Full wwPDB X-ray Structure Validation Report (i)

Nov 2, 2023 – 09:09 PM EDT

PDB ID	:	3V97
Title	:	Crystal structure of bifunctional methyltransferase YcbY (RlmLK) from Escherichia coli, SAH binding
Authors	:	Su, X.D.; Wang, K.T.
Deposited on	:	2011-12-23
Resolution	:	2.20 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 (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:

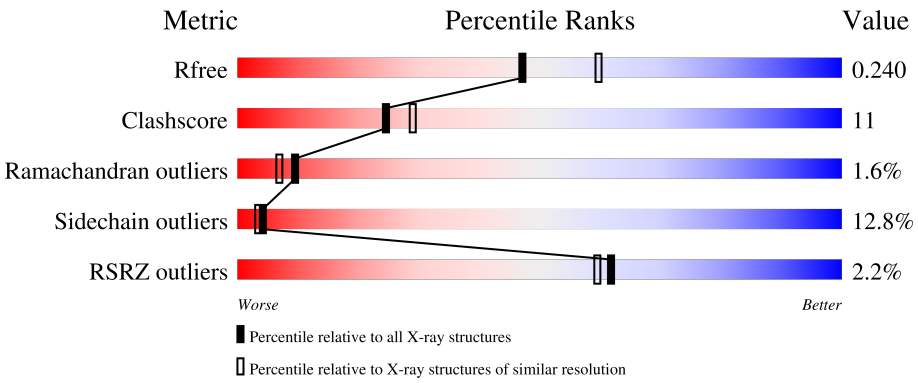
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	703	.% 70% 19% 5% • 5%
1	B	703	4% 69% 16% 5% • 9%
2	C	2	50% 50%
2	D	2	50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	803	-	X	-	-
4	GOL	A	804	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10697 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 Ribosomal RNA large subunit methyltransferase L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	667	5139	3262	901	954	22	0	0	0
1	B	641	4898	3106	857	914	21	0	0	0

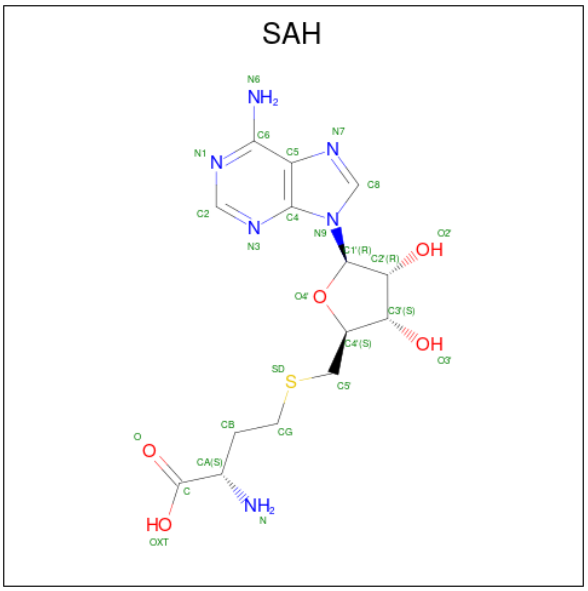
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	expression tag	UNP P75864
B	0	ALA	-	expression tag	UNP P75864

- Molecule 2 is an oligosaccharide called 6-O-octanoyl-beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose.

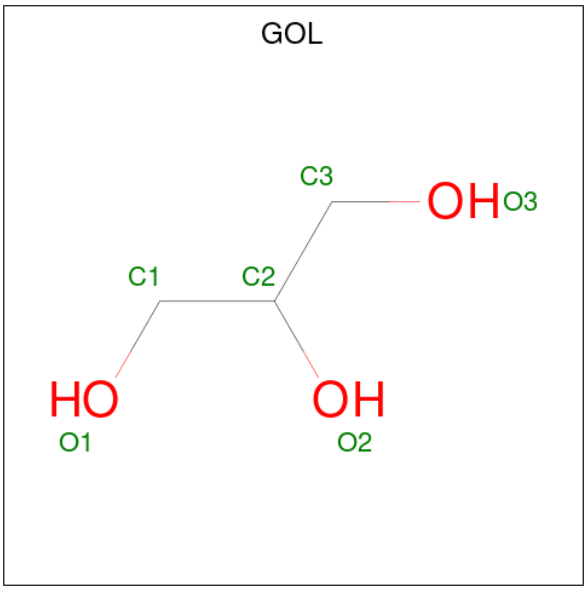
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	C	2	31	19	12	0	0	0
2	D	2	30	18	12	0	0	0

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	6	3	3	0	0
			Total	C	O		
4	A	1	6	3	3	0	0
			Total	C	O		
4	B	1	6	3	3	0	0
			Total	C	O		
4	B	1	6	3	3	0	0

- Molecule 5 is water.

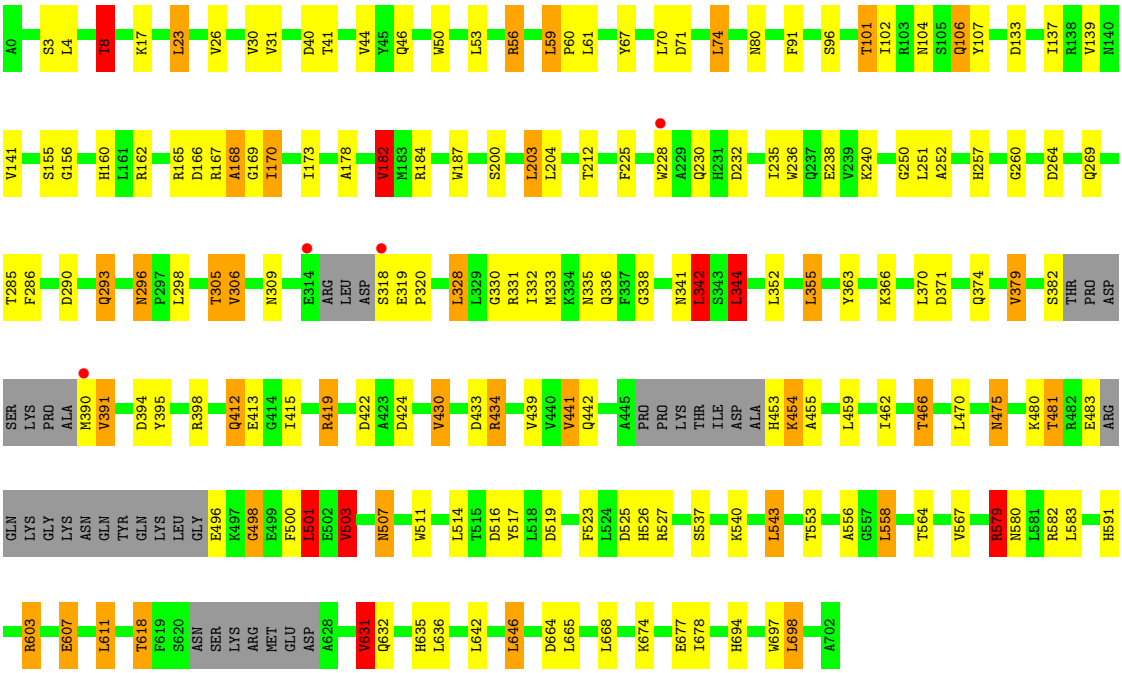
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	270	270	270	0	0
			Total	O		
5	B	201	201	201	0	0

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.

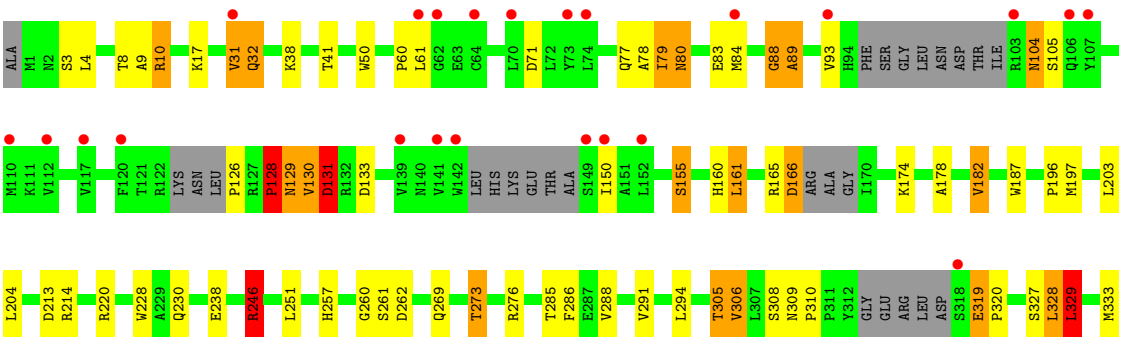
• Molecule 1: Ribosomal RNA large subunit methyltransferase L

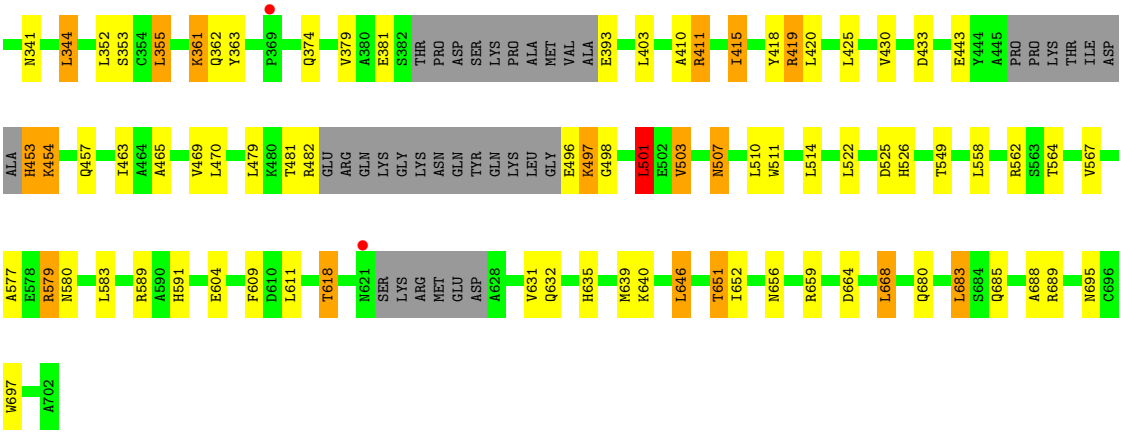
Chain A:



• Molecule 1: Ribosomal RNA large subunit methyltransferase L

Chain B:





- Molecule 2: 6-O-octanoyl-beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain C: 50% 50%

