Full wwPDB X-ray Structure Validation Report (i)

Nov 3, 2023 – 05:10 AM EDT

PDB ID	:	3V8V
Title	:	Crystal structure of bifunctional methyltransferase YcbY (RlmLK) from Escherichia coli, SAM binding
Authors	:	Su, X.D.; Wang, K.T.
Deposited on	:	2011-12-23
Resolution	:	2.60 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:

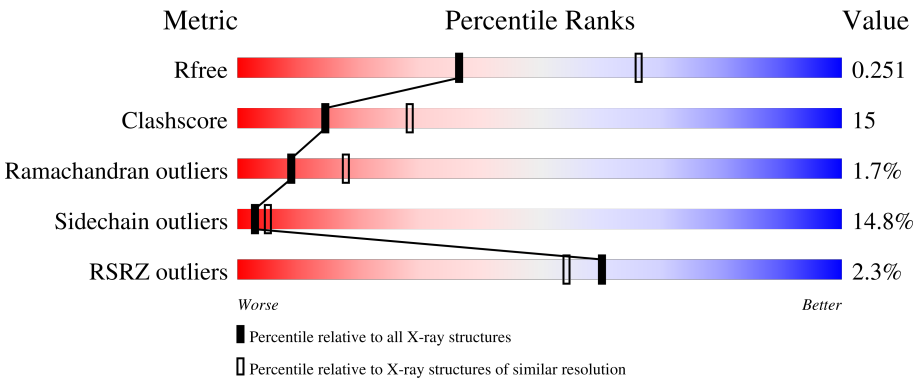
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	702	68% 22% 5% 5%
1	B	702	4% 63% 20% 6% • 9%
2	C	2	50% 50%
2	D	2	50% 50%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10456 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.

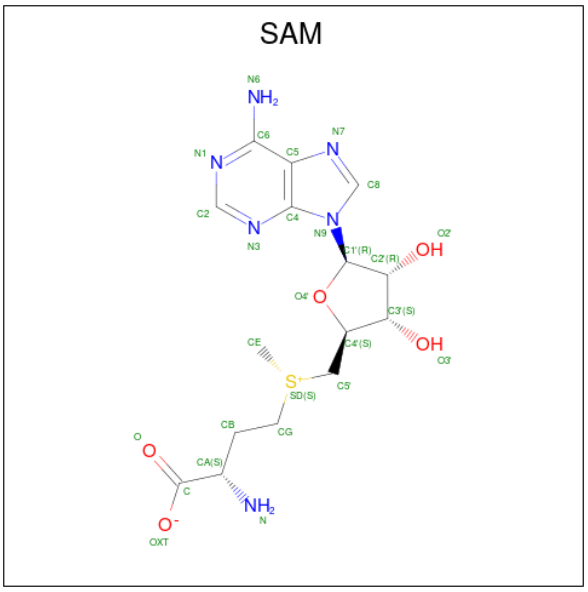
- Molecule 1 is a protein called Ribosomal RNA large subunit methyltransferase L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	664	5139	3269	901	946	23	0	1	0
1	B	636	4788	3035	836	895	22	0	1	0

- 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-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	26	14	6	5	1	0	0
			Total	C	N	O	S		
3	A	1	19	10	5	3	1	0	0
			Total	C	N	O	S		
3	B	1	26	14	6	5	1	0	0
			Total	C	N	O	S		
3	B	1	25	14	6	4	1	0	0

- Molecule 4 is water.

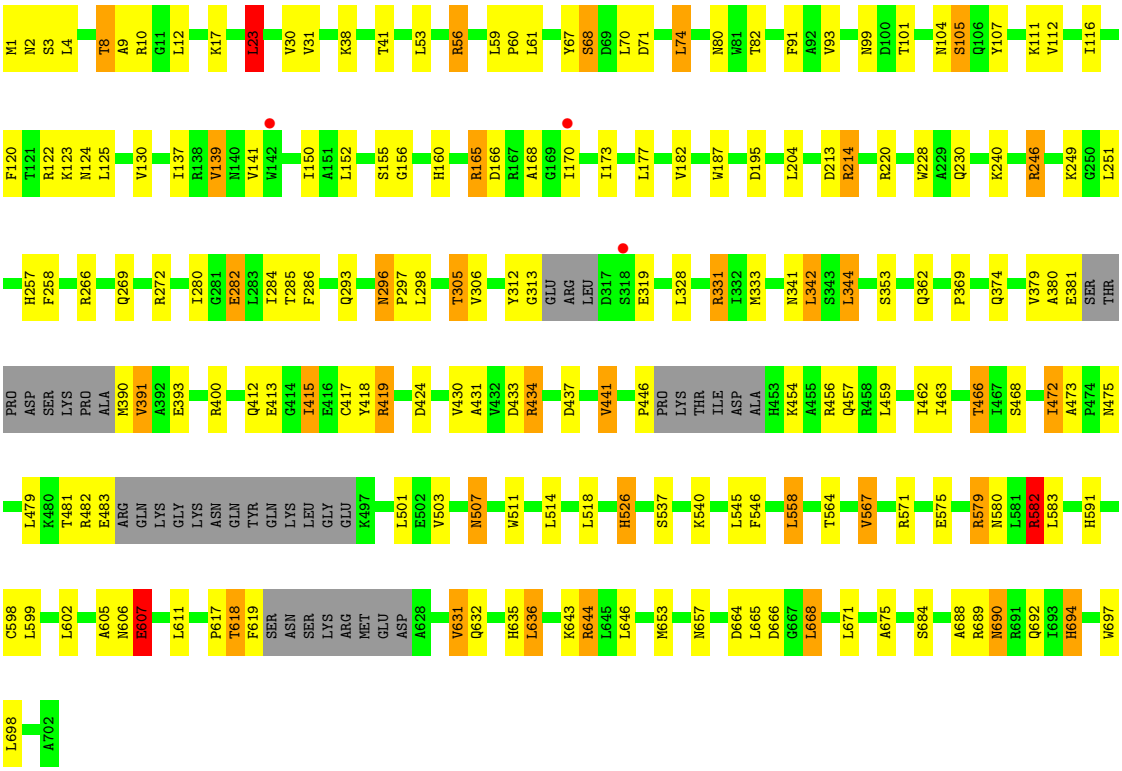
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	211	211	211	0	0
			Total	O		
4	B	161	161	161	0	0

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.

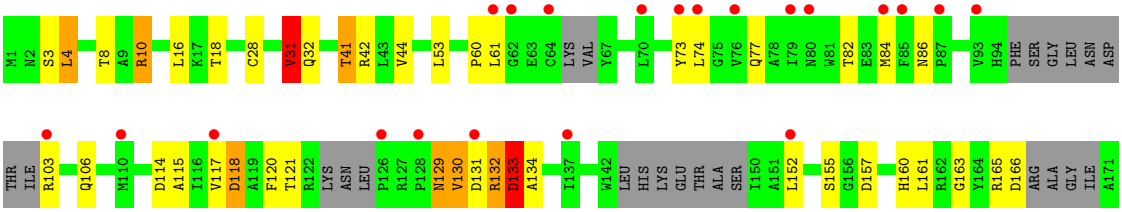
• Molecule 1: Ribosomal RNA large subunit methyltransferase L

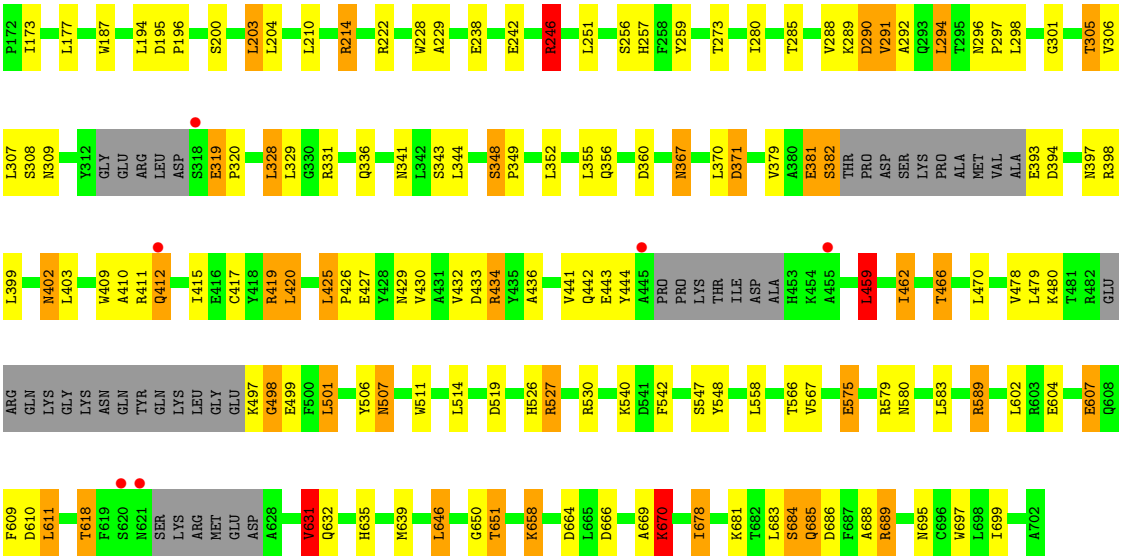
Chain A: 68% 22% 5% 5%



• Molecule 1: Ribosomal RNA large subunit methyltransferase L

Chain B: 4% 63% 20% 6% • 9%





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

Chain C:

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

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.72Å 140.59Å 102.10Å 90.00° 101.88° 90.00°	Depositor
Resolution (Å)	42.57 – 2.60 42.57 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.6 (42.57-2.60) 94.6 (42.57-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.89 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.182 , 0.247 0.191 , 0.251	Depositor DCC
R_{free} test set	3015 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å^2)	55.8	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 61.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10456	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% 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: TRV, GLC, SAM

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	0.91	1/5248 (0.0%)	0.95	15/7115 (0.2%)
1	B	0.82	1/4882 (0.0%)	0.92	12/6625 (0.2%)
All	All	0.86	2/10130 (0.0%)	0.94	27/13740 (0.2%)

