Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 07:50 AM EDT

PDB ID	:	6W89
Title	:	Structure of DNMT3A (R882H) in complex with CGA DNA
Authors	:	Anteneh, H.; Song, J.
Deposited on	:	2020-03-20
Resolution	:	2.50 Å(reported)

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

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

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

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

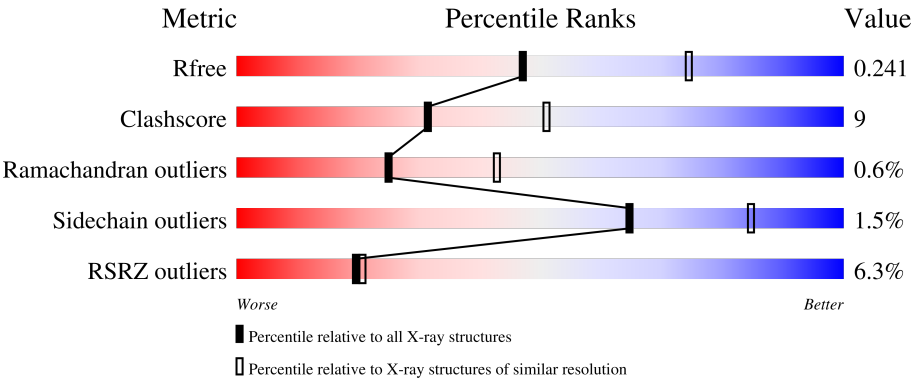
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	285	85% 15%
1	D	285	% 90% 10%
1	G	285	87% 13%
1	J	285	% 88% 12%
2	B	209	13% 67% 26% 7%

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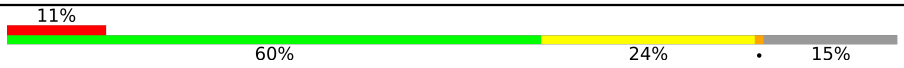
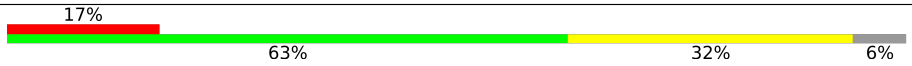
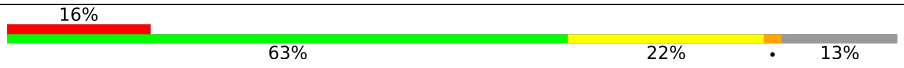
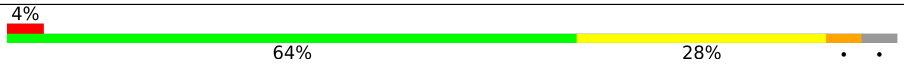
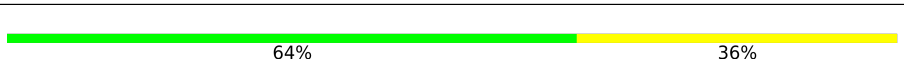
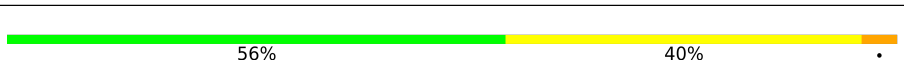
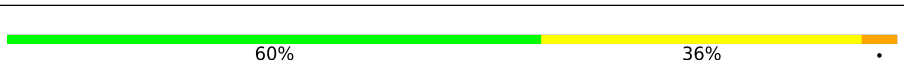
Mol	Chain	Length	Quality of chain
2	C	209	
2	H	209	
2	I	209	
3	E	25	
3	F	25	
3	K	25	
3	L	25	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 17145 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 DNA (cytosine-5)-methyltransferase 3A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	2	0
			2284	1458	407	406	13			
1	D	285	Total	C	N	O	S	0	3	0
			2300	1469	413	405	13			
1	G	284	Total	C	N	O	S	0	3	0
			2289	1462	410	404	13			
1	J	285	Total	C	N	O	S	0	4	0
			2308	1474	414	407	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	882	HIS	ARG	engineered mutation	UNP Q9Y6K1
D	882	HIS	ARG	engineered mutation	UNP Q9Y6K1
G	882	HIS	ARG	engineered mutation	UNP Q9Y6K1
J	882	HIS	ARG	engineered mutation	UNP Q9Y6K1