- Molecule 2: 6-O-octanoyl-beta-D-fructofuranose-(2-1)-alpha-D-glucopyranose

Chain D: 50% 50%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.65Å 140.83Å 102.87Å 90.00° 102.30° 90.00°	Depositor
Resolution (Å)	49.91 – 2.20 49.91 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.1 (49.91-2.20) 96.2 (49.91-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.186 , 0.234 0.194 , 0.240	Depositor DCC
R_{free} test set	4970 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	42.5	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 43.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10697	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% 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: GLC, TRV, SAH, GOL

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	1.14	8/5243 (0.2%)	1.09	31/7108 (0.4%)
1	B	0.96	3/4990 (0.1%)	1.01	17/6763 (0.3%)
All	All	1.05	11/10233 (0.1%)	1.05	48/13871 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	238	GLU	CG-CD	6.60	1.61	1.51
1	A	238	GLU	CG-CD	6.59	1.61	1.51
1	A	631	VAL	CB-CG1	-6.17	1.39	1.52
1	A	556	ALA	CA-CB	6.11	1.65	1.52
1	A	200	SER	CA-CB	5.19	1.60	1.52
1	A	441	VAL	CB-CG1	-5.19	1.42	1.52
1	B	609	PHE	CE2-CZ	5.14	1.47	1.37
1	A	252	ALA	CA-CB	5.03	1.63	1.52
1	B	50	TRP	CE3-CZ3	5.02	1.47	1.38
1	A	523	PHE	CD2-CE2	5.01	1.49	1.39
1	A	395	TYR	CD2-CE2	-5.00	1.31	1.39

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	246	ARG	NE-CZ-NH1	11.48	126.04	120.30
1	B	589	ARG	NE-CZ-NH1	9.07	124.83	120.30
1	B	246	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	A	579	ARG	NE-CZ-NH1	-7.93	116.33	120.30
1	B	589	ARG	NE-CZ-NH2	-7.77	116.41	120.30
1	A	501	LEU	CB-CG-CD2	7.62	123.95	111.00
1	A	56	ARG	NE-CZ-NH2	-7.21	116.70	120.30
1	A	344	LEU	CB-CG-CD1	7.13	123.12	111.00
1	B	562	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	A	503	VAL	CG1-CB-CG2	6.73	121.67	110.90
1	B	246	ARG	CD-NE-CZ	6.53	132.75	123.60
1	B	683	LEU	CB-CG-CD2	6.40	121.88	111.00
1	B	501	LEU	CA-CB-CG	6.37	129.94	115.30
1	A	419	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	A	342	LEU	CB-CG-CD2	6.29	121.69	111.00
1	A	631	VAL	CG1-CB-CG2	6.28	120.94	110.90
1	A	582	ARG	CB-CG-CD	-6.18	95.52	111.60
1	A	306	VAL	CG1-CB-CG2	6.18	120.78	110.90
1	A	434	ARG	N-CA-CB	-6.15	99.52	110.60
1	A	203	LEU	CB-CG-CD1	6.15	121.45	111.00
1	A	422	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	A	182	VAL	CG1-CB-CG2	5.96	120.44	110.90
1	A	8	THR	CB-CA-C	-5.85	95.81	111.60
1	B	214	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	A	611	LEU	CB-CG-CD2	5.73	120.74	111.00
1	A	23	LEU	CA-CB-CG	5.71	128.44	115.30
1	B	683	LEU	CA-CB-CG	5.67	128.34	115.30
1	A	355	LEU	CA-CB-CG	5.64	128.28	115.30
1	A	419	ARG	CB-CG-CD	-5.64	96.93	111.60
1	A	498	GLY	N-CA-C	5.64	127.19	113.10
1	B	128	PRO	N-CA-CB	5.63	110.06	103.30
1	B	126	PRO	N-CA-CB	5.63	110.05	103.30
1	A	543	LEU	CB-CG-CD2	5.48	120.32	111.00
1	A	631	VAL	CB-CA-C	-5.45	101.06	111.40
1	B	579	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	501	LEU	CA-CB-CG	5.34	127.58	115.30
1	A	558	LEU	CB-CG-CD1	5.28	119.97	111.00
1	A	527	ARG	CG-CD-NE	5.27	122.87	111.80
1	A	646	LEU	CB-CG-CD2	5.26	119.94	111.00
1	A	162	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	B	525	ASP	CB-CG-OD2	5.20	122.97	118.30
1	B	646	LEU	CB-CG-CD2	5.20	119.83	111.00
1	B	498	GLY	N-CA-C	5.19	126.09	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	276	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	59	LEU	CA-CB-CG	5.14	127.12	115.30
1	A	422	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	424	ASP	CB-CG-OD1	-5.02	113.78	118.30
1	A	430	VAL	CG1-CB-CG2	5.01	118.92	110.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	498	GLY	Peptide
1	B	453	HIS	Peptide

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	5139	0	4995	117	1
1	B	4898	0	4719	94	0
2	C	31	0	7	3	0
2	D	30	0	7	3	0
3	A	52	0	38	0	0
3	B	52	0	38	2	0
4	A	12	0	16	5	0
4	B	12	0	16	3	0
5	A	270	0	0	16	0
5	B	201	0	0	12	0
All	All	10697	0	9836	218	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 11.