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	B	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	282	GLU	CG-CD	5.53	1.60	1.51
1	B	499	GLU	CG-CD	5.52	1.60	1.51

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	214	ARG	NE-CZ-NH2	-7.87	116.37	120.30
1	B	459	LEU	CA-CB-CG	7.58	132.72	115.30
1	B	246	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	A	579	ARG	NE-CZ-NH2	7.02	123.81	120.30
1	A	56	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	B	246	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	A	214	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	631	VAL	CB-CA-C	-6.10	99.81	111.40
1	A	4	LEU	CA-CB-CG	-6.09	101.28	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	686	ASP	CB-CG-OD1	5.98	123.69	118.30
1	A	437	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	195	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	579	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	B	402	ASN	CB-CA-C	5.58	121.56	110.40
1	A	220	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	498	GLY	N-CA-C	5.54	126.95	113.10
1	A	558	LEU	CB-CG-CD1	5.41	120.20	111.00
1	A	23	LEU	CA-CB-CG	5.36	127.63	115.30
1	B	501	LEU	CA-CB-CG	5.32	127.54	115.30
1	B	4	LEU	CA-CB-CG	5.27	127.42	115.30
1	A	56	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	589	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	220	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	B	434	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	342	LEU	CA-CB-CG	5.09	127.02	115.30
1	A	582	ARG	CB-CG-CD	-5.08	98.39	111.60
1	B	214	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	131	ASP	Peptide
1	B	498	GLY	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	5025	143	1
1	B	4788	0	4539	155	0
2	C	31	0	7	3	0
2	D	30	0	7	3	0
3	A	45	0	31	0	0
3	B	51	0	38	5	0
4	A	211	0	0	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	161	0	0	29	0
All	All	10456	0	9647	304	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 15.

