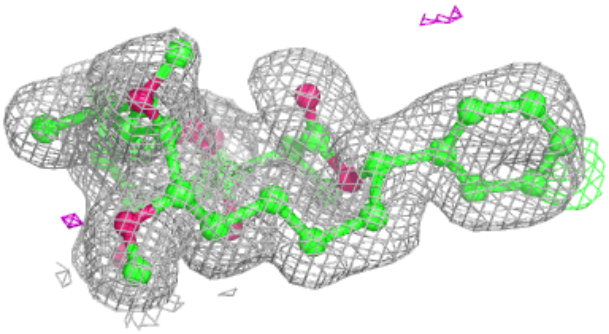


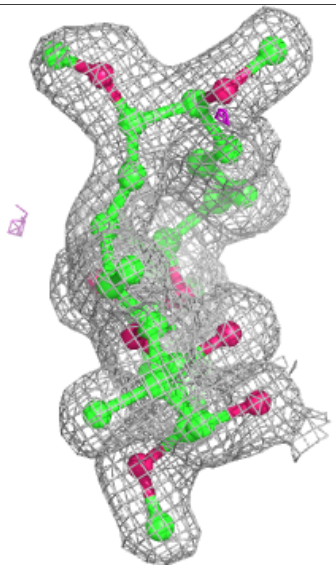


Electron density around S1A C 1550:

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

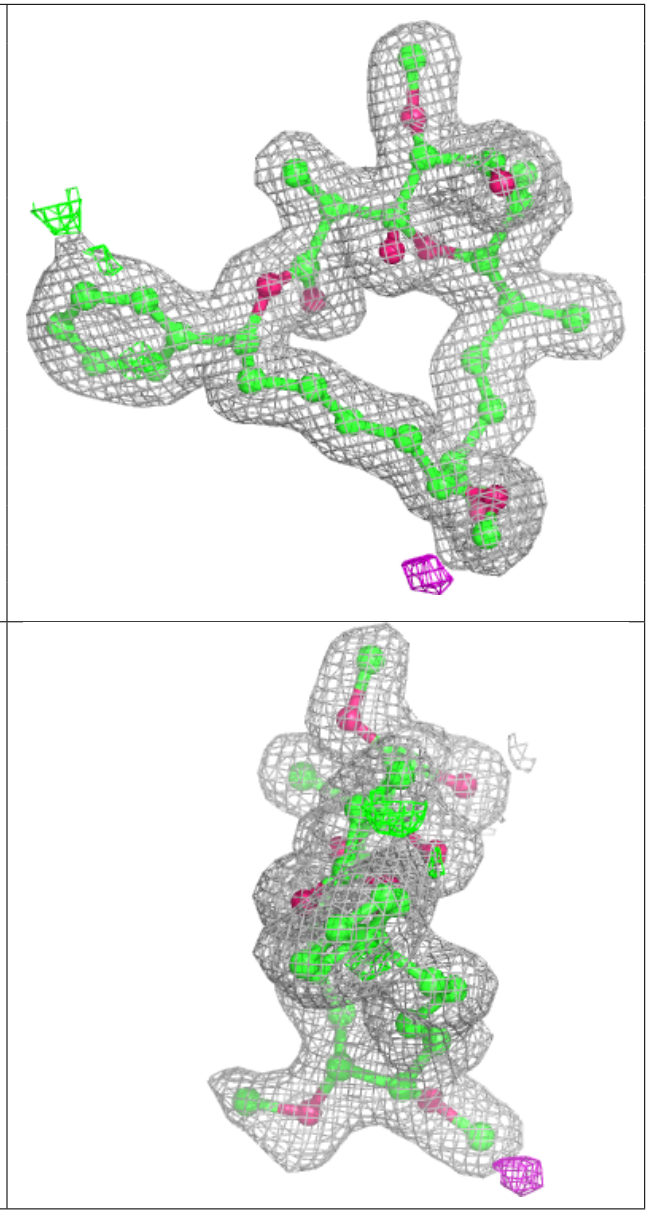






Electron density around S1A B 1567:

$2mF_o$-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.