All (218) 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:C:1:GLC:C1	2:C:1:GLC:O5	1.64	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1:GLC:C1	2:D:1:GLC:O5	1.68	1.40
1:B:341:ASN:HB2	5:B:1040:HOH:O	1.38	1.21
1:B:88:GLY:HA2	1:B:89:ALA:HB2	1.44	1.00
1:A:412:GLN:HG3	5:A:1089:HOH:O	1.62	0.99
1:B:273:THR:HG22	5:B:1088:HOH:O	1.61	0.98
1:B:165:ARG:HG3	1:B:166:ASP:H	1.32	0.95
1:B:680:GLN:HG2	5:B:1068:HOH:O	1.66	0.94
1:A:603:ARG:HG2	1:A:603:ARG:HH21	1.35	0.92
1:A:507:ASN:H	1:A:507:ASN:HD22	1.13	0.92
1:A:160:HIS:HD2	5:A:985:HOH:O	1.51	0.91
2:C:1:GLC:O5	2:C:1:GLC:C2	2.20	0.90
1:B:511:TRP:H	1:B:580:ASN:HD21	1.20	0.89
1:B:507:ASN:H	1:B:507:ASN:HD22	1.20	0.89
1:B:309:ASN:HD22	3:B:801:SAH:HN1	1.21	0.87
1:A:454:LYS:HG2	1:A:455:ALA:N	1.91	0.86
1:B:410:ALA:O	1:B:411:ARG:CB	2.23	0.84
1:A:525:ASP:OD1	1:A:694:HIS:HD2	1.60	0.83
1:A:309:ASN:OD1	4:A:803:GOL:H32	1.79	0.82
1:A:104:ASN:HD22	1:A:107:TYR:H	1.28	0.81
1:B:128:PRO:O	1:B:129:ASN:HB2	1.80	0.79
1:B:497:LYS:CB	5:B:1100:HOH:O	2.33	0.75
1:B:78:ALA:O	1:B:79:ILE:HB	1.87	0.75
1:B:635:HIS:HE1	1:B:664:ASP:H	1.35	0.75
1:A:475:ASN:H	1:A:475:ASN:HD22	1.33	0.74
1:A:511:TRP:H	1:A:580:ASN:HD21	1.36	0.74
1:A:454:LYS:HG2	1:A:455:ALA:H	1.50	0.74
1:A:579:ARG:HD2	4:A:804:GOL:O2	1.88	0.73
1:A:674:LYS:HE2	5:A:1109:HOH:O	1.88	0.73
1:A:166:ASP:HB2	5:A:1036:HOH:O	1.89	0.71
1:B:128:PRO:O	1:B:129:ASN:CB	2.38	0.71
1:A:419:ARG:HD2	1:A:433:ASP:OD1	1.91	0.70
1:A:618:THR:HA	1:A:631:VAL:HG22	1.74	0.70
1:B:507:ASN:H	1:B:507:ASN:ND2	1.89	0.70
1:A:500:PHE:CE1	4:A:804:GOL:H11	2.27	0.70
1:B:481:THR:HG22	1:B:482:ARG:O	1.91	0.70
1:A:257:HIS:HE1	1:A:285:THR:OG1	1.74	0.69
1:B:419:ARG:HD2	1:B:433:ASP:OD1	1.93	0.69
4:B:803:GOL:H31	5:B:1042:HOH:O	1.93	0.68
1:A:156:GLY:HA3	5:A:1095:HOH:O	1.94	0.68
2:D:1:GLC:O5	2:D:1:GLC:C2	2.28	0.68
1:A:525:ASP:OD1	1:A:694:HIS:CD2	2.46	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:ASN:HD22	1:A:507:ASN:N	1.90	0.67
1:A:511:TRP:H	1:A:580:ASN:ND2	1.92	0.67
1:B:511:TRP:H	1:B:580:ASN:ND2	1.91	0.67
1:A:56:ARG:NH2	1:A:156:GLY:O	2.27	0.67
1:B:130:VAL:O	1:B:131:ASP:HB3	1.95	0.67
1:B:257:HIS:HE1	1:B:285:THR:OG1	1.77	0.67
1:A:160:HIS:CD2	5:A:985:HOH:O	2.36	0.66
1:A:462:ILE:O	1:A:466:THR:CG2	2.44	0.66
1:A:165:ARG:HG3	1:A:166:ASP:H	1.61	0.66
1:A:187:TRP:HA	1:A:305:THR:HG21	1.78	0.66
1:A:390:MET:O	1:A:391:VAL:HG12	1.94	0.66
1:A:475:ASN:HD22	1:A:475:ASN:N	1.92	0.66
1:A:603:ARG:HH21	1:A:603:ARG:CG	2.07	0.65
2:D:1:GLC:C1	2:D:1:GLC:C5	2.63	0.65
1:B:88:GLY:HA2	1:B:89:ALA:CB	2.16	0.65
1:B:328:LEU:O	1:B:329:LEU:CB	2.44	0.65
1:A:413:GLU:HB2	1:A:415:ILE:HD12	1.79	0.64
1:B:88:GLY:CA	1:B:89:ALA:HB2	2.23	0.64
1:B:83:GLU:OE2	1:B:83:GLU:HA	1.97	0.64
1:B:187:TRP:HD1	1:B:305:THR:HG23	1.63	0.64
1:B:618:THR:HG21	5:B:1005:HOH:O	1.97	0.64
1:A:232:ASP:CG	1:A:235:ILE:HD12	2.18	0.63
1:B:213:ASP:OD1	1:B:246:ARG:HG2	1.99	0.62
1:B:309:ASN:OD1	4:B:803:GOL:H32	2.00	0.62
1:A:133:ASP:CB	5:A:1139:HOH:O	2.48	0.62
1:A:481:THR:O	5:A:1164:HOH:O	2.16	0.62
1:A:413:GLU:CB	1:A:415:ILE:HD12	2.29	0.61
1:A:462:ILE:O	1:A:466:THR:HG22	2.00	0.61
1:B:695:ASN:HD22	1:B:697:TRP:HE1	1.47	0.61
1:A:507:ASN:H	1:A:507:ASN:ND2	1.92	0.61
1:B:415:ILE:HD11	1:B:418:TYR:HB3	1.83	0.61
1:B:688:ALA:O	1:B:689:ARG:CB	2.45	0.61
1:A:305:THR:HB	1:A:341:ASN:HB3	1.83	0.60
1:B:618:THR:HG22	5:B:960:HOH:O	2.01	0.60
1:A:454:LYS:CG	1:A:455:ALA:H	2.15	0.59
1:A:106:GLN:HE21	1:A:106:GLN:HA	1.66	0.59
1:A:296:ASN:ND2	1:A:298:LEU:H	2.00	0.59
1:A:454:LYS:CG	1:A:455:ALA:N	2.64	0.58
1:A:228:TRP:CZ2	1:A:230:GLN:HB2	2.38	0.58
1:B:564:THR:OG1	1:B:591:HIS:HD2	1.85	0.58
2:C:1:GLC:C1	2:C:1:GLC:C5	2.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ASN:H	1:A:336:GLN:HE21	1.52	0.57
1:A:496:GLU:HA	1:A:516:ASP:CG	2.24	0.57
1:A:228:TRP:CE2	1:A:230:GLN:HB2	2.39	0.57
1:A:635:HIS:HE1	1:A:664:ASP:H	1.50	0.57
1:B:246:ARG:HG2	1:B:246:ARG:HH11	1.70	0.57
1:B:309:ASN:ND2	3:B:801:SAH:HN1	1.96	0.56
1:A:419:ARG:CD	1:A:433:ASP:OD1	2.53	0.56
1:A:439:VAL:HG21	1:A:470:LEU:HD23	1.87	0.56
1:B:306:VAL:HG13	1:B:333:MET:HE2	1.87	0.56
1:B:80:ASN:OD1	1:B:83:GLU:HG2	2.05	0.56
1:B:640:LYS:HE2	5:B:1056:HOH:O	2.04	0.56
1:A:187:TRP:HD1	1:A:305:THR:HG23	1.71	0.56
1:B:510:LEU:HD13	1:B:522:LEU:HD13	1.88	0.55
1:B:496:GLU:O	1:B:497:LYS:CB	2.54	0.55
1:A:165:ARG:HG3	1:A:166:ASP:N	2.22	0.54
1:A:603:ARG:HG2	1:A:603:ARG:NH2	2.10	0.54
1:B:465:ALA:O	1:B:469:VAL:HG23	2.07	0.54
1:B:155:SER:O	1:B:220:ARG:NH2	2.41	0.53
1:B:651:THR:HG22	5:B:1046:HOH:O	2.08	0.53
1:B:104:ASN:ND2	1:B:105:SER:H	2.06	0.53
1:A:8:THR:CG2	1:A:53:LEU:O	2.57	0.53
1:A:454:LYS:HD3	5:A:1155:HOH:O	2.07	0.53
1:B:9:ALA:O	1:B:10:ARG:O	2.27	0.53
1:B:187:TRP:HA	1:B:305:THR:HG21	1.91	0.53
1:B:361:LYS:HG3	1:B:362:GLN:N	2.23	0.53
1:A:8:THR:HG22	1:A:53:LEU:O	2.08	0.52
1:A:462:ILE:O	1:A:466:THR:HG23	2.07	0.52
1:B:178:ALA:O	1:B:182:VAL:HG13	2.10	0.52
1:B:419:ARG:CD	1:B:433:ASP:OD1	2.56	0.52
1:B:639:MET:CE	1:B:652:ILE:HD13	2.40	0.52
1:A:40:ASP:OD1	1:A:40:ASP:C	2.48	0.51
1:A:677:GLU:HB2	1:A:697:TRP:CZ3	2.45	0.51
1:B:165:ARG:HG3	1:B:166:ASP:N	2.12	0.51
1:B:635:HIS:CE1	1:B:664:ASP:H	2.22	0.51
1:A:330:GLY:CA	1:A:355:LEU:HD13	2.41	0.51
1:B:104:ASN:HD22	1:B:105:SER:H	1.59	0.51
1:B:31:VAL:HG12	1:B:31:VAL:O	2.11	0.51
1:A:390:MET:O	1:A:391:VAL:CG1	2.60	0.50
1:A:333:MET:CE	1:A:342:LEU:HG	2.42	0.50
1:B:306:VAL:CG1	1:B:333:MET:CE	2.89	0.50
1:A:306:VAL:HG22	1:A:342:LEU:HD23	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:HIS:N	5:A:1155:HOH:O	2.44	0.49
1:B:160:HIS:CE1	1:B:161:LEU:HD13	2.47	0.49
1:B:213:ASP:OD1	1:B:246:ARG:CG	2.59	0.49
1:A:70:LEU:HG	1:A:74:LEU:HD22	1.93	0.49
1:A:391:VAL:HG22	1:A:391:VAL:O	2.13	0.49
1:A:475:ASN:H	1:A:475:ASN:ND2	2.05	0.49
1:A:212:THR:O	1:A:250:GLY:HA3	2.13	0.48
1:A:632:GLN:O	1:A:635:HIS:HD2	1.96	0.48
1:B:631:VAL:O	1:B:635:HIS:HB3	2.13	0.48
1:A:564:THR:OG1	1:A:591:HIS:HD2	1.97	0.48
1:A:413:GLU:CB	1:A:415:ILE:CD1	2.92	0.48
1:A:4:LEU:HD21	1:A:44:VAL:HG22	1.95	0.47
1:A:305:THR:CG2	5:A:977:HOH:O	2.61	0.47
1:A:674:LYS:CE	5:A:1109:HOH:O	2.55	0.47
1:B:463:ILE:HD11	1:B:479:LEU:HD13	1.96	0.47
1:B:262:ASP:O	1:B:288:VAL:HA	2.14	0.47
1:B:549:THR:O	1:B:577:ALA:HA	2.14	0.47
1:B:327:SER:C	1:B:328:LEU:O	2.47	0.47
1:B:344:LEU:O	1:B:374:GLN:HA	2.14	0.47
1:B:353:SER:HB3	1:B:457:GLN:HG2	1.96	0.47
1:B:639:MET:HG3	1:B:668:LEU:HD11	1.97	0.47
1:B:352:LEU:O	1:B:355:LEU:HD22	2.15	0.47
1:A:67:TYR:C	1:A:101:THR:HG21	2.35	0.47
1:A:330:GLY:N	1:A:355:LEU:HD13	2.30	0.46
1:A:501:LEU:HD13	1:A:503:VAL:HG23	1.97	0.46
1:A:104:ASN:ND2	1:A:107:TYR:H	2.06	0.46
1:A:236:TRP:CE2	1:A:240:LYS:HD2	2.51	0.46
1:B:305:THR:CG2	5:B:974:HOH:O	2.64	0.46
1:B:507:ASN:HD22	1:B:507:ASN:N	2.00	0.46
1:B:579:ARG:HG3	4:B:804:GOL:O2	2.15	0.46
1:A:290:ASP:HB3	1:A:293:GLN:OE1	2.16	0.46
1:A:46:GLN:O	1:A:50:TRP:HB2	2.16	0.45
1:A:618:THR:HG22	5:A:966:HOH:O	2.16	0.45
1:B:656:ASN:ND2	1:B:695:ASN:HD21	2.13	0.45
1:A:232:ASP:OD2	1:A:235:ILE:HD12	2.17	0.45
1:A:500:PHE:CD1	4:A:804:GOL:H11	2.51	0.45
1:B:165:ARG:O	1:B:166:ASP:HB3	2.16	0.45
1:B:228:TRP:CD1	1:B:230:GLN:HB2	2.52	0.45
1:A:419:ARG:HA	1:A:433:ASP:OD1	2.16	0.45
1:B:31:VAL:O	1:B:32:GLN:O	2.34	0.45
1:B:306:VAL:HG13	1:B:333:MET:CE	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:639:MET:HE3	1:B:652:ILE:HD13	1.98	0.45
1:A:398:ARG:NE	5:A:1119:HOH:O	2.49	0.45
1:B:269:GLN:O	1:B:273:THR:HG23	2.17	0.45
1:A:165:ARG:CG	1:A:166:ASP:H	2.25	0.44
1:A:257:HIS:CE1	1:A:285:THR:OG1	2.63	0.44
1:B:319:GLU:HA	1:B:320:PRO:HD3	1.73	0.44
1:A:296:ASN:HD22	1:A:298:LEU:H	1.64	0.44
1:A:296:ASN:HD22	1:A:296:ASN:C	2.19	0.44
1:A:517:TYR:HB2	1:A:519:ASP:O	2.17	0.44
1:A:264:ASP:OD1	1:A:264:ASP:C	2.56	0.44
1:B:501:LEU:HD13	1:B:503:VAL:HG23	2.00	0.44
1:A:496:GLU:HA	1:A:516:ASP:OD1	2.18	0.44
1:A:187:TRP:CD1	1:A:305:THR:HG23	2.52	0.43
1:A:3:SER:O	1:A:60:PRO:HD2	2.19	0.43
1:A:678:ILE:HG21	1:A:698:LEU:HD22	2.00	0.43
1:A:328:LEU:O	1:A:332:ILE:HG13	2.19	0.43
1:B:306:VAL:HG11	1:B:333:MET:SD	2.58	0.43
1:B:260:GLY:O	1:B:286:PHE:HA	2.19	0.43
1:A:260:GLY:O	1:A:286:PHE:HA	2.19	0.43
1:B:246:ARG:HG2	1:B:246:ARG:NH1	2.30	0.43
1:B:78:ALA:O	1:B:79:ILE:CB	2.53	0.43
1:A:319:GLU:HA	1:A:320:PRO:HD3	1.88	0.43
1:A:366:LYS:HD3	1:A:371:ASP:OD1	2.19	0.43
1:B:196:PRO:HD2	1:B:308:SER:HB2	2.01	0.43
1:A:184:ARG:HB3	1:A:363:TYR:CE2	2.54	0.42
1:B:187:TRP:CD1	1:B:305:THR:HG23	2.49	0.42
1:A:187:TRP:HA	1:A:305:THR:CG2	2.49	0.42
1:A:413:GLU:HB3	1:A:415:ILE:CD1	2.50	0.42
1:A:591:HIS:HE1	5:A:1137:HOH:O	2.01	0.42
1:A:102:ILE:HD12	1:A:102:ILE:N	2.35	0.42
1:A:173:ILE:HD11	1:A:309:ASN:ND2	2.35	0.41
1:A:540:LYS:HA	1:A:540:LYS:HD3	1.72	0.41
1:B:3:SER:O	1:B:60:PRO:HD2	2.20	0.41
1:B:306:VAL:HG11	1:B:333:MET:CE	2.50	0.41
1:A:178:ALA:O	1:A:182:VAL:HG13	2.21	0.41
1:B:197:MET:SD	1:B:310:PRO:HB3	2.60	0.41
1:A:500:PHE:CZ	4:A:804:GOL:H11	2.54	0.41
1:A:553:THR:HG23	1:A:564:THR:HB	2.03	0.41
1:A:41:THR:OG1	1:A:235:ILE:HD13	2.20	0.41
1:A:168:ALA:HA	1:A:169:GLY:HA3	1.56	0.41
1:A:618:THR:HG23	5:A:984:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:SER:OG	1:B:38:LYS:HE3	2.20	0.41
1:A:91:PHE:HA	1:A:137:ILE:O	2.21	0.41
1:B:305:THR:HG22	5:B:974:HOH:O	2.20	0.41
1:B:564:THR:OG1	1:B:591:HIS:CD2	2.72	0.41
1:A:225:PHE:HZ	1:A:236:TRP:CE2	2.39	0.40
1:B:393:GLU:HB2	5:B:965:HOH:O	2.20	0.40
1:B:632:GLN:O	1:B:635:HIS:HD2	2.04	0.40
1:A:352:LEU:HD23	1:A:352:LEU:HA	1.86	0.40
1:B:328:LEU:O	1:B:329:LEU:HB3	2.18	0.40
1:B:453:HIS:O	1:B:454:LYS:CB	2.69	0.40
1:A:338:GLY:HA2	1:A:379:VAL:HG22	2.04	0.40
1:A:344:LEU:O	1:A:374:GLN:HA	2.21	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)
1:A:71:ASP:OD1	1:A:331:ARG:NH1[1_455]	2.16	0.04