All (304) 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:D:1:GLC:O5	2:D:1:GLC:C1	1.65	1.43
2:C:1:GLC:C1	2:C:1:GLC:O5	1.65	1.41
3:B:801:SAM:H8	4:B:1047:HOH:O	1.09	1.26
1:B:165:ARG:HG3	1:B:166:ASP:H	1.05	1.19
1:A:165:ARG:HG3	1:A:166:ASP:H	0.99	1.15
1:B:651:THR:HG22	4:B:983:HOH:O	1.46	1.15
1:B:669:ALA:O	1:B:670:LYS:CB	2.02	1.02
1:B:669:ALA:O	1:B:670:LYS:HB3	1.20	1.02
1:A:165:ARG:HG3	1:A:166:ASP:N	1.76	0.99
1:A:165:ARG:CG	1:A:166:ASP:H	1.78	0.97
2:D:1:GLC:O5	2:D:1:GLC:C2	2.18	0.92
1:A:507:ASN:H	1:A:507:ASN:HD22	1.11	0.91
1:B:73:TYR:CE1	1:B:115:ALA:HB2	2.04	0.91
1:A:246:ARG:HH11	1:A:246:ARG:HG2	1.38	0.89
1:A:446:PRO:HD2	4:A:1099:HOH:O	1.72	0.89
1:B:165:ARG:HG3	1:B:166:ASP:N	1.86	0.89
1:B:511:TRP:H	1:B:580:ASN:HD21	1.18	0.88
1:A:419:ARG:HD2	1:A:433:ASP:OD1	1.78	0.84
1:B:133:ASP:HA	4:B:1039:HOH:O	1.78	0.83
1:A:137:ILE:HD12	1:A:228[B]:TRP:HE3	1.43	0.82
1:B:635:HIS:HE1	1:B:664:ASP:H	1.27	0.81
1:B:685:GLN:N	4:B:1027:HOH:O	1.65	0.81
1:B:84[A]:MET:CE	1:B:84[A]:MET:HA	2.09	0.80
1:B:618:THR:HA	1:B:631:VAL:CG2	2.11	0.80
1:B:319:GLU:HG2	4:B:955:HOH:O	1.82	0.80
1:A:511:TRP:H	1:A:580:ASN:HD21	1.26	0.80
1:A:618:THR:HA	1:A:631:VAL:HG22	1.62	0.79
1:B:478:VAL:CB	4:B:1052:HOH:O	2.30	0.79
1:A:415:ILE:HD11	1:A:418:TYR:HB3	1.66	0.78
1:B:196:PRO:HB3	4:B:1030:HOH:O	1.84	0.77
1:B:462:ILE:O	1:B:466:THR:HG22	1.85	0.76
1:A:434:ARG:HD2	4:A:926:HOH:O	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:SER:HB3	4:A:1096:HOH:O	1.87	0.75
1:B:173:ILE:HG23	1:B:177:LEU:HD23	1.67	0.74
1:A:296:ASN:C	1:A:296:ASN:HD22	1.89	0.74
1:B:530:ARG:HD3	4:B:1034:HOH:O	1.88	0.73
1:A:67:TYR:O	1:A:68:SER:O	2.06	0.73
1:B:157:ASP:OD1	1:B:222:ARG:NH1	2.21	0.73
1:B:511:TRP:H	1:B:580:ASN:ND2	1.85	0.73
1:B:84[A]:MET:HA	1:B:84[A]:MET:HE3	1.69	0.73
1:A:296:ASN:ND2	1:A:298:LEU:H	1.87	0.72
1:A:381:GLU:HB2	4:A:1018:HOH:O	1.87	0.72
1:A:690:ASN:C	1:A:690:ASN:HD22	1.93	0.72
1:B:165:ARG:CG	1:B:166:ASP:H	1.88	0.72
1:B:441:VAL:O	1:B:479:LEU:O	2.08	0.72
1:B:684:SER:O	4:B:1033:HOH:O	2.07	0.72
1:A:617:PRO:HG2	4:A:1076:HOH:O	1.89	0.71
1:B:507:ASN:HD22	1:B:507:ASN:H	1.37	0.71
1:B:246:ARG:HG2	1:B:246:ARG:HH11	1.55	0.71
1:A:257:HIS:HE1	1:A:285:THR:OG1	1.73	0.70
1:B:8:THR:HG23	1:B:16:LEU:HD22	1.73	0.70
1:B:684:SER:O	1:B:685:GLN:CB	2.39	0.70
1:A:511:TRP:H	1:A:580:ASN:ND2	1.90	0.69
1:A:319:GLU:HB2	4:A:1016:HOH:O	1.93	0.69
1:A:618:THR:HA	1:A:631:VAL:CG2	2.23	0.69
1:A:462:ILE:O	1:A:466:THR:HG22	1.93	0.68
1:A:104:ASN:HD22	1:A:107:TYR:H	1.40	0.68
1:A:56:ARG:NH2	1:A:156:GLY:O	2.27	0.68
1:B:73:TYR:CD1	1:B:115:ALA:HB2	2.29	0.68
1:A:567:VAL:HG22	1:A:598:CYS:SG	2.34	0.68
1:B:8:THR:HG22	1:B:53:LEU:O	1.94	0.68
1:B:73:TYR:CE1	1:B:115:ALA:CB	2.77	0.68
1:A:419:ARG:CD	1:A:433:ASP:OD1	2.42	0.67
1:A:605:ALA:O	1:A:644:ARG:NH2	2.25	0.66
1:B:294:LEU:HD21	4:B:1030:HOH:O	1.94	0.66
1:A:17:LYS:HE3	4:A:963:HOH:O	1.96	0.66
1:A:526:HIS:ND1	1:A:694:HIS:HD2	1.94	0.66
1:B:548:TYR:HB2	3:B:802:SAM:HG2	1.76	0.66
1:A:472:ILE:HG23	1:A:473:ALA:H	1.61	0.66
1:B:575:GLU:HG3	1:B:579:ARG:HH12	1.61	0.66
1:B:639:MET:HE1	1:B:699:ILE:HG21	1.77	0.66
1:A:582:ARG:NH2	1:B:163:GLY:O	2.30	0.65
1:A:305:THR:HB	1:A:341:ASN:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:TRP:HD1	1:A:305:THR:HG23	1.61	0.65
1:A:99:ASN:HB2	4:A:981:HOH:O	1.96	0.64
1:A:462:ILE:O	1:A:466:THR:CG2	2.45	0.64
1:B:132:ARG:C	1:B:134:ALA:H	2.00	0.64
1:A:8:THR:HG22	1:A:53:LEU:O	1.97	0.64
1:A:507:ASN:H	1:A:507:ASN:ND2	1.91	0.64
1:A:507:ASN:HD22	1:A:507:ASN:N	1.89	0.64
1:B:28:CYS:HB2	4:B:1012:HOH:O	1.98	0.64
1:B:257:HIS:HE1	1:B:285:THR:OG1	1.80	0.64
1:A:1:MET:N	4:A:1038:HOH:O	2.30	0.63
1:A:228[A]:TRP:NE1	1:A:230:GLN:HB2	2.13	0.63
1:A:213:ASP:OD1	1:A:246:ARG:HG2	1.99	0.63
1:B:305:THR:HB	1:B:341:ASN:HB3	1.81	0.63
1:B:3:SER:O	1:B:60:PRO:HD2	1.97	0.63
1:A:70:LEU:HG	1:A:74:LEU:HD22	1.80	0.63
1:B:84[A]:MET:HE3	1:B:84[A]:MET:CA	2.26	0.63
1:A:690:ASN:ND2	1:A:692:GLN:H	1.97	0.62
1:A:306:VAL:HG13	1:A:333:MET:HE1	1.82	0.62
1:B:604:GLU:CB	4:B:1007:HOH:O	2.46	0.62
1:A:296:ASN:HD22	1:A:298:LEU:H	1.47	0.62
1:A:165:ARG:HA	4:A:1069:HOH:O	2.01	0.61
1:A:380:ALA:O	1:A:381:GLU:CB	2.48	0.61
1:B:381:GLU:CB	4:B:1060:HOH:O	2.47	0.61
1:B:646:LEU:HD22	1:B:650:GLY:HA3	1.82	0.61
1:B:31:VAL:O	1:B:31:VAL:HG13	2.01	0.61
1:B:194:LEU:HD21	4:B:1030:HOH:O	2.01	0.60
1:B:635:HIS:CE1	1:B:664:ASP:H	2.14	0.60
1:B:688:ALA:O	1:B:689:ARG:CB	2.48	0.60
1:A:3:SER:O	1:A:60:PRO:HD2	2.02	0.60
1:A:187:TRP:HA	1:A:305:THR:HG21	1.84	0.60
1:A:257:HIS:HD2	4:A:1080:HOH:O	1.85	0.59
1:B:328:LEU:HD23	1:B:331:ARG:NH2	2.16	0.59
1:B:695:ASN:HD22	1:B:697:TRP:HE1	1.49	0.59
1:B:507:ASN:H	1:B:507:ASN:ND2	2.00	0.59
1:A:137:ILE:HD12	1:A:228[B]:TRP:CE3	2.32	0.59
1:B:8:THR:CG2	1:B:16:LEU:HD22	2.33	0.59
1:B:187:TRP:HD1	1:B:305:THR:HG23	1.68	0.58
1:B:430:VAL:HG21	1:B:462:ILE:CD1	2.34	0.58
1:B:497:LYS:N	4:B:998:HOH:O	2.36	0.58
1:A:635:HIS:HE1	1:A:664:ASP:H	1.52	0.57
1:A:463:ILE:CD1	1:A:479:LEU:HD22	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:MET:CB	4:A:1058:HOH:O	2.52	0.57
1:A:10:ARG:HG2	4:A:986:HOH:O	2.05	0.56
1:B:479:LEU:O	1:B:480:LYS:HB2	2.05	0.56
1:A:463:ILE:HD11	1:A:479:LEU:HD22	1.86	0.56
1:B:309:ASN:HD21	3:B:801:SAM:HB2	1.69	0.56
1:B:397:ASN:HA	4:B:978:HOH:O	2.04	0.56
1:B:393:GLU:HB2	4:B:949:HOH:O	2.04	0.56
1:B:397:ASN:ND2	4:B:978:HOH:O	2.38	0.56
1:A:9:ALA:HB3	1:A:12:LEU:HD12	1.87	0.56
1:B:575:GLU:HG3	1:B:579:ARG:NH1	2.21	0.56
1:A:545:LEU:HD23	1:A:567:VAL:HG13	1.87	0.56
1:B:412:GLN:HE21	1:B:412:GLN:HA	1.69	0.56
1:B:443:GLU:OE2	1:B:459:LEU:HD22	2.06	0.55
1:B:589:ARG:HG2	1:B:589:ARG:O	2.05	0.55
1:B:427:GLU:OE2	1:B:427:GLU:N	2.33	0.55
1:A:8:THR:HG22	4:A:921:HOH:O	2.05	0.55
1:A:91:PHE:HA	1:A:137:ILE:O	2.06	0.55
1:A:296:ASN:HD22	1:A:297:PRO:N	2.03	0.55
1:A:482:ARG:CB	4:A:1040:HOH:O	2.54	0.55
1:B:684:SER:O	1:B:685:GLN:HB3	2.07	0.55
1:A:400:ARG:HD3	4:A:1020:HOH:O	2.07	0.54
1:B:84[A]:MET:HE1	1:B:229:ALA:HB3	1.88	0.54
1:B:639:MET:CE	1:B:699:ILE:HG21	2.36	0.54
1:B:246:ARG:HG2	1:B:246:ARG:NH1	2.17	0.54
2:C:1:GLC:C1	2:C:1:GLC:C5	2.71	0.54
1:A:8:THR:CG2	1:A:53:LEU:O	2.54	0.54
1:A:165:ARG:CG	1:A:166:ASP:N	2.47	0.54
1:A:246:ARG:HG2	1:A:246:ARG:NH1	2.12	0.54
1:A:579:ARG:NH2	4:A:983:HOH:O	2.41	0.54
1:B:666:ASP:O	1:B:669:ALA:O	2.25	0.54
1:A:137:ILE:CD1	1:A:228[B]:TRP:HE3	2.20	0.53
1:A:694:HIS:HB3	4:A:1060:HOH:O	2.08	0.53
1:A:353:SER:OG	1:A:457:GLN:HG2	2.09	0.53
1:B:292:ALA:HA	1:B:328:LEU:HD11	1.90	0.53
1:B:73:TYR:HE1	1:B:115:ALA:HB2	1.68	0.53
1:A:319:GLU:OE2	1:A:456:ARG:NH2	2.42	0.52
1:B:479:LEU:O	1:B:480:LYS:CB	2.56	0.52
1:B:187:TRP:CD1	1:B:305:THR:HG23	2.45	0.52
1:A:168:ALA:HB1	4:A:1072:HOH:O	2.09	0.52
1:B:309:ASN:ND2	3:B:801:SAM:HB2	2.23	0.52
1:A:390:MET:O	1:A:391:VAL:HG12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:VAL:HG22	1:A:139:VAL:HG22	1.92	0.52
1:B:618:THR:HA	1:B:631:VAL:HG22	1.88	0.52
1:B:540:LYS:HB3	1:B:610:ASP:HB2	1.92	0.52
1:B:419:ARG:HD2	1:B:433:ASP:OD1	2.09	0.52
1:B:430:VAL:HA	4:B:1059:HOH:O	2.09	0.52
1:B:429:ASN:HD21	1:B:444:TYR:HB2	1.75	0.52
1:A:481:THR:OG1	1:A:482:ARG:N	2.39	0.51
1:B:290:ASP:OD2	3:B:801:SAM:N6	2.42	0.51
1:B:210:LEU:O	1:B:210:LEU:HD23	2.11	0.51
1:A:431:ALA:O	1:A:441:VAL:HA	2.11	0.51
1:B:214:ARG:HD3	1:B:280:ILE:HD13	1.93	0.51
1:B:618:THR:HG21	4:B:939:HOH:O	2.10	0.51
1:A:526:HIS:CE1	1:A:694:HIS:HD2	2.28	0.51
1:B:430:VAL:HG21	1:B:462:ILE:HD12	1.91	0.51
1:B:419:ARG:CD	1:B:433:ASP:OD1	2.59	0.51
1:B:542:PHE:CD1	1:B:611:LEU:HD13	2.45	0.51
1:A:107:TYR:HA	4:A:1084:HOH:O	2.10	0.50
1:A:635:HIS:CE1	1:A:664:ASP:H	2.27	0.50
1:B:381:GLU:O	1:B:382:SER:HB2	2.11	0.50
1:A:472:ILE:HG12	1:A:473:ALA:N	2.27	0.50
1:B:117:VAL:O	1:B:118:ASP:HB3	2.11	0.50
2:D:1:GLC:C1	2:D:1:GLC:C5	2.74	0.50
1:A:82:THR:HA	1:A:120:PHE:CE2	2.47	0.49
1:A:30:VAL:HG13	4:A:1106:HOH:O	2.11	0.49
1:A:296:ASN:C	1:A:296:ASN:ND2	2.62	0.49
1:B:203:LEU:HB2	4:B:993:HOH:O	2.12	0.49
1:A:391:VAL:O	1:A:391:VAL:HG13	2.13	0.49
1:A:258:PHE:HB2	1:A:284:ILE:HG12	1.95	0.49
1:B:519:ASP:HB3	4:B:947:HOH:O	2.13	0.49
1:A:305:THR:CG2	4:A:1062:HOH:O	2.60	0.49
1:A:472:ILE:HG23	1:A:473:ALA:N	2.26	0.49
1:A:643:LYS:HE2	1:A:671:LEU:O	2.13	0.48
1:B:352:LEU:O	1:B:355:LEU:HD23	2.13	0.48
1:A:619:PHE:C	4:A:1097:HOH:O	2.51	0.48
1:B:10:ARG:CB	4:B:1022:HOH:O	2.61	0.48
1:B:635:HIS:O	1:B:639:MET:HG2	2.13	0.48
1:B:631:VAL:O	1:B:635:HIS:HB3	2.13	0.48
1:B:187:TRP:HA	1:B:305:THR:HG21	1.96	0.48
1:B:152:LEU:HD22	1:B:228:TRP:CD2	2.49	0.48
1:B:417:CYS:HA	1:B:434:ARG:O	2.13	0.48
1:A:631:VAL:HG23	4:A:1091:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:ARG:C	1:B:134:ALA:N	2.67	0.48
1:A:571:ARG:O	1:A:575:GLU:HG2	2.13	0.48
1:B:348:SER:N	1:B:349:PRO:HD3	2.29	0.48
1:A:579:ARG:NH1	4:A:941:HOH:O	2.47	0.47
1:B:542:PHE:HD1	1:B:611:LEU:HD13	1.80	0.47
1:A:413:GLU:HB3	1:A:415:ILE:HG23	1.96	0.47
1:A:305:THR:HG21	1:A:341:ASN:HD22	1.79	0.47
1:A:23:LEU:HD23	1:A:23:LEU:O	2.15	0.47
1:A:306:VAL:HG13	1:A:333:MET:CE	2.46	0.46
1:A:369:PRO:HG2	4:A:1085:HOH:O	2.14	0.46
1:B:349:PRO:HD2	4:B:953:HOH:O	2.15	0.46
1:B:292:ALA:HA	1:B:328:LEU:CD1	2.45	0.46
1:B:420:LEU:HA	1:B:420:LEU:HD12	1.62	0.46
1:B:371:ASP:N	1:B:371:ASP:OD1	2.49	0.46
1:A:173:ILE:HG23	1:A:177:LEU:HD23	1.96	0.46
1:A:312:TYR:O	1:A:313:GLY:C	2.54	0.46
1:A:41:THR:HG23	4:A:974:HOH:O	2.16	0.46
1:A:228[A]:TRP:CE2	1:A:230:GLN:HB2	2.50	0.46
1:B:84[B]:MET:HG2	1:B:228:TRP:CZ2	2.51	0.46
1:B:442:GLN:HB3	4:B:943:HOH:O	2.16	0.46
1:B:684:SER:O	1:B:685:GLN:HB2	2.14	0.46
1:A:344:LEU:O	1:A:374:GLN:HA	2.16	0.46
1:A:564:THR:OG1	1:A:591:HIS:HD2	1.98	0.45
1:B:257:HIS:CE1	1:B:285:THR:OG1	2.65	0.45
1:B:166:ASP:HB2	4:B:1026:HOH:O	2.17	0.45
1:B:319:GLU:HA	1:B:320:PRO:HD3	1.74	0.45
1:A:152:LEU:HD22	1:A:228[B]:TRP:CD2	2.52	0.45
1:B:443:GLU:HA	4:B:1059:HOH:O	2.16	0.45
1:A:240:LYS:HE2	4:A:950:HOH:O	2.16	0.45
1:A:591:HIS:HE1	4:A:1013:HOH:O	1.98	0.45
1:A:417:CYS:HA	1:A:434:ARG:O	2.16	0.45
1:A:632:GLN:O	1:A:635:HIS:HD2	2.00	0.45
1:B:103:ARG:O	1:B:106:GLN:HB2	2.17	0.45
1:A:400:ARG:CD	4:A:1020:HOH:O	2.62	0.45
1:A:446:PRO:HA	4:A:1035:HOH:O	2.16	0.44
1:B:305:THR:HG22	4:B:929:HOH:O	2.17	0.44
1:A:472:ILE:HG12	1:A:473:ALA:H	1.81	0.44
1:B:132:ARG:O	1:B:134:ALA:N	2.36	0.44
1:A:690:ASN:C	1:A:690:ASN:ND2	2.66	0.44
1:B:607:GLU:H	1:B:607:GLU:HG2	1.53	0.44
1:A:82:THR:HG21	1:A:123:LYS:HD2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:668:LEU:HD23	1:A:675:ALA:HB2	2.00	0.44
1:B:194:LEU:HD23	1:B:195:ASP:N	2.33	0.44
1:B:214:ARG:CD	1:B:280:ILE:HD13	2.48	0.44
1:B:352:LEU:O	1:B:355:LEU:CD2	2.66	0.44
1:A:56:ARG:HA	1:A:155:SER:OG	2.17	0.44
1:A:160:HIS:H	1:A:160:HIS:CD2	2.35	0.43
1:A:475:ASN:HB2	4:A:1073:HOH:O	2.17	0.43
1:B:632:GLN:HB2	1:B:658:LYS:HE3	1.99	0.43
1:B:399:LEU:O	1:B:403:LEU:HB2	2.18	0.43
1:A:380:ALA:O	1:A:381:GLU:HB2	2.18	0.43
1:A:380:ALA:O	1:A:381:GLU:HB3	2.17	0.43
1:A:546:PHE:CD1	1:A:617:PRO:HD3	2.53	0.43
1:A:657:ASN:HB3	1:A:694:HIS:ND1	2.33	0.43
1:A:214:ARG:HD2	1:A:280:ILE:HD13	2.00	0.43
2:C:1:GLC:O5	2:C:1:GLC:C2	2.30	0.43
1:A:82:THR:HA	1:A:120:PHE:CZ	2.53	0.43
1:B:296:ASN:HA	1:B:297:PRO:HD3	1.88	0.43
1:A:112:VAL:O	1:A:116:ILE:HG13	2.19	0.43
1:A:214:ARG:CD	1:A:280:ILE:HD13	2.49	0.43
1:B:160:HIS:CD2	1:B:160:HIS:H	2.37	0.43
1:B:432:VAL:HG22	1:B:441:VAL:HG22	2.01	0.43
1:A:2:ASN:O	1:A:38:LYS:HA	2.19	0.42
1:B:403:LEU:HD23	1:B:403:LEU:O	2.19	0.42
1:A:272:ARG:NH1	1:A:286:PHE:O	2.52	0.42
1:B:129:ASN:O	1:B:130:VAL:CB	2.67	0.42
1:B:296:ASN:HB2	1:B:336:GLN:HG2	2.01	0.42
1:B:367:ASN:OD1	1:B:367:ASN:C	2.57	0.42
1:B:398:ARG:HE	1:B:402:ASN:HD22	1.68	0.42
1:B:410:ALA:O	1:B:411:ARG:CB	2.66	0.42
1:A:653:MET:HA	1:A:697:TRP:O	2.20	0.42
1:A:602:LEU:HA	1:A:602:LEU:HD23	1.78	0.42
1:B:196:PRO:HD2	1:B:308:SER:HB2	2.00	0.42
1:B:355:LEU:O	1:B:356:GLN:HB2	2.19	0.42
1:B:695:ASN:ND2	1:B:697:TRP:HE1	2.16	0.42
1:B:506:TYR:CE2	1:B:527:ARG:HG3	2.55	0.42
1:B:429:ASN:ND2	1:B:444:TYR:HB2	2.35	0.42
1:A:526:HIS:ND1	1:A:694:HIS:CD2	2.82	0.42
1:A:606:ASN:O	1:A:607:GLU:O	2.38	0.42
1:B:242:GLU:O	1:B:246:ARG:HB2	2.19	0.42
1:B:425:LEU:HA	1:B:426:PRO:HD3	1.80	0.42
1:B:618:THR:HA	1:B:631:VAL:HG23	1.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:THR:HG22	4:A:1062:HOH:O	2.21	0.41
1:A:636:LEU:HD22	1:A:671:LEU:HD11	2.01	0.41
1:A:187:TRP:CD1	1:A:305:THR:HG23	2.50	0.41
1:A:305:THR:CB	1:A:341:ASN:HB3	2.50	0.41
1:A:152:LEU:HD22	1:A:228[B]:TRP:CE2	2.55	0.41
1:B:165:ARG:CG	1:B:166:ASP:N	2.62	0.41
1:A:462:ILE:O	1:A:466:THR:HG23	2.18	0.41
1:B:678:ILE:H	1:B:678:ILE:HG13	1.73	0.41
1:A:369:PRO:HD2	4:A:1085:HOH:O	2.20	0.41
1:B:114:ASP:HA	1:B:115:ALA:HA	1.94	0.41
1:B:607:GLU:HG3	1:B:609:PHE:CZ	2.56	0.41
1:B:194:LEU:HD23	1:B:194:LEU:C	2.41	0.41
1:B:259:TYR:CD2	1:B:259:TYR:N	2.89	0.41
1:B:632:GLN:O	1:B:635:HIS:HD2	2.04	0.41
1:A:688:ALA:C	1:A:690:ASN:H	2.23	0.41
1:B:187:TRP:HA	1:B:305:THR:CG2	2.51	0.41
1:B:602:LEU:HA	1:B:602:LEU:HD23	1.91	0.41
1:A:618:THR:HG22	4:A:937:HOH:O	2.20	0.40
1:B:86:ASN:HD22	1:B:86:ASN:HA	1.74	0.40
1:B:547:SER:CB	1:B:566:THR:HG23	2.51	0.40
1:B:291:VAL:O	1:B:294:LEU:HB2	2.21	0.40
1:B:497:LYS:N	4:B:997:HOH:O	2.53	0.40
1:B:409:TRP:C	1:B:410:ALA:O	2.57	0.40
1:A:580:ASN:HD22	1:A:580:ASN:HA	1.69	0.40
1:B:41:THR:O	1:B:44:VAL:HB	2.21	0.40
1:B:307:LEU:HA	1:B:343:SER:O	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]	2.10	0.10