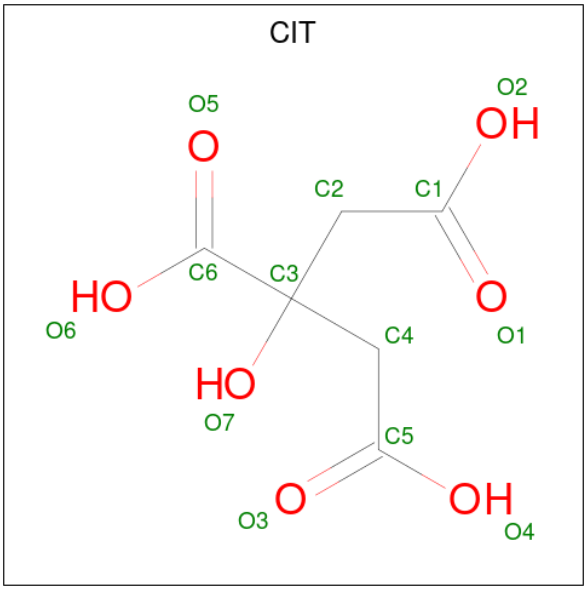
- Molecule 2 is a protein called DNA (cytosine-5)-methyltransferase 3-like.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	194	Total	C	N	O	S	0	1	0
			1464	953	241	267	3			
2	C	178	Total	C	N	O	S	0	0	0
			1275	823	215	235	2			
2	H	197	Total	C	N	O	S	0	0	0
			1477	966	242	265	4			
2	I	182	Total	C	N	O	S	0	0	0
			1314	851	224	237	2			

- Molecule 3 is a DNA chain called CGA DNA (25-MER).

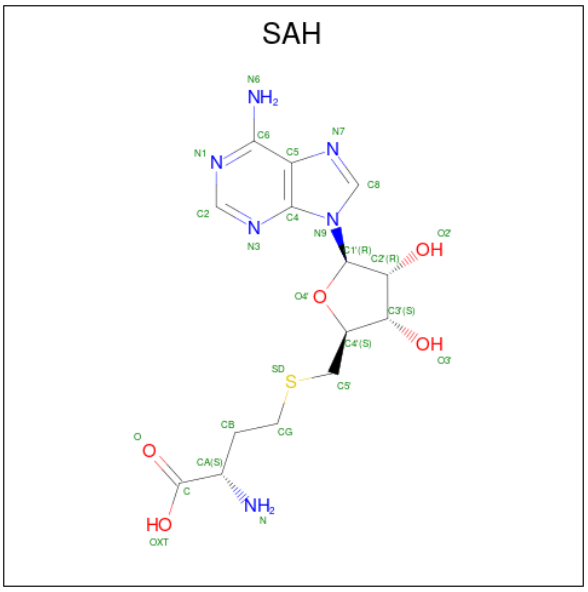
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	24	Total	C	N	O	P	0	0	0
			489	235	88	143	23			
3	F	25	Total	C	N	O	P	0	0	0
			510	245	93	148	24			
3	K	25	Total	C	N	O	P	0	0	0
			510	245	93	148	24			
3	L	25	Total	C	N	O	P	0	0	0
			510	245	93	148	24			

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	6	7		
4	D	1	Total	C	O	0	0
			13	6	7		
4	G	1	Total	C	O	0	0
			13	6	7		
4	J	1	Total	C	O	0	0
			13	6	7		

- Molecule 5 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O S 26 14 6 5 1	0	0
5	D	1	Total C N O S 26 14 6 5 1	0	0
5	G	1	Total C N O S 26 14 6 5 1	0	0
5	J	1	Total C N O S 26 14 6 5 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	69	Total O 69 69	0	0
6	B	12	Total O 12 12	0	0
6	D	41	Total O 41 41	0	0
6	C	3	Total O 3 3	0	0
6	E	2	Total O 2 2	0	0
6	F	2	Total O 2 2	0	0
6	G	56	Total O 56 56	0	0
6	H	4	Total O 4 4	0	0

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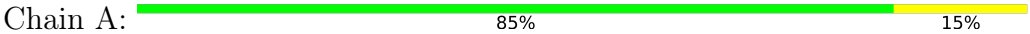
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	J	51	Total O 51 51	0	0
6	I	7	Total O 7 7	0	0
6	K	5	Total O 5 5	0	0
6	L	7	Total O 7 7	0	0

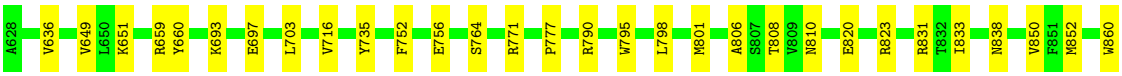
3 Residue-property plots (i)

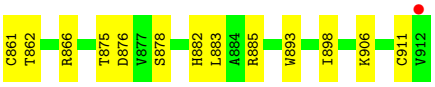
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA (cytosine-5)-methyltransferase 3A

Chain A:

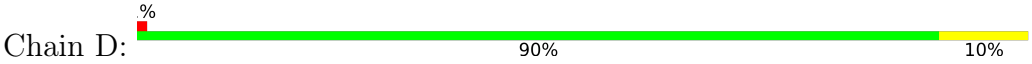






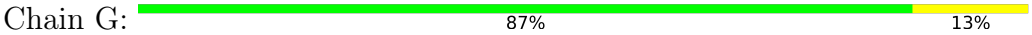
• Molecule 1: DNA (cytosine-5)-methyltransferase 3A