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	655/703 (93%)	630 (96%)	20 (3%)	5 (1%)	19 19
1	B	621/703 (88%)	586 (94%)	19 (3%)	16 (3%)	5 3
All	All	1276/1406 (91%)	1216 (95%)	39 (3%)	21 (2%)	9 7

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	ILE

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Mol	Chain	Res	Type
1	B	10	ARG
1	B	32	GLN
1	B	129	ASN
1	B	131	ASP
1	B	381	GLU
1	B	411	ARG
1	B	497	LYS
1	A	167	ARG
1	A	168	ALA
1	B	89	ALA
1	B	454	LYS
1	B	88	GLY
1	B	133	ASP
1	B	329	LEU
1	A	607	GLU
1	B	79	ILE
1	A	391	VAL
1	B	128	PRO
1	B	130	VAL
1	B	31	VAL

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	517/581 (89%)	449 (87%)	68 (13%)	4 3
1	B	488/581 (84%)	427 (88%)	61 (12%)	4 4
All	All	1005/1162 (86%)	876 (87%)	129 (13%)	4 3

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	17	LYS
1	A	23	LEU

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Mol	Chain	Res	Type
1	A	26	VAL
1	A	30	VAL
1	A	31	VAL
1	A	59	LEU
1	A	61	LEU
1	A	74	LEU
1	A	80	ASN
1	A	96	SER
1	A	101	THR
1	A	106	GLN
1	A	139	VAL
1	A	141	VAL
1	A	155	SER
1	A	170	ILE
1	A	182	VAL
1	A	203	LEU
1	A	204	LEU
1	A	251	LEU
1	A	269	GLN
1	A	293	GLN
1	A	296	ASN
1	A	305	THR
1	A	318	SER
1	A	328	LEU
1	A	335	ASN
1	A	342	LEU
1	A	344	LEU
1	A	370	LEU
1	A	379	VAL
1	A	382	SER
1	A	394	ASP
1	A	412	GLN
1	A	430	VAL
1	A	434	ARG
1	A	441	VAL
1	A	442	GLN
1	A	454	LYS
1	A	459	LEU
1	A	466	THR
1	A	475	ASN
1	A	480	LYS
1	A	481	THR

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Mol	Chain	Res	Type
1	A	483	GLU
1	A	501	LEU
1	A	503	VAL
1	A	507	ASN
1	A	514	LEU
1	A	526	HIS
1	A	537	SER
1	A	543	LEU
1	A	558	LEU
1	A	567	VAL
1	A	579	ARG
1	A	583	LEU
1	A	603	ARG
1	A	607	GLU
1	A	611	LEU
1	A	618	THR
1	A	631	VAL
1	A	636	LEU
1	A	642	LEU
1	A	646	LEU
1	A	665	LEU
1	A	668	LEU
1	A	698	LEU
1	B	4	LEU
1	B	8	THR
1	B	17	LYS
1	B	41	THR
1	B	61	LEU
1	B	71	ASP
1	B	77	GLN
1	B	80	ASN
1	B	84	MET
1	B	93	VAL
1	B	104	ASN
1	B	131	ASP
1	B	150	ILE
1	B	155	SER
1	B	161	LEU
1	B	166	ASP
1	B	174	LYS
1	B	182	VAL
1	B	203	LEU

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Mol	Chain	Res	Type
1	B	204	LEU
1	B	246	ARG
1	B	251	LEU
1	B	261	SER
1	B	273	THR
1	B	291	VAL
1	B	294	LEU
1	B	305	THR
1	B	306	VAL
1	B	319	GLU
1	B	328	LEU
1	B	329	LEU
1	B	344	LEU
1	B	355	LEU
1	B	361	LYS
1	B	363	TYR
1	B	379	VAL
1	B	403	LEU
1	B	415	ILE
1	B	419	ARG
1	B	420	LEU
1	B	425	LEU
1	B	430	VAL
1	B	443	GLU
1	B	470	LEU
1	B	501	LEU
1	B	503	VAL
1	B	507	ASN
1	B	514	LEU
1	B	526	HIS
1	B	558	LEU
1	B	567	VAL
1	B	583	LEU
1	B	604	GLU
1	B	611	LEU
1	B	618	THR
1	B	646	LEU
1	B	651	THR
1	B	659	ARG
1	B	668	LEU
1	B	683	LEU
1	B	685	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	80	ASN
1	A	94	HIS
1	A	104	ASN
1	A	106	GLN
1	A	257	HIS
1	A	269	GLN
1	A	296	ASN
1	A	336	GLN
1	A	402	ASN
1	A	412	GLN
1	A	475	ASN
1	A	507	ASN
1	A	580	ASN
1	A	591	HIS
1	A	635	HIS
1	A	685	GLN
1	A	694	HIS
1	B	22	ASN
1	B	77	GLN
1	B	86	ASN
1	B	104	ASN
1	B	160	HIS
1	B	257	HIS
1	B	309	ASN
1	B	507	ASN
1	B	580	ASN
1	B	591	HIS
1	B	635	HIS
1	B	676	GLN
1	B	680	GLN
1	B	695	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)

4 monosaccharides 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	GLC	C	1	2	11,11,12	9.87	6 (54%)	15,15,17	3.49	10 (66%)
2	TRV	C	2	2	19,20,21	2.16	6 (31%)	19,27,28	1.74	4 (21%)
2	GLC	D	1	2	11,11,12	10.36	6 (54%)	15,15,17	3.26	9 (60%)
2	TRV	D	2	2	18,19,21	2.44	5 (27%)	18,26,28	1.64	2 (11%)

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	GLC	C	1	2	-	0/2/19/22	0/1/1/1
2	TRV	C	2	2	-	9/14/33/34	0/1/1/1
2	GLC	D	1	2	-	0/2/19/22	0/1/1/1
2	TRV	D	2	2	-	3/13/32/34	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	GLC	C4-C5	-20.51	1.09	1.53
2	C	1	GLC	C4-C5	-20.18	1.10	1.53
2	D	1	GLC	C1-C2	-18.28	1.10	1.52
2	C	1	GLC	C1-C2	-16.94	1.13	1.52
2	D	1	GLC	O5-C1	15.20	1.68	1.43
2	C	1	GLC	O5-C1	12.91	1.64	1.43
2	C	1	GLC	C2-C3	10.48	1.67	1.52
2	D	1	GLC	O5-C5	8.85	1.61	1.43
2	D	1	GLC	C2-C3	8.18	1.64	1.52
2	C	1	GLC	O5-C5	7.49	1.58	1.43
2	D	1	GLC	C4-C3	6.94	1.70	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	TRV	O1N-C1N	6.73	1.42	1.22
2	C	1	GLC	C4-C3	6.58	1.69	1.52
2	C	2	TRV	O1N-C1N	5.50	1.38	1.22
2	D	2	TRV	C1-C2	-4.41	1.45	1.52
2	D	2	TRV	O2-C2	3.84	1.47	1.40
2	C	2	TRV	O5-C5	3.79	1.52	1.43
2	C	2	TRV	C1-C2	-3.66	1.46	1.52
2	C	2	TRV	O2-C2	2.51	1.45	1.40
2	C	2	TRV	O6-C1N	2.43	1.40	1.33
2	D	2	TRV	O5-C2	-2.42	1.39	1.43
2	C	2	TRV	O5-C2	-2.40	1.39	1.43
2	D	2	TRV	O6-C1N	2.13	1.39	1.33

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1	GLC	O2-C2-C1	6.43	122.31	109.15
2	C	1	GLC	O2-C2-C1	5.96	121.34	109.15
2	C	1	GLC	O2-C2-C3	-5.88	98.36	110.14
2	C	1	GLC	O4-C4-C5	5.46	122.86	109.30
2	D	1	GLC	O3-C3-C2	5.15	119.86	109.99
2	D	2	TRV	O6-C1N-O1N	-5.15	110.60	123.59
2	D	1	GLC	O4-C4-C5	5.11	121.98	109.30
2	C	2	TRV	O6-C1N-O1N	-5.02	110.91	123.59
2	C	1	GLC	O5-C1-C2	-4.70	103.52	110.77
2	C	1	GLC	O3-C3-C2	4.51	118.63	109.99
2	D	1	GLC	C1-O5-C5	-4.21	106.49	112.19
2	D	1	GLC	O3-C3-C4	4.11	119.84	110.35
2	C	1	GLC	O4-C4-C3	-3.39	102.51	110.35
2	D	1	GLC	O4-C4-C3	-2.83	103.80	110.35
2	C	1	GLC	C1-C2-C3	2.81	113.12	109.67
2	C	1	GLC	C2-C3-C4	-2.64	106.32	110.89
2	D	2	TRV	O4-C4-C5	2.55	118.42	111.05
2	C	2	TRV	O2-C2-O5	2.51	114.34	109.50
2	C	1	GLC	O6-C6-C5	-2.49	102.76	111.29
2	C	2	TRV	O6-C1N-C2N	2.44	119.57	111.91
2	D	1	GLC	O2-C2-C3	-2.44	105.25	110.14
2	D	1	GLC	C2-C3-C4	2.37	115.00	110.89
2	C	2	TRV	O1N-C1N-C2N	-2.31	114.73	123.73
2	C	1	GLC	O5-C5-C6	-2.21	103.74	107.20
2	D	1	GLC	O6-C6-C5	-2.11	104.05	111.29

There are no chirality outliers.