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	653/702 (93%)	616 (94%)	31 (5%)	6 (1%)	17 35
1	B	615/702 (88%)	560 (91%)	39 (6%)	16 (3%)	5 9
All	All	1268/1404 (90%)	1176 (93%)	70 (6%)	22 (2%)	9 18

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	SER
1	A	472	ILE
1	B	130	VAL
1	A	607	GLU
1	B	31	VAL
1	B	32	GLN
1	B	118	ASP
1	B	132	ARG
1	B	133	ASP
1	B	367	ASN
1	B	381	GLU
1	B	670	LYS
1	B	685	GLN
1	B	10	ARG
1	B	120	PHE
1	A	689	ARG
1	B	689	ARG
1	A	170	ILE
1	B	129	ASN
1	B	436	ALA
1	A	391	VAL
1	B	301	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	519/581 (89%)	444 (86%)	75 (14%)	3 5
1	B	466/581 (80%)	396 (85%)	70 (15%)	3 5
All	All	985/1162 (85%)	840 (85%)	145 (15%)	3 5

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	23	LEU
1	A	31	VAL
1	A	59	LEU
1	A	61	LEU
1	A	74	LEU
1	A	80	ASN
1	A	101	THR
1	A	105	SER
1	A	111	LYS
1	A	122	ARG
1	A	124	ASN
1	A	125	LEU
1	A	130	VAL
1	A	139	VAL
1	A	141	VAL
1	A	150	ILE
1	A	165	ARG
1	A	182	VAL
1	A	204	LEU
1	A	246	ARG
1	A	249	LYS
1	A	251	LEU
1	A	266	ARG
1	A	269	GLN
1	A	282	GLU
1	A	293	GLN
1	A	296	ASN
1	A	305	THR
1	A	328	LEU
1	A	331	ARG
1	A	342	LEU
1	A	344	LEU
1	A	362	GLN
1	A	379	VAL

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Mol	Chain	Res	Type
1	A	393	GLU
1	A	412	GLN
1	A	415	ILE
1	A	419	ARG
1	A	424	ASP
1	A	430	VAL
1	A	434	ARG
1	A	441	VAL
1	A	454	LYS
1	A	459	LEU
1	A	466	THR
1	A	468	SER
1	A	483	GLU
1	A	501	LEU
1	A	503	VAL
1	A	507	ASN
1	A	514	LEU
1	A	518	LEU
1	A	526	HIS
1	A	537	SER
1	A	540	LYS
1	A	558	LEU
1	A	567	VAL
1	A	582	ARG
1	A	583	LEU
1	A	599	LEU
1	A	607	GLU
1	A	611	LEU
1	A	618	THR
1	A	631	VAL
1	A	636	LEU
1	A	644	ARG
1	A	646	LEU
1	A	665	LEU
1	A	666	ASP
1	A	668	LEU
1	A	684	SER
1	A	690	ASN
1	A	694	HIS
1	A	698	LEU
1	B	4	LEU
1	B	18	THR