All (12) torsion outliers are listed below:

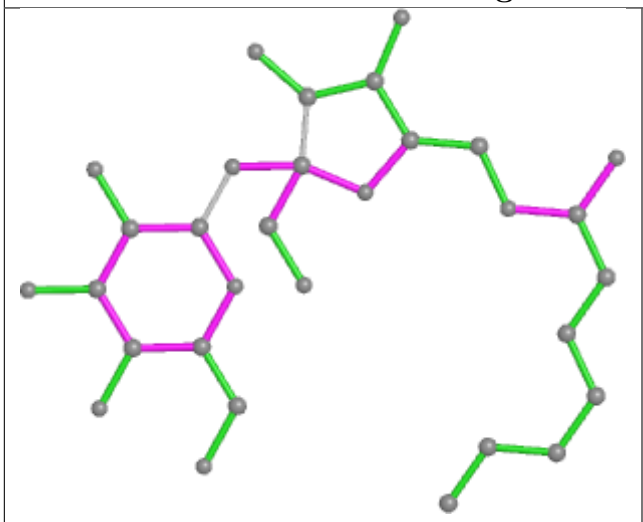
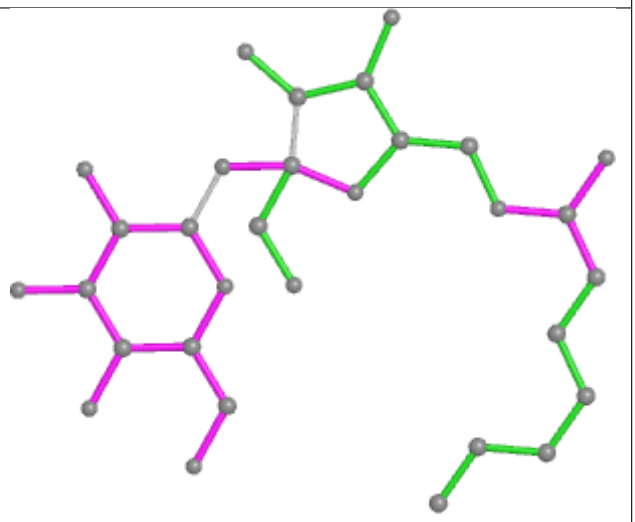
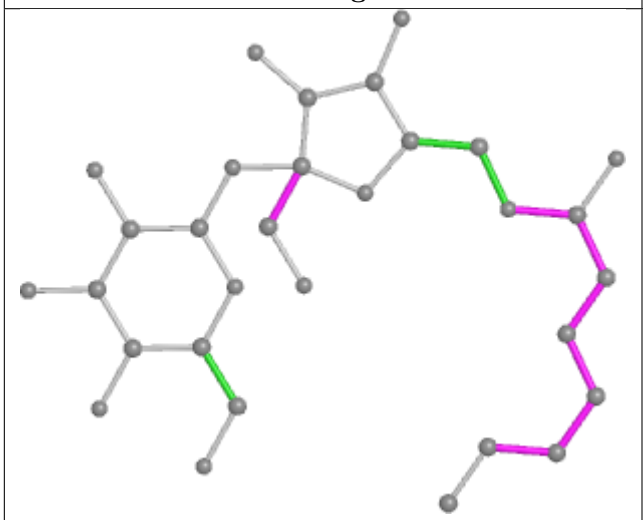
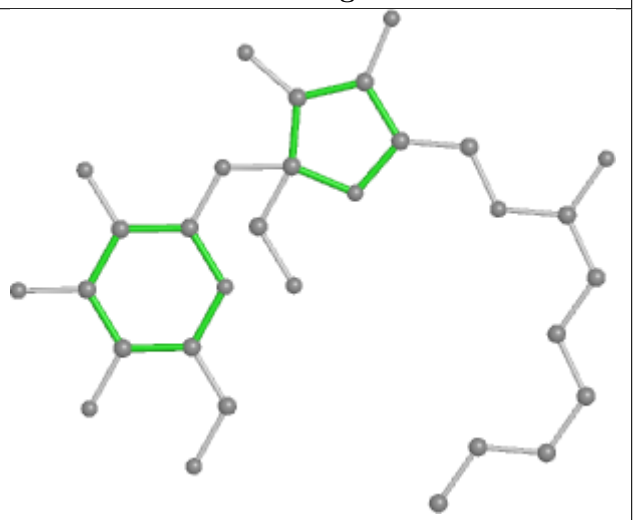
Mol	Chain	Res	Type	Atoms
2	C	2	TRV	O1-C1-C2-O2
2	C	2	TRV	O1-C1-C2-C3
2	C	2	TRV	C3N-C4N-C5N-C6N
2	C	2	TRV	O1-C1-C2-O5
2	C	2	TRV	C1N-C2N-C3N-C4N
2	C	2	TRV	C2N-C3N-C4N-C5N
2	D	2	TRV	C2N-C3N-C4N-C5N
2	D	2	TRV	C3N-C4N-C5N-C6N
2	C	2	TRV	O1N-C1N-O6-C6
2	C	2	TRV	C4N-C5N-C6N-C7N
2	D	2	TRV	O1N-C1N-O6-C6
2	C	2	TRV	O1N-C1N-C2N-C3N

There are no ring outliers.

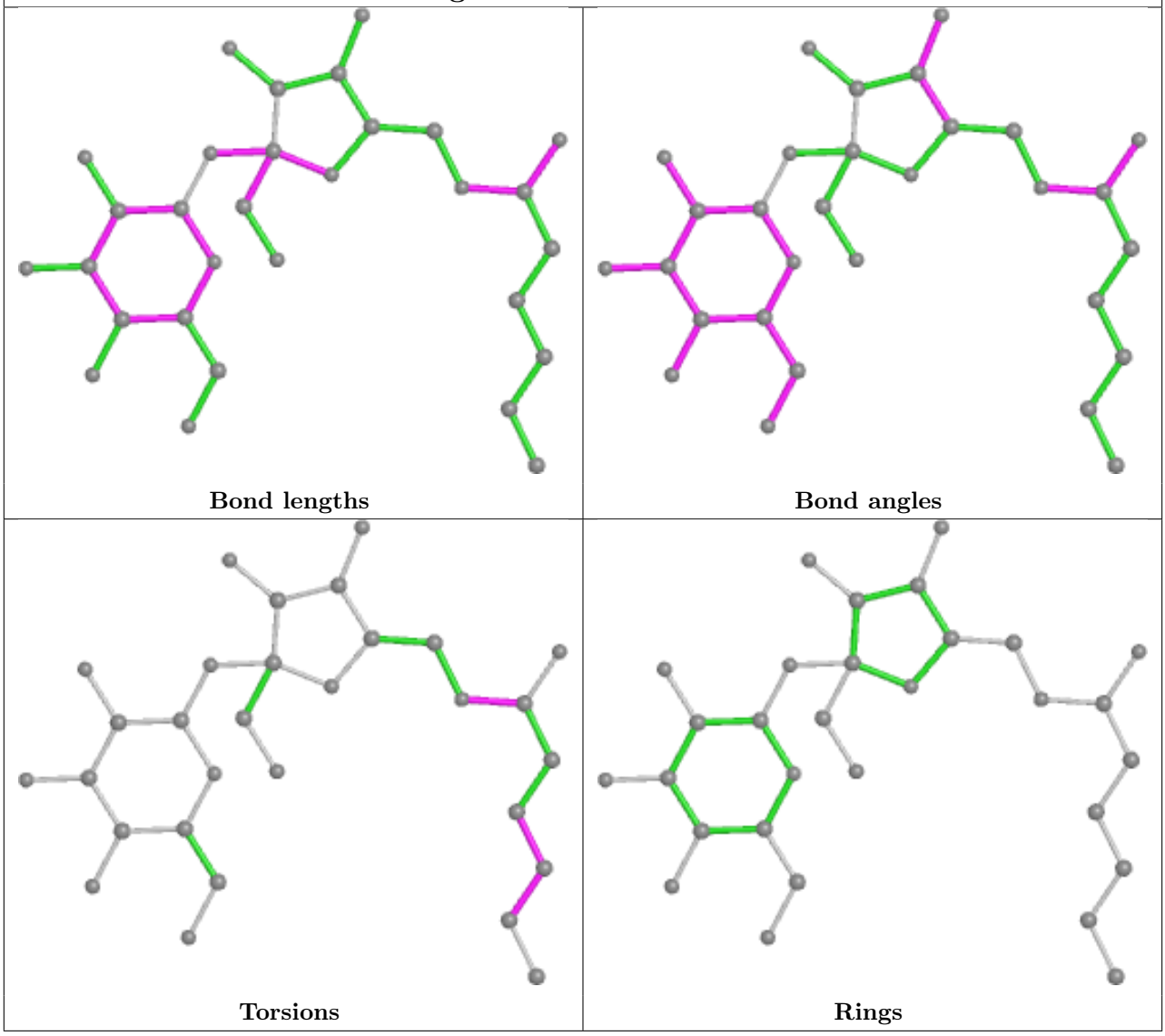
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	GLC	3	0
2	C	1	GLC	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain C	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain D



5.6 Ligand geometry (i)

8 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	SAH	A	801	-	24,28,28	1.37	4 (16%)	25,40,40	1.66	7 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GOL	A	804	-	5,5,5	0.74	0	5,5,5	1.16	0
4	GOL	A	803	-	5,5,5	2.10	2 (40%)	5,5,5	2.22	4 (80%)
3	SAH	B	801	-	24,28,28	1.41	3 (12%)	25,40,40	1.49	5 (20%)
4	GOL	B	803	-	5,5,5	0.91	0	5,5,5	0.96	0
4	GOL	B	804	-	5,5,5	0.84	0	5,5,5	1.11	0
3	SAH	A	802	-	24,28,28	0.93	0	25,40,40	1.76	6 (24%)
3	SAH	B	802	-	24,28,28	1.20	2 (8%)	25,40,40	2.33	10 (40%)

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	SAH	A	801	-	-	0/11/31/31	0/3/3/3
4	GOL	A	804	-	-	0/4/4/4	-
4	GOL	A	803	-	-	0/4/4/4	-
3	SAH	B	801	-	-	0/11/31/31	0/3/3/3
4	GOL	B	803	-	-	0/4/4/4	-
4	GOL	B	804	-	-	0/4/4/4	-
3	SAH	A	802	-	-	2/11/31/31	0/3/3/3
3	SAH	B	802	-	-	3/11/31/31	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	SAH	C4-N3	-3.84	1.30	1.35
3	A	801	SAH	C8-N7	3.67	1.41	1.34
4	A	803	GOL	O2-C2	3.30	1.53	1.43
3	B	801	SAH	C2-N3	2.56	1.36	1.32
4	A	803	GOL	O3-C3	2.55	1.53	1.42
3	B	801	SAH	C8-N7	2.55	1.39	1.34
3	A	801	SAH	O3'-C3'	2.50	1.48	1.43
3	A	801	SAH	C2-N3	2.44	1.36	1.32
3	B	802	SAH	CB-CG	2.31	1.60	1.51
3	B	802	SAH	C5-C4	2.09	1.46	1.40
3	A	801	SAH	C5-C4	2.07	1.46	1.40

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	802	SAH	CB-CG-SD	-5.12	101.83	113.31
3	B	802	SAH	O4'-C4'-C5'	-4.57	97.07	108.83
3	A	802	SAH	N3-C2-N1	-3.68	122.92	128.68
3	B	802	SAH	OXT-C-O	-3.55	116.02	124.09
3	B	802	SAH	N3-C2-N1	-3.51	123.19	128.68
3	A	802	SAH	O4'-C4'-C5'	-3.38	100.13	108.83
3	B	801	SAH	O4'-C1'-C2'	-3.29	102.12	106.93
3	A	802	SAH	CB-CG-SD	-3.25	106.01	113.31
3	B	802	SAH	CB-CA-C	3.25	118.03	110.30
3	B	801	SAH	N3-C2-N1	-3.11	123.82	128.68
3	A	801	SAH	C4-C5-N7	-3.07	106.20	109.40
3	B	801	SAH	C4-C5-N7	-2.96	106.31	109.40
3	A	801	SAH	O4'-C1'-C2'	-2.85	102.76	106.93
3	B	802	SAH	OXT-C-CA	2.79	122.89	113.38
3	B	802	SAH	CB-CA-N	-2.76	102.94	110.17
3	A	801	SAH	N3-C2-N1	-2.72	124.42	128.68
3	B	802	SAH	C5'-C4'-C3'	-2.72	108.26	115.06
3	A	802	SAH	OXT-C-O	-2.71	117.93	124.09
4	A	803	GOL	O3-C3-C2	2.63	122.79	110.20
3	A	801	SAH	CB-CA-N	2.56	116.89	110.17
3	B	802	SAH	C4'-C5'-SD	-2.56	104.58	113.78
3	A	802	SAH	CB-CA-C	2.49	116.23	110.30
3	B	801	SAH	C1'-N9-C4	-2.48	122.29	126.64
4	A	803	GOL	C3-C2-C1	-2.42	102.28	111.70
3	A	801	SAH	C5-C6-N6	-2.42	116.68	120.35
3	A	801	SAH	N6-C6-N1	2.34	123.42	118.57
3	A	802	SAH	C5'-SD-CG	-2.29	95.41	102.27
3	B	802	SAH	C1'-N9-C4	-2.27	122.65	126.64
4	A	803	GOL	O2-C2-C1	2.25	119.05	109.12
3	B	801	SAH	OXT-C-CA	2.10	120.55	113.38
4	A	803	GOL	O1-C1-C2	2.08	120.16	110.20
3	A	801	SAH	C1'-N9-C4	-2.02	123.09	126.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	SAH	CA-CB-CG-SD
3	B	802	SAH	O4'-C4'-C5'-SD
3	B	802	SAH	C3'-C4'-C5'-SD
3	B	802	SAH	CA-CB-CG-SD
3	A	802	SAH	C3'-C4'-C5'-SD

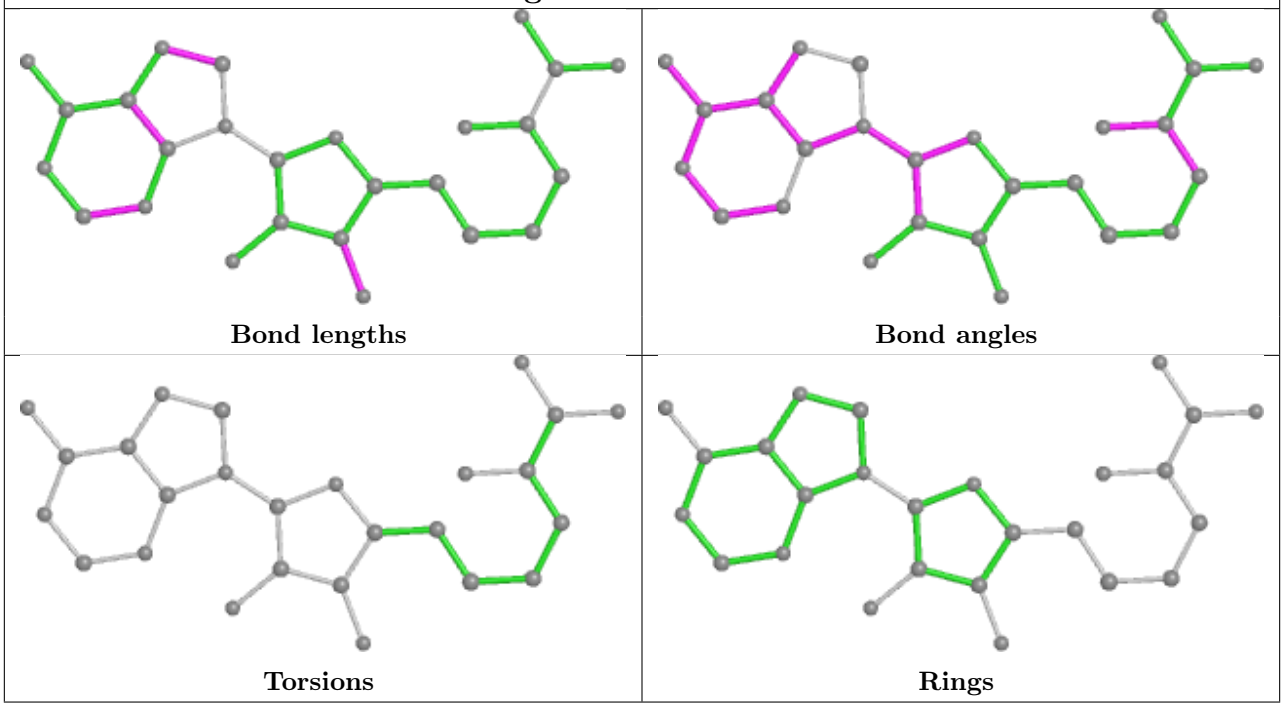
There are no ring outliers.

5 monomers are involved in 10 short contacts:

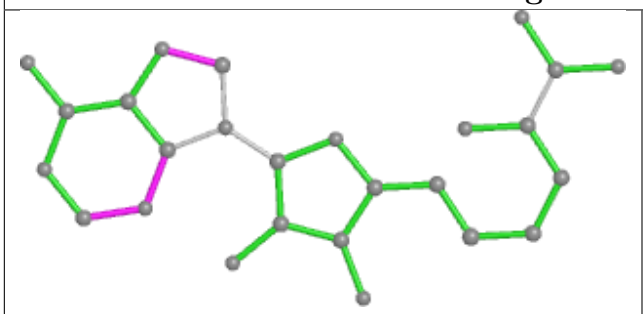
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	804	GOL	4	0
4	A	803	GOL	1	0
3	B	801	SAH	2	0
4	B	803	GOL	2	0
4	B	804	GOL	1	0

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.