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Mol	Chain	Res	Type
1	B	31	VAL
1	B	41	THR
1	B	42	ARG
1	B	61	LEU
1	B	74	LEU
1	B	77	GLN
1	B	82	THR
1	B	121	THR
1	B	133	ASP
1	B	155	SER
1	B	161	LEU
1	B	200	SER
1	B	203	LEU
1	B	204	LEU
1	B	238	GLU
1	B	246	ARG
1	B	251	LEU
1	B	256	SER
1	B	273	THR
1	B	288	VAL
1	B	289	LYS
1	B	290	ASP
1	B	291	VAL
1	B	294	LEU
1	B	298	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	348	SER
1	B	360	ASP
1	B	370	LEU
1	B	371	ASP
1	B	379	VAL
1	B	382	SER
1	B	394	ASP
1	B	412	GLN
1	B	415	ILE
1	B	419	ARG
1	B	420	LEU

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Mol	Chain	Res	Type
1	B	425	LEU
1	B	459	LEU
1	B	462	ILE
1	B	466	THR
1	B	470	LEU
1	B	501	LEU
1	B	507	ASN
1	B	514	LEU
1	B	526	HIS
1	B	527	ARG
1	B	558	LEU
1	B	567	VAL
1	B	575	GLU
1	B	583	LEU
1	B	607	GLU
1	B	611	LEU
1	B	618	THR
1	B	631	VAL
1	B	646	LEU
1	B	651	THR
1	B	658	LYS
1	B	670	LYS
1	B	678	ILE
1	B	681	LYS
1	B	683	LEU
1	B	684	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	80	ASN
1	A	104	ASN
1	A	160	HIS
1	A	257	HIS
1	A	269	GLN
1	A	293	GLN
1	A	296	ASN
1	A	309	ASN
1	A	341	ASN
1	A	402	ASN
1	A	507	ASN

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Mol	Chain	Res	Type
1	A	509	HIS
1	A	580	ASN
1	A	591	HIS
1	A	635	HIS
1	A	685	GLN
1	A	690	ASN
1	A	694	HIS
1	B	77	GLN
1	B	86	ASN
1	B	140	ASN
1	B	160	HIS
1	B	257	HIS
1	B	309	ASN
1	B	336	GLN
1	B	397	ASN
1	B	402	ASN
1	B	412	GLN
1	B	429	ASN
1	B	507	ASN
1	B	580	ASN
1	B	591	HIS
1	B	608	GLN
1	B	635	HIS
1	B	676	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	10.35	6 (54%)	15,15,17	3.20	6 (40%)
2	TRV	C	2	2	19,20,21	2.18	5 (26%)	19,27,28	2.12	6 (31%)
2	GLC	D	1	2	11,11,12	10.74	6 (54%)	15,15,17	2.95	7 (46%)
2	TRV	D	2	2	18,19,21	2.59	6 (33%)	18,26,28	1.82	3 (16%)

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	-	8/14/33/34	0/1/1/1
2	GLC	D	1	2	-	0/2/19/22	0/1/1/1
2	TRV	D	2	2	-	6/13/32/34	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	-22.19	1.06	1.53
2	C	1	GLC	C4-C5	-21.57	1.07	1.53
2	D	1	GLC	C1-C2	-19.82	1.06	1.52
2	C	1	GLC	C1-C2	-19.33	1.08	1.52
2	D	1	GLC	O5-C1	13.90	1.65	1.43
2	C	1	GLC	O5-C1	13.86	1.65	1.43
2	D	1	GLC	C2-C3	8.92	1.65	1.52
2	C	1	GLC	C2-C3	7.85	1.64	1.52
2	D	1	GLC	O5-C5	7.40	1.58	1.43
2	D	1	GLC	C4-C3	7.16	1.70	1.52
2	D	2	TRV	O1N-C1N	6.81	1.42	1.22
2	C	1	GLC	C4-C3	6.63	1.69	1.52
2	C	1	GLC	O5-C5	6.48	1.56	1.43
2	D	2	TRV	C1-C2	-4.84	1.44	1.52
2	C	2	TRV	O2-C2	4.82	1.49	1.40
2	C	2	TRV	C1-C2	-4.44	1.45	1.52
2	C	2	TRV	O1N-C1N	4.37	1.35	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	TRV	O5-C2	-3.59	1.37	1.43
2	D	2	TRV	O2-C2	3.53	1.46	1.40
2	D	2	TRV	O6-C1N	3.52	1.43	1.33
2	C	2	TRV	O6-C1N	2.50	1.40	1.33
2	D	2	TRV	C2N-C1N	2.49	1.58	1.50
2	C	2	TRV	O5-C2	-2.44	1.39	1.43

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1	GLC	O2-C2-C1	7.06	123.59	109.15
2	D	1	GLC	O4-C4-C5	6.09	124.41	109.30
2	D	1	GLC	O2-C2-C1	5.98	121.38	109.15
2	D	2	TRV	O6-C1N-O1N	-5.14	110.62	123.59
2	C	1	GLC	O4-C4-C5	4.98	121.66	109.30
2	C	1	GLC	O4-C4-C3	-4.81	99.22	110.35
2	C	2	TRV	O1N-C1N-C2N	-4.72	105.32	123.73
2	C	1	GLC	O5-C5-C6	-4.63	99.95	107.20
2	C	2	TRV	O1-C1-C2	4.58	121.59	111.86
2	D	1	GLC	O5-C1-C2	-4.26	104.19	110.77
2	C	1	GLC	O2-C2-C3	-3.73	102.67	110.14
2	C	2	TRV	O4-C4-C3	3.40	122.33	112.15
2	C	2	TRV	O6-C1N-O1N	-3.39	115.03	123.59
2	D	1	GLC	O3-C3-C2	3.33	116.36	109.99
2	C	1	GLC	O3-C3-C2	3.06	115.86	109.99
2	D	1	GLC	O5-C5-C4	-2.90	103.78	110.83
2	C	2	TRV	C4N-C3N-C2N	2.77	123.14	113.19
2	D	2	TRV	O6-C1N-C2N	2.56	119.95	111.91
2	D	2	TRV	O6-C6-C5	2.43	113.59	108.43
2	D	1	GLC	C1-O5-C5	2.42	115.47	112.19
2	C	2	TRV	O6-C1N-C2N	2.40	119.45	111.91
2	D	1	GLC	C1-C2-C3	-2.25	106.90	109.67

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2	TRV	O1-C1-C2-O2
2	D	2	TRV	O1-C1-C2-O2
2	D	2	TRV	C2N-C3N-C4N-C5N
2	C	2	TRV	C3N-C4N-C5N-C6N
2	D	2	TRV	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	C	2	TRV	O1N-C1N-O6-C6
2	D	2	TRV	C3N-C4N-C5N-C6N
2	C	2	TRV	O1-C1-C2-O5
2	D	2	TRV	C1N-C2N-C3N-C4N
2	C	2	TRV	O1-C1-C2-C3
2	D	2	TRV	O1-C1-C2-O5
2	C	2	TRV	C2N-C3N-C4N-C5N
2	C	2	TRV	O5-C5-C6-O6
2	C	2	TRV	O1N-C1N-C2N-C3N

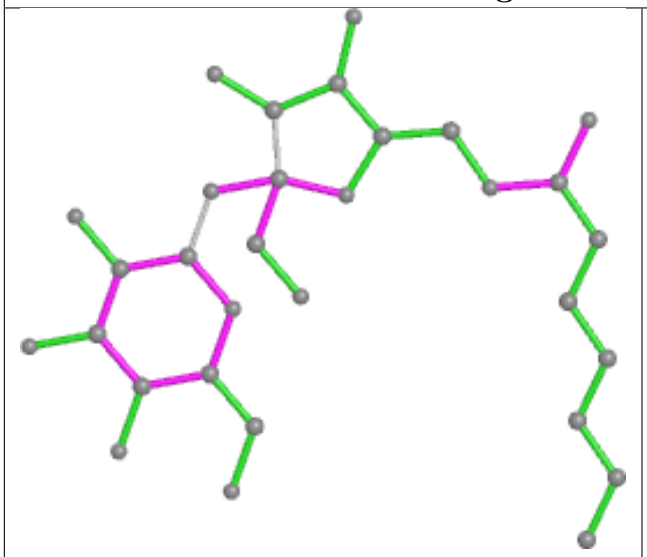
There are no ring outliers.