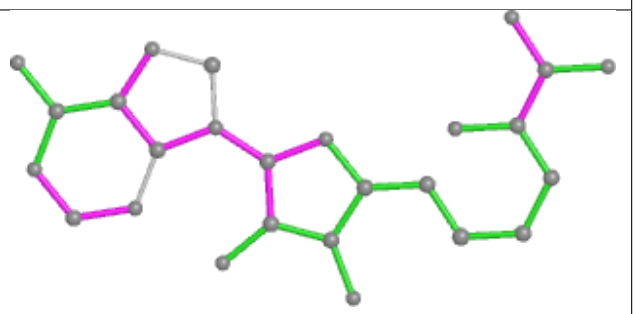
Ligand SAH A 801



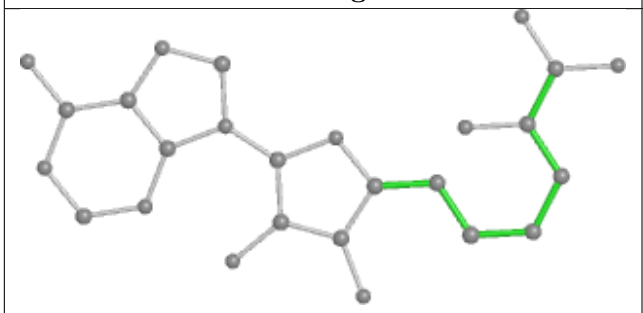
Ligand SAH B 801



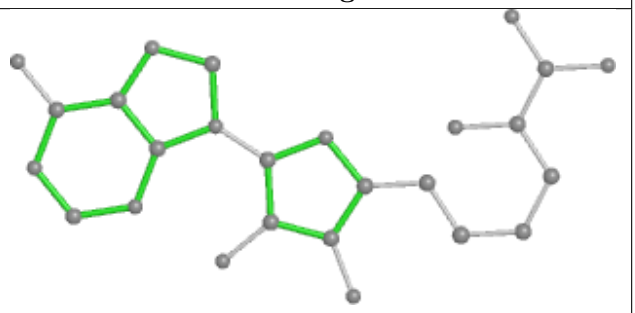
Bond lengths



Bond angles

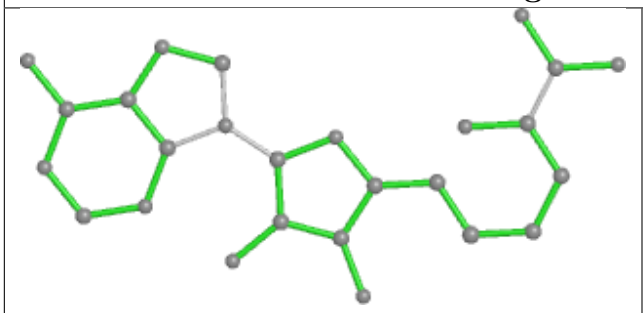


Torsions

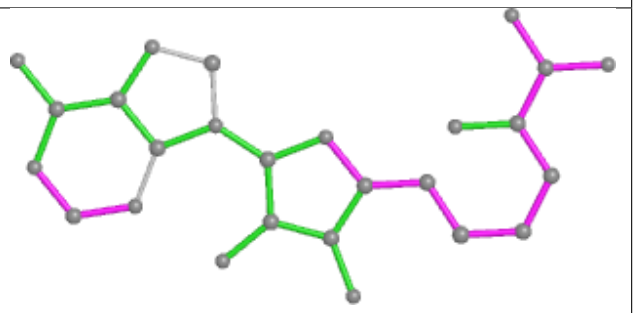


Rings

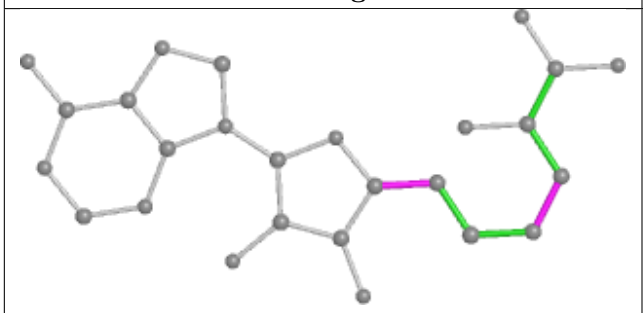
Ligand SAH A 802



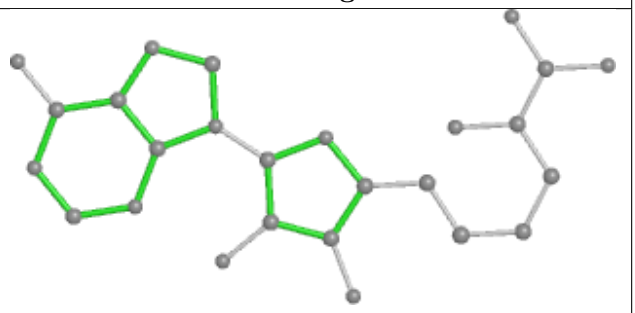
Bond lengths



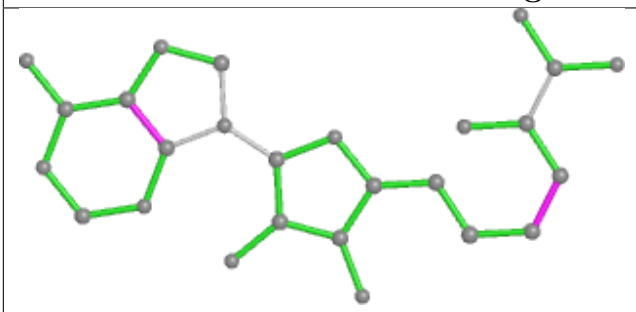
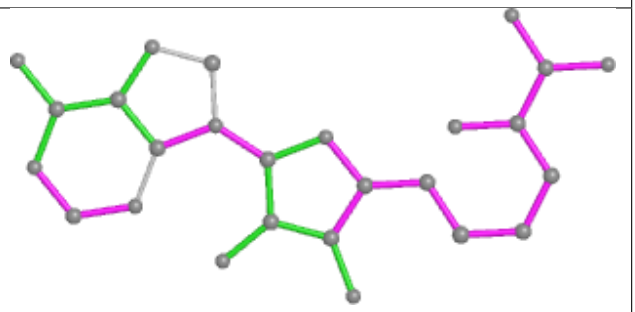
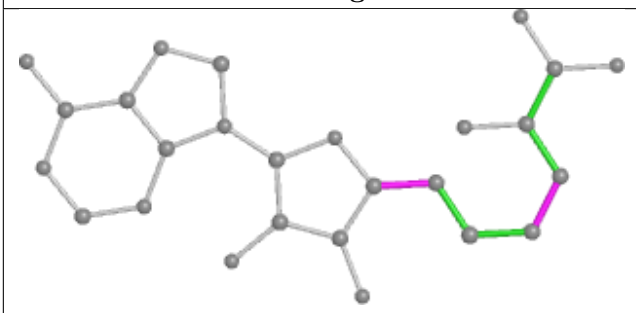
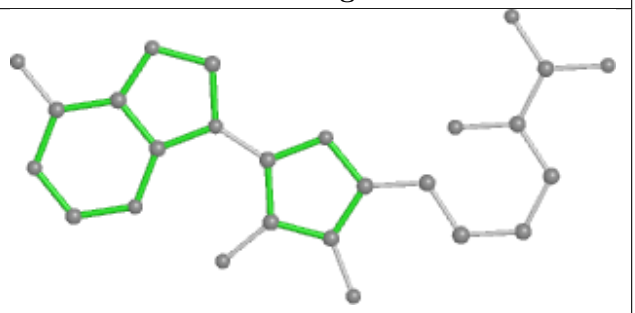
Bond angles



Torsions



Rings

Ligand SAH B 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

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	667/703 (94%)	-0.23	4 (0%)	89	88	25, 45, 73, 96	0
1	B	641/703 (91%)	0.05	25 (3%)	39	37	29, 57, 91, 125	0
All	All	1308/1406 (93%)	-0.09	29 (2%)	62	59	25, 50, 86, 125	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	150	ILE	5.6
1	B	64	CYS	3.9
1	B	61	LEU	3.7
1	B	93	VAL	3.6
1	B	107	TYR	3.4
1	B	369	PRO	3.4
1	B	103	ARG	3.3
1	B	84	MET	3.2
1	B	110	MET	3.2
1	B	149	SER	3.1
1	B	112	VAL	3.1
1	B	73	TYR	3.0
1	B	141	VAL	3.0
1	A	390	MET	2.9
1	B	117	VAL	2.8
1	B	152	LEU	2.8
1	B	106	GLN	2.7
1	B	31	VAL	2.7
1	B	120	PHE	2.7
1	B	74	LEU	2.6
1	B	70	LEU	2.6
1	B	318	SER	2.6
1	B	621	ASN	2.6
1	B	142	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	314	GLU	2.5
1	B	62	GLY	2.5
1	B	139	VAL	2.5
1	A	318	SER	2.2
1	A	228	TRP	2.2

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)

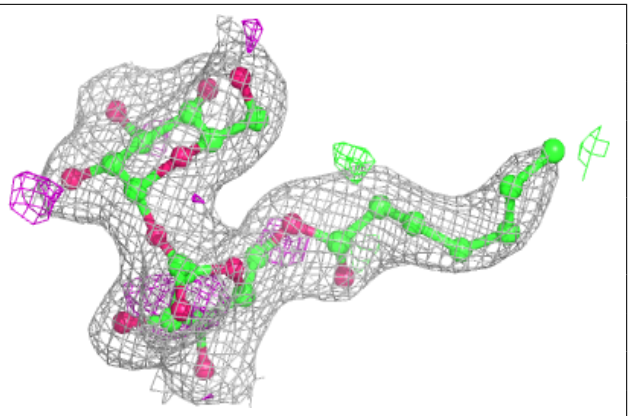
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

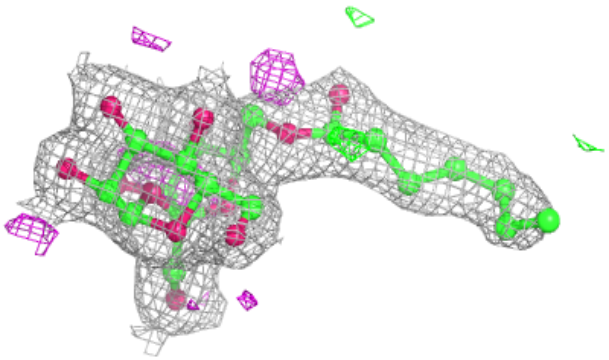
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	D	1	11/12	0.94	0.11	37,41,45,47	0
2	TRV	D	2	19/21	0.95	0.15	41,45,61,62	0
2	GLC	C	1	11/12	0.96	0.13	29,34,39,40	0
2	TRV	C	2	20/21	0.96	0.13	27,36,57,58	0

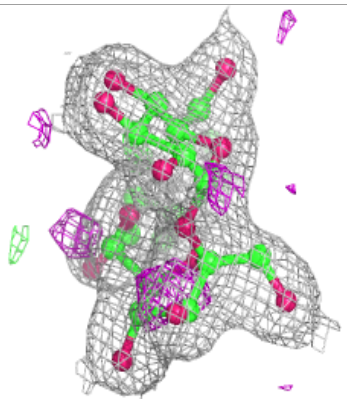
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

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

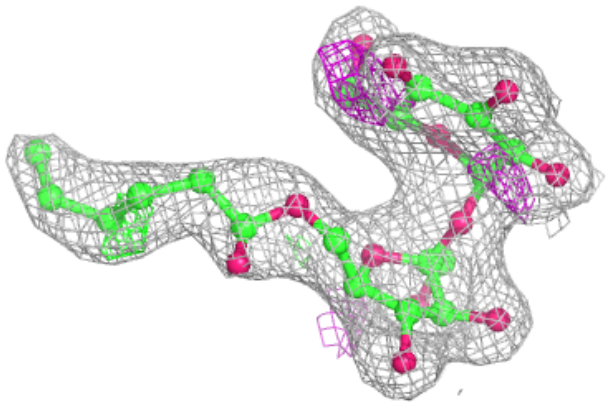


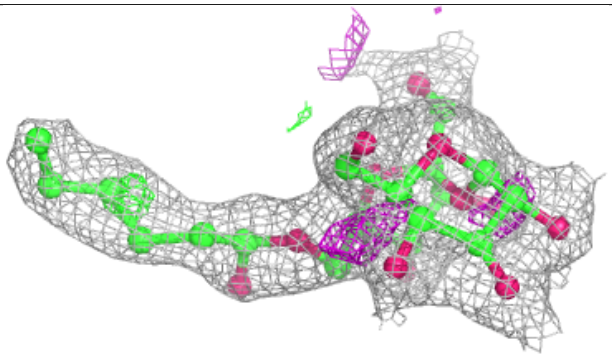


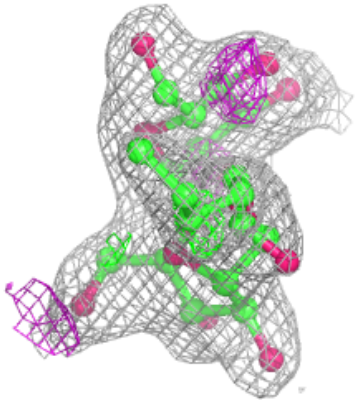


Electron density around Chain D:

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







6.4 Ligands (i)

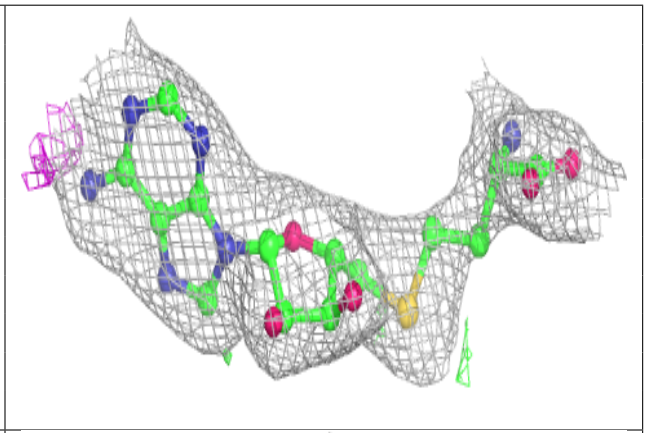
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

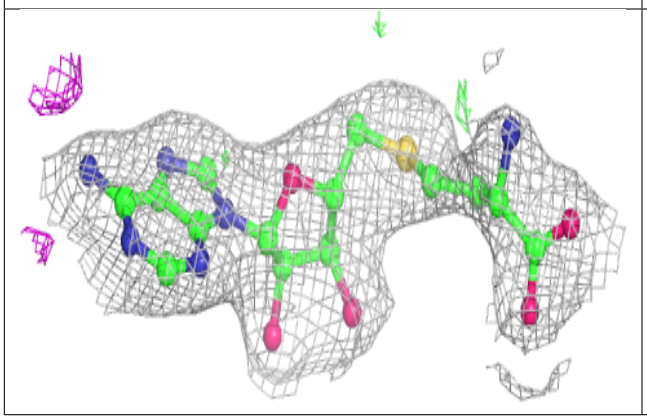
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	A	804	6/6	0.67	0.21	63,67,68,70	0
4	GOL	B	804	6/6	0.74	0.21	59,65,66,72	0
4	GOL	A	803	6/6	0.84	0.15	35,43,43,49	0
4	GOL	B	803	6/6	0.88	0.15	56,61,63,66	0
3	SAH	B	801	26/26	0.95	0.12	44,50,64,64	0
3	SAH	A	802	26/26	0.96	0.12	33,40,44,45	0
3	SAH	B	802	26/26	0.96	0.11	38,41,46,53	0
3	SAH	A	801	26/26	0.98	0.10	29,37,41,43	0

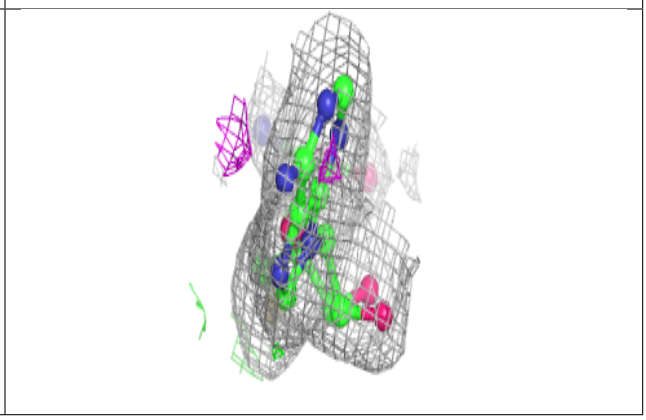
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAH B 801:

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

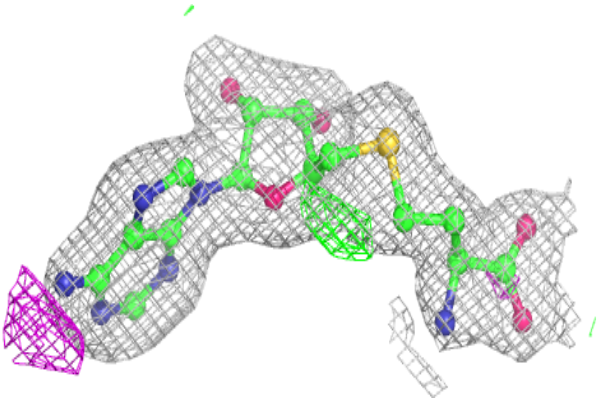


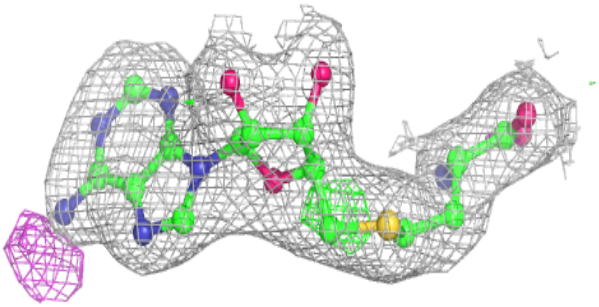


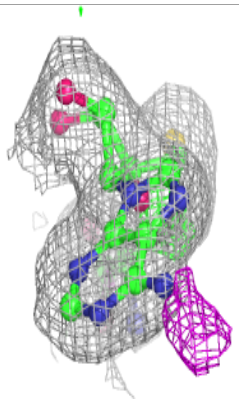


Electron density around SAH A 802:

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

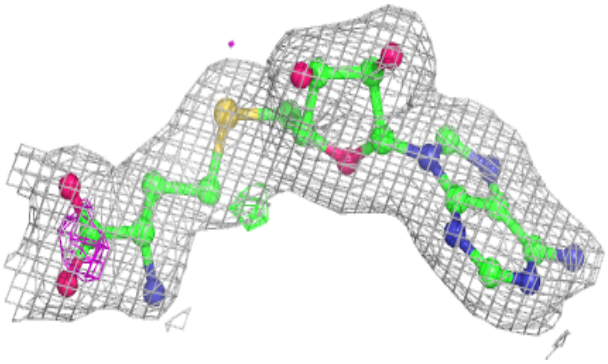


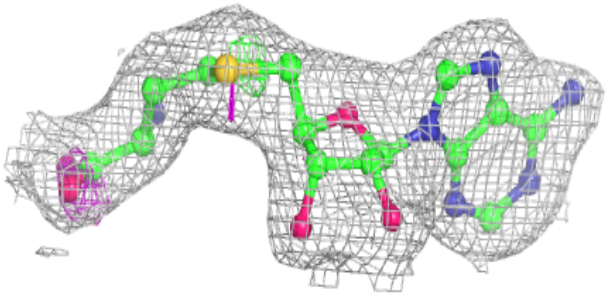


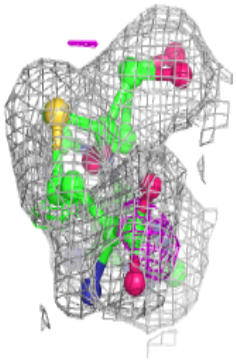


Electron density around SAH B 802:

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

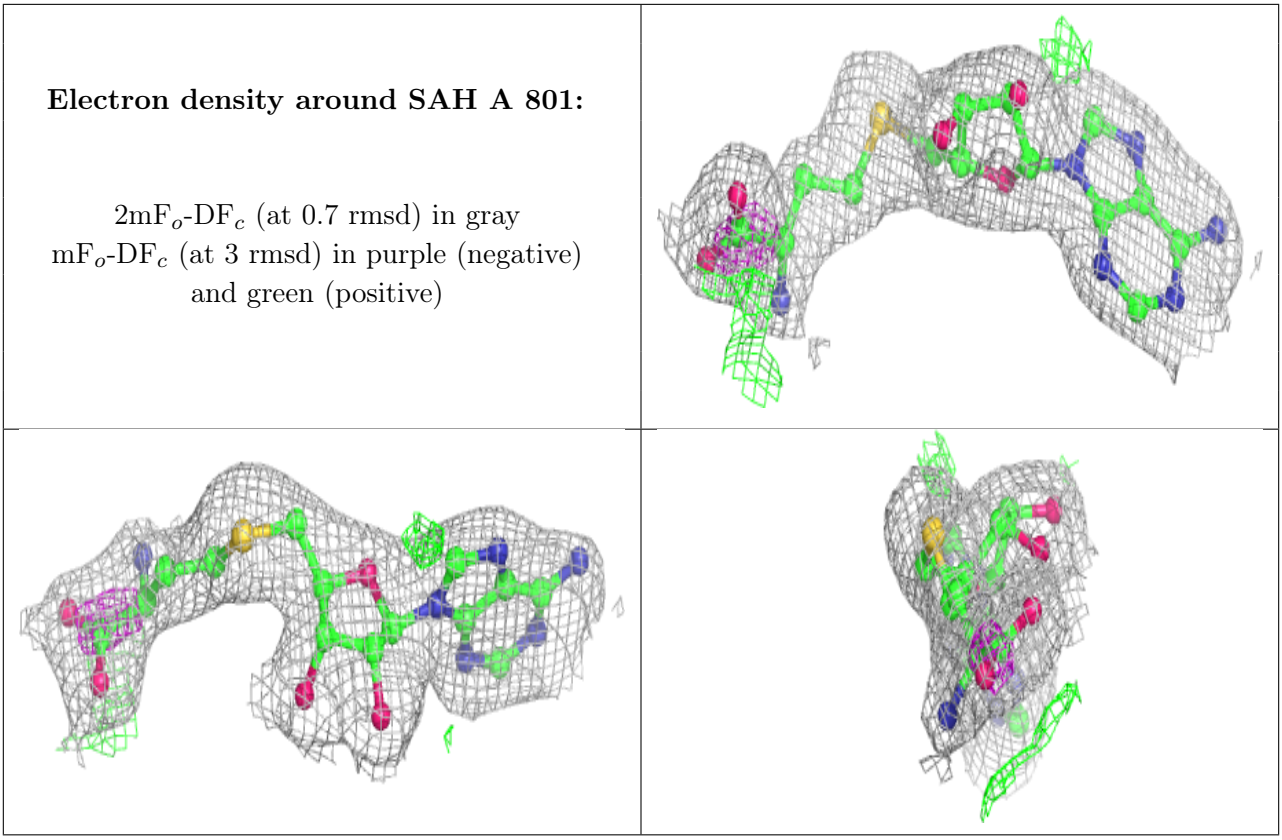






Electron density around SAH A 801:

$2mF_o$-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.