2 monomers are involved in 6 short contacts:

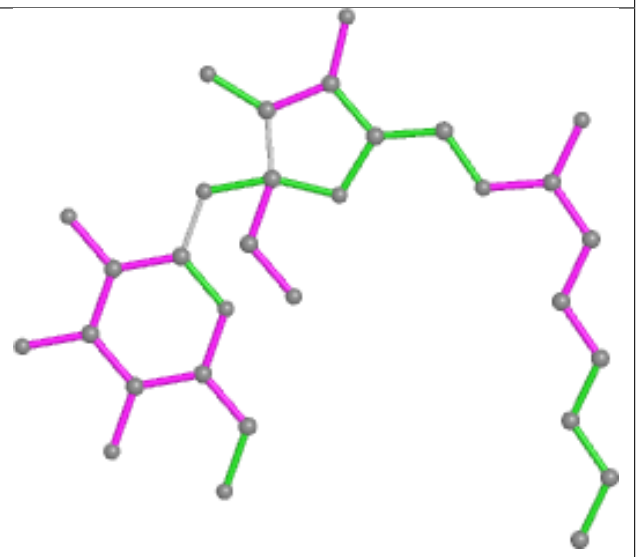
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	GLC	3	0
2	C	1	GLC	3	0

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

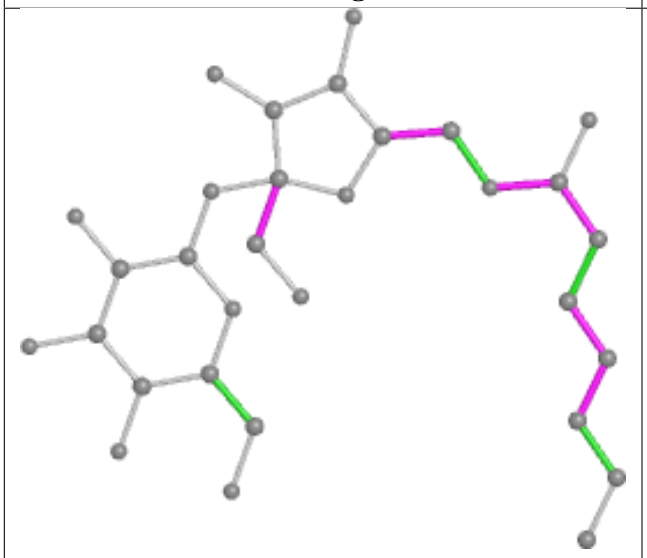
Oligosaccharide Chain C



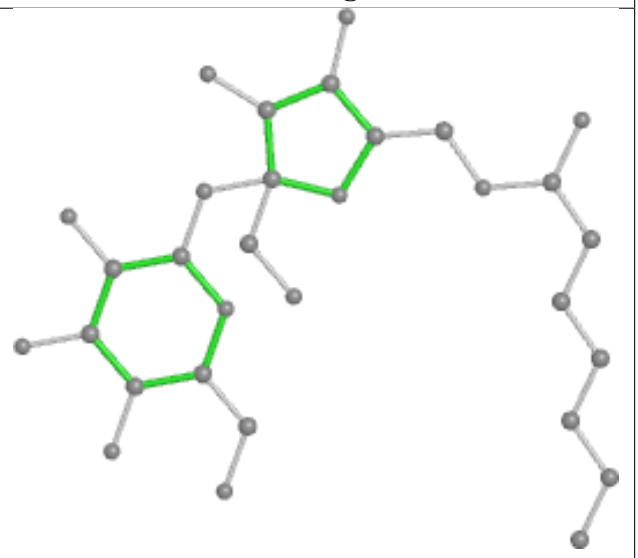
Bond lengths



Bond angles

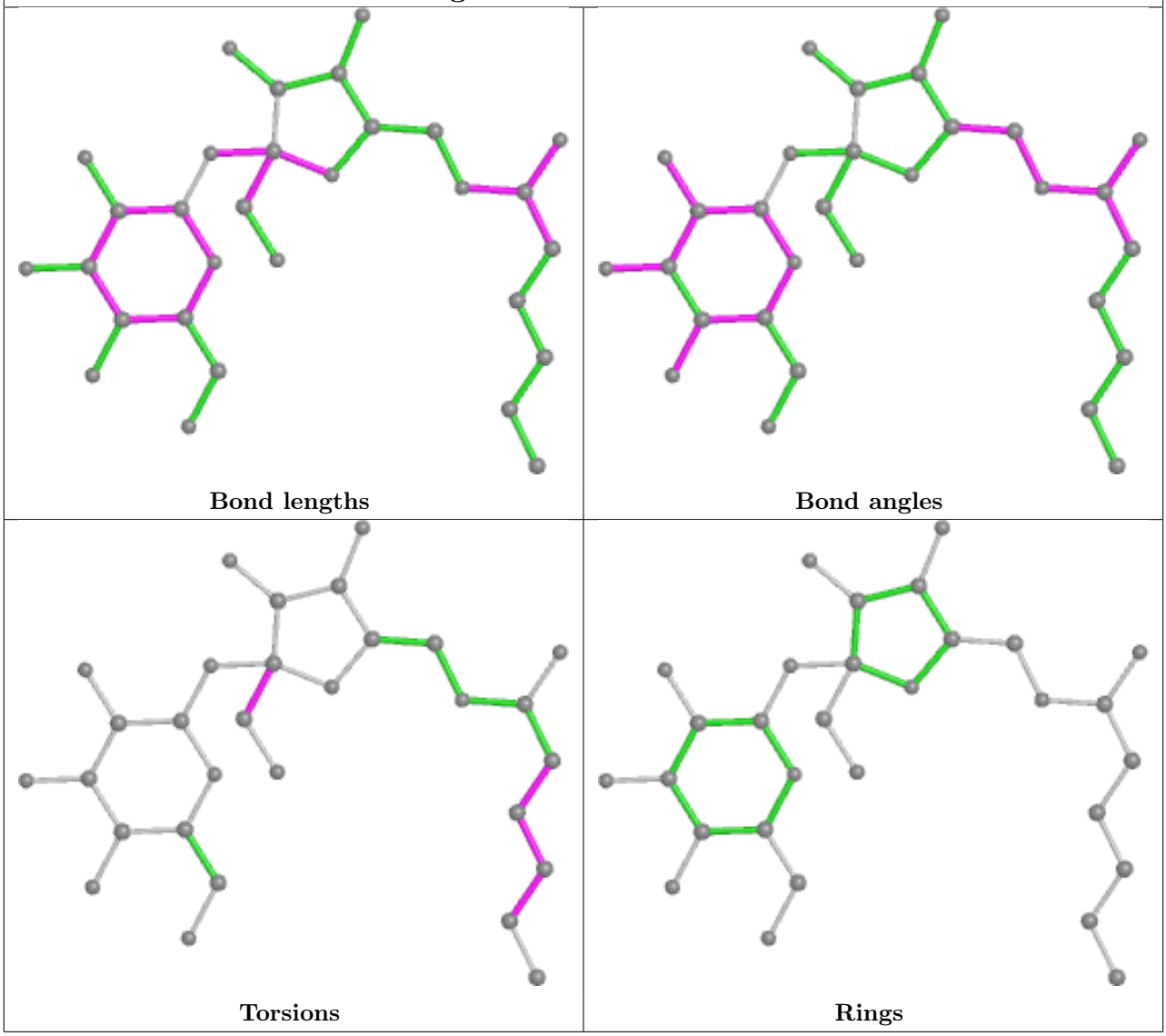


Torsions



Rings

Oligosaccharide Chain D



5.6 Ligand geometry (i)

4 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	SAM	A	802	-	18,21,29	1.34	2 (11%)	18,31,42	1.63	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SAM	B	801	-	24,28,29	1.45	2 (8%)	25,40,42	1.47	4 (16%)
3	SAM	B	802	-	23,27,29	1.21	2 (8%)	20,38,42	1.30	1 (5%)
3	SAM	A	801	-	24,28,29	1.31	1 (4%)	25,40,42	1.72	5 (20%)

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	SAM	A	802	-	-	0/2/22/33	0/3/3/3
3	SAM	B	801	-	-	2/11/31/33	0/3/3/3
3	SAM	B	802	-	-	4/8/29/33	0/3/3/3
3	SAM	A	801	-	-	6/11/31/33	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	SAM	C2-N3	5.47	1.40	1.32
3	A	801	SAM	C2-N3	3.87	1.38	1.32
3	A	802	SAM	C2-N3	3.69	1.38	1.32
3	B	802	SAM	C2-N3	3.28	1.37	1.32
3	B	801	SAM	C2-N1	3.17	1.39	1.33
3	A	802	SAM	C2-N1	2.72	1.39	1.33
3	B	802	SAM	O4'-C4'	-2.39	1.39	1.45

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	801	SAM	N3-C2-N1	-6.20	118.99	128.68
3	A	802	SAM	N3-C2-N1	-4.96	120.92	128.68
3	B	801	SAM	N3-C2-N1	-4.10	122.28	128.68
3	B	802	SAM	N3-C2-N1	-3.81	122.72	128.68
3	A	801	SAM	OXT-C-O	-2.66	118.05	124.09
3	A	802	SAM	C1'-N9-C4	-2.66	121.97	126.64
3	A	801	SAM	O4'-C1'-C2'	-2.62	103.09	106.93
3	B	801	SAM	O4'-C1'-C2'	-2.60	103.13	106.93
3	B	801	SAM	OXT-C-O	-2.59	118.20	124.09
3	B	801	SAM	OXT-C-CA	2.36	121.43	113.38
3	A	802	SAM	O2'-C2'-C3'	2.20	118.95	111.82
3	A	801	SAM	C4-C5-N7	-2.14	107.16	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	801	SAM	OXT-C-CA	2.13	120.65	113.38

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	SAM	C-CA-CB-CG
3	B	801	SAM	O4'-C4'-C5'-SD
3	B	802	SAM	O-C-CA-CB
3	B	802	SAM	C-CA-CB-CG
3	A	801	SAM	N-CA-CB-CG
3	B	801	SAM	C3'-C4'-C5'-SD
3	B	802	SAM	C3'-C4'-C5'-SD
3	A	801	SAM	C4'-C5'-SD-CG
3	A	801	SAM	OXT-C-CA-CB
3	B	802	SAM	CA-CB-CG-SD
3	A	801	SAM	O-C-CA-N
3	A	801	SAM	O-C-CA-CB

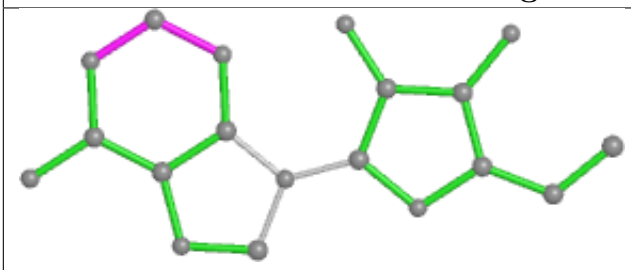
There are no ring outliers.

2 monomers are involved in 5 short contacts:

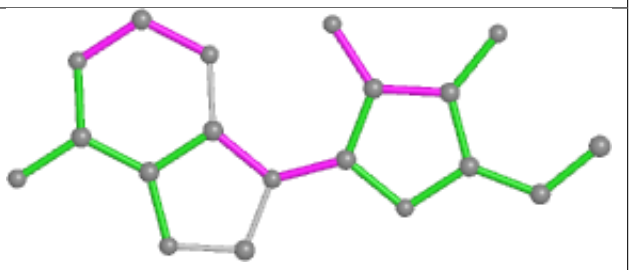
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	801	SAM	4	0
3	B	802	SAM	1	0

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.

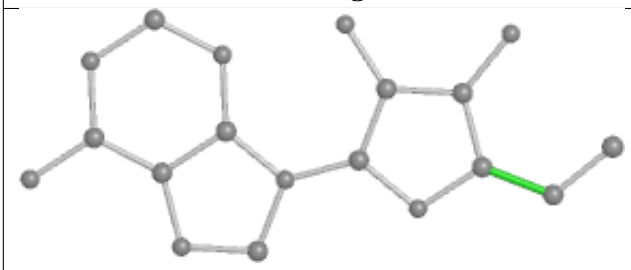
Ligand SAM A 802



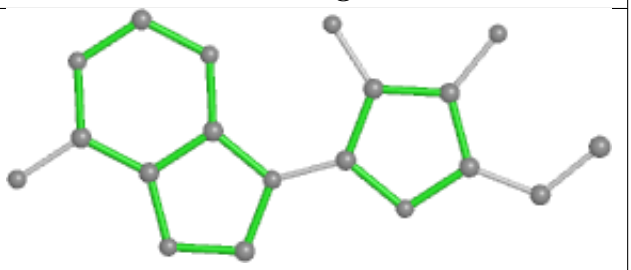
Bond lengths



Bond angles

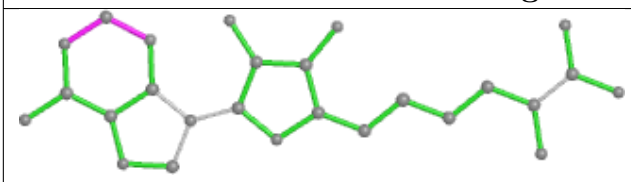


Torsions

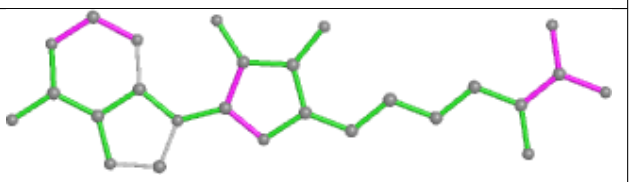


Rings

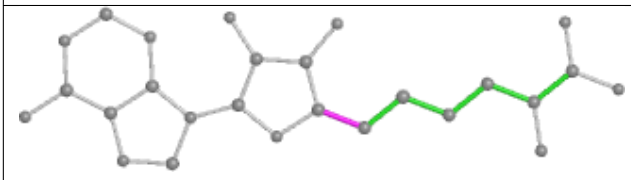
Ligand SAM B 801



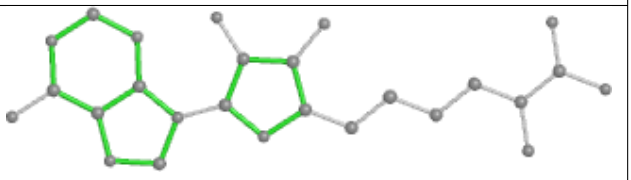
Bond lengths



Bond angles

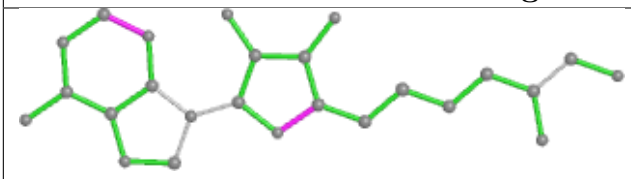


Torsions

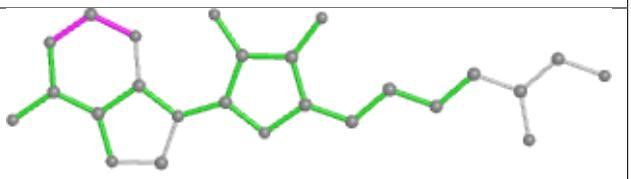


Rings

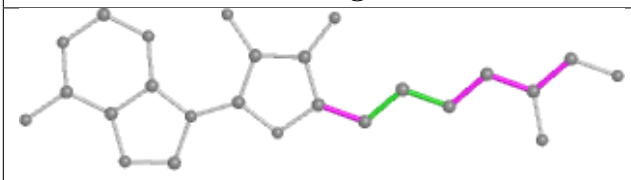
Ligand SAM B 802



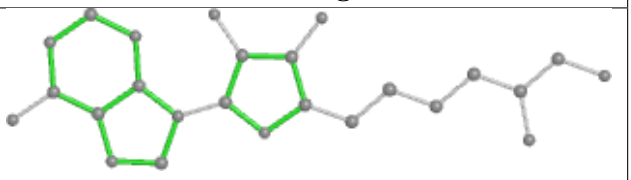
Bond lengths



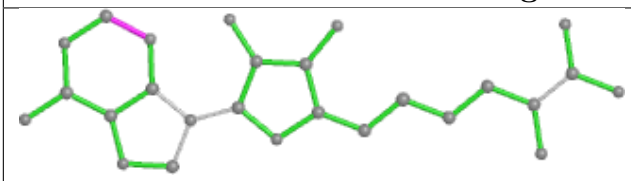
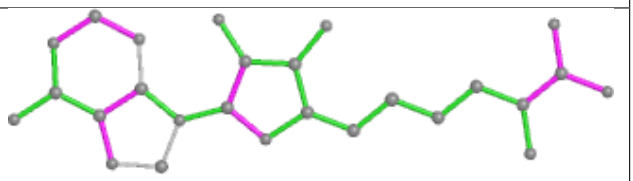
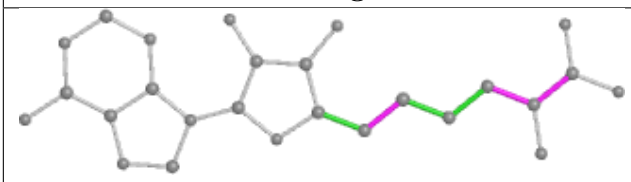
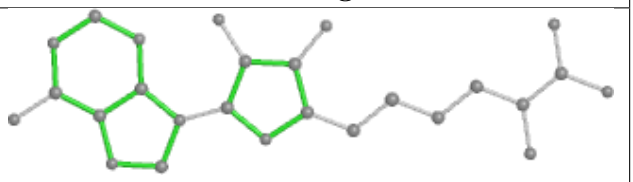
Bond angles



Torsions



Rings

Ligand SAM A 801	
 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	664/702 (94%)	-0.40	3 (0%)	91	89	33, 55, 85, 101	0
1	B	636/702 (90%)	-0.19	27 (4%)	36	29	33, 69, 112, 139	0
All	All	1300/1404 (92%)	-0.29	30 (2%)	60	54	33, 62, 100, 139	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	61	LEU	4.2
1	B	131	ASP	3.7
1	B	318	SER	3.6
1	B	62	GLY	3.5
1	B	85	PHE	3.5
1	B	64	CYS	3.3
1	B	117	VAL	3.1
1	B	455	ALA	3.0
1	A	142	TRP	2.9
1	B	84[A]	MET	2.9
1	B	110	MET	2.9
1	B	103	ARG	2.8
1	B	74	LEU	2.8
1	B	137	ILE	2.8
1	B	70	LEU	2.7
1	B	152	LEU	2.6
1	A	318	SER	2.5
1	B	128	PRO	2.4
1	B	620	SER	2.4
1	B	87	PRO	2.4
1	B	73	TYR	2.3
1	B	93	VAL	2.3
1	B	76	VAL	2.1
1	B	126	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	621	ASN	2.1
1	B	412	GLN	2.1
1	B	445	ALA	2.1
1	A	170	ILE	2.1
1	B	80	ASN	2.1
1	B	79	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

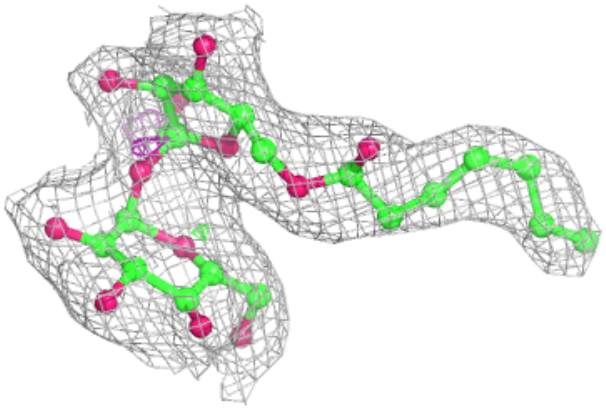
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

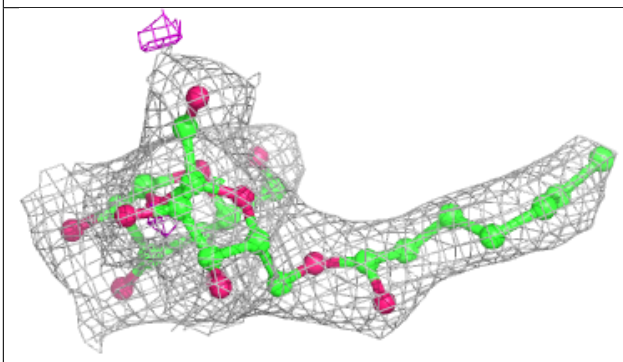
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLC	C	1	11/12	0.96	0.16	31,41,43,44	0
2	TRV	D	2	19/21	0.96	0.17	49,58,69,72	0
2	GLC	D	1	11/12	0.97	0.13	48,52,53,55	0
2	TRV	C	2	20/21	0.97	0.16	34,43,50,50	0

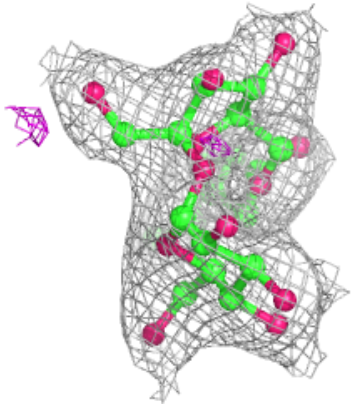
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

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)

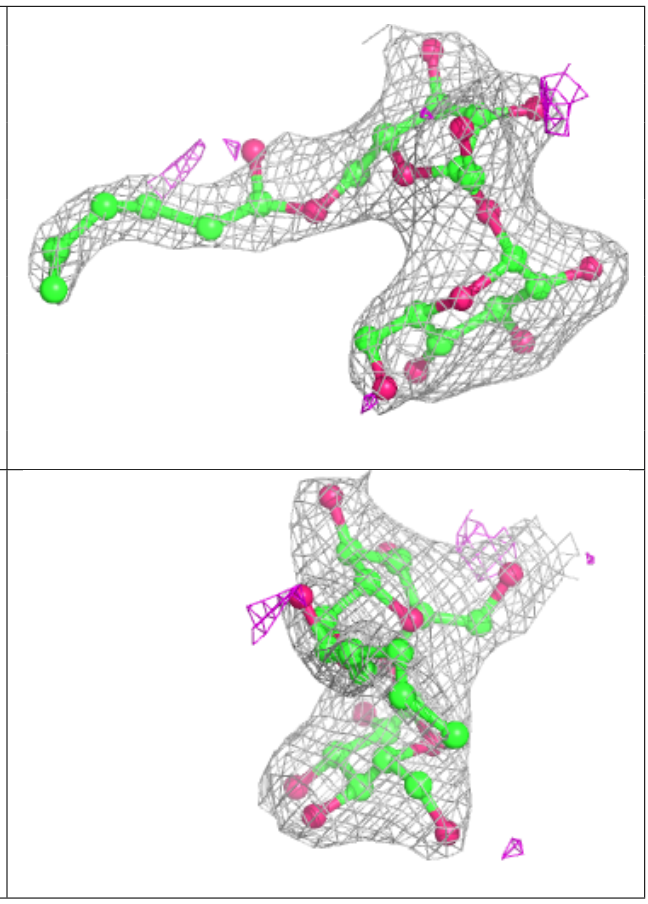






Electron density around Chain D:

$2mF_o$-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)

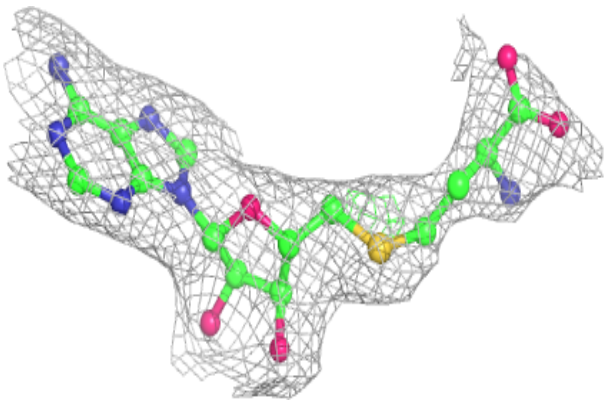
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

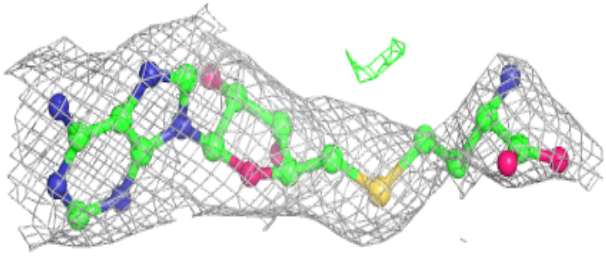
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SAM	B	801	26/27	0.94	0.17	54,76,98,99	0
3	SAM	B	802	25/27	0.96	0.15	52,58,84,85	0
3	SAM	A	801	26/27	0.97	0.13	35,49,81,81	0
3	SAM	A	802	19/27	0.97	0.13	65,69,71,74	0

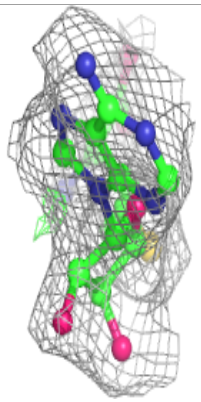
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAM 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)

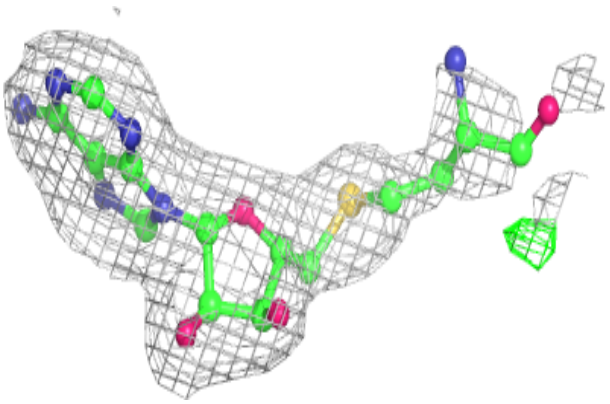


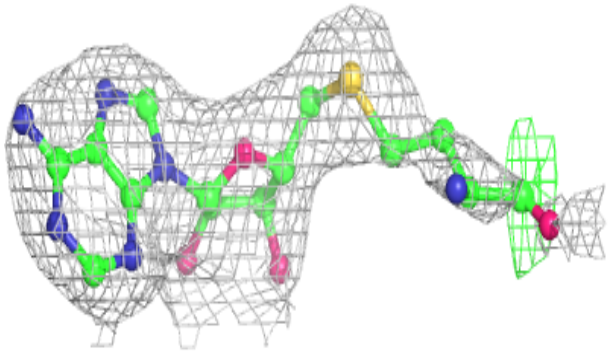


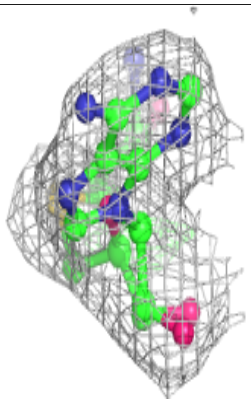


Electron density around SAM B 802:

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

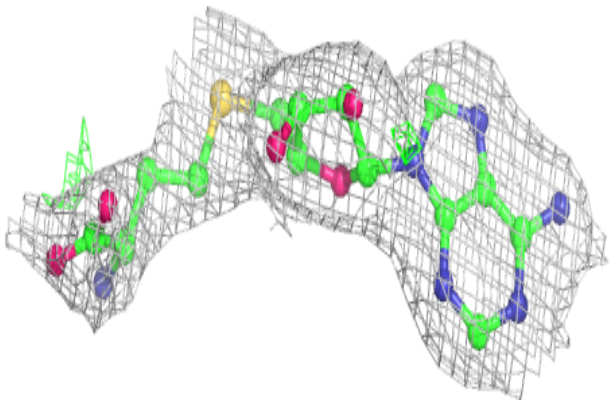


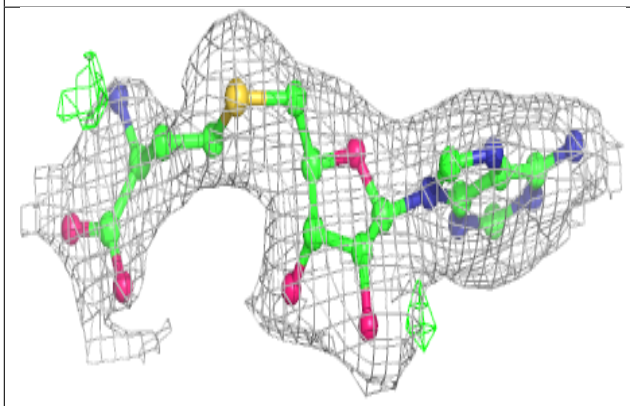


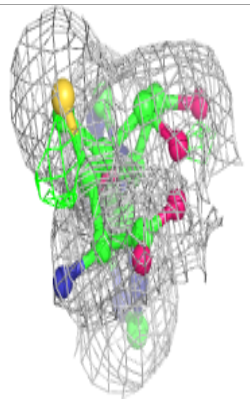


Electron density around SAM A 801:

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

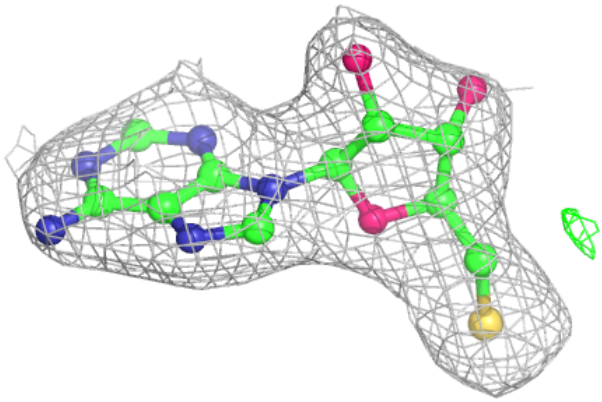


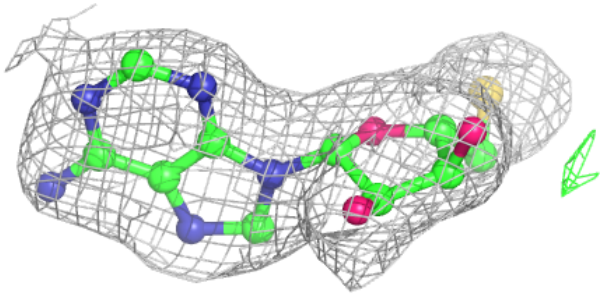


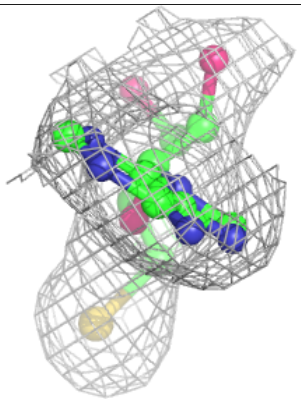


Electron density around SAM A 802:

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







6.5 Other polymers (i)

There are no such residues in this entry.