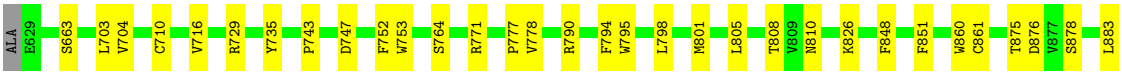
Chain D:



• Molecule 1: DNA (cytosine-5)-methyltransferase 3A

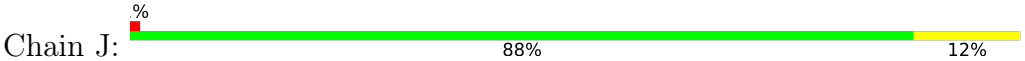
Chain G:

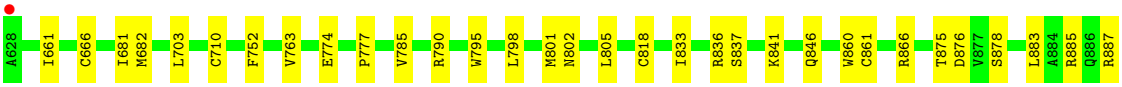


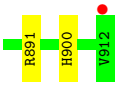


• Molecule 1: DNA (cytosine-5)-methyltransferase 3A

Chain J:

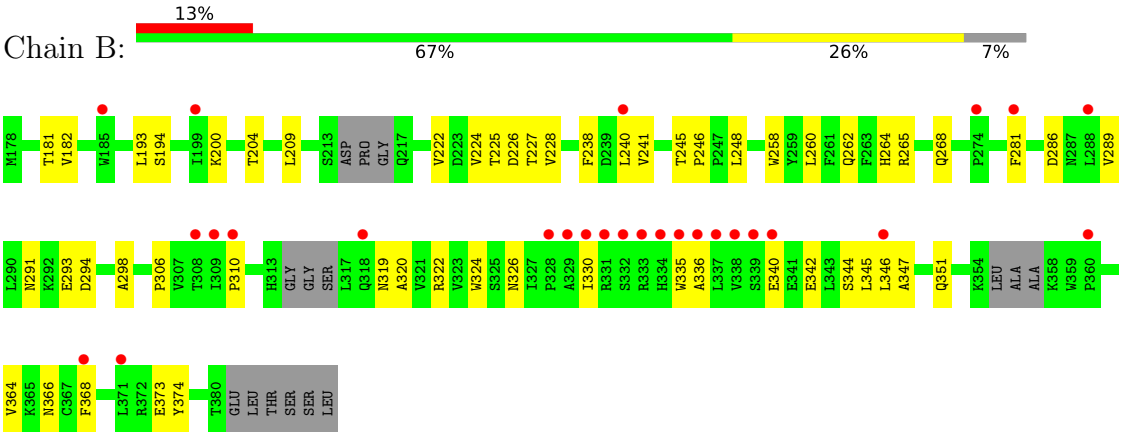






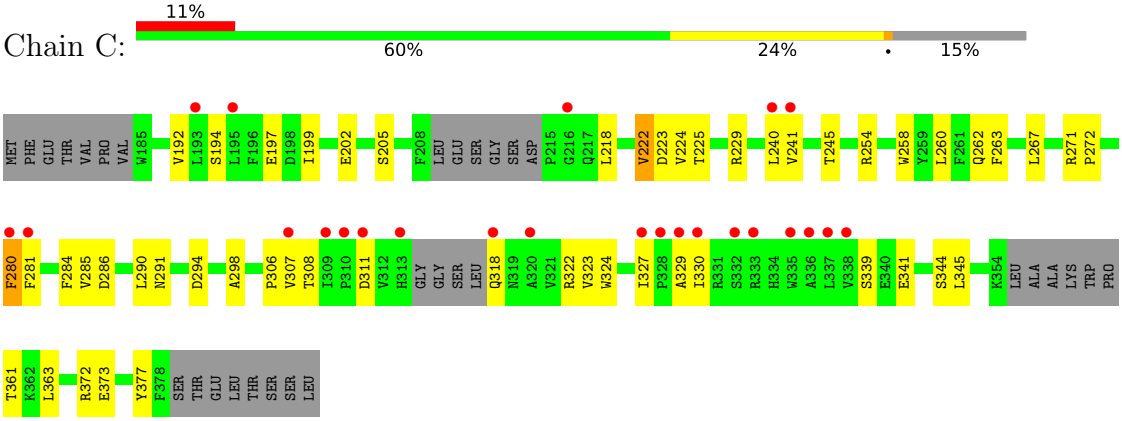
• Molecule 2: DNA (cytosine-5)-methyltransferase 3-like

Chain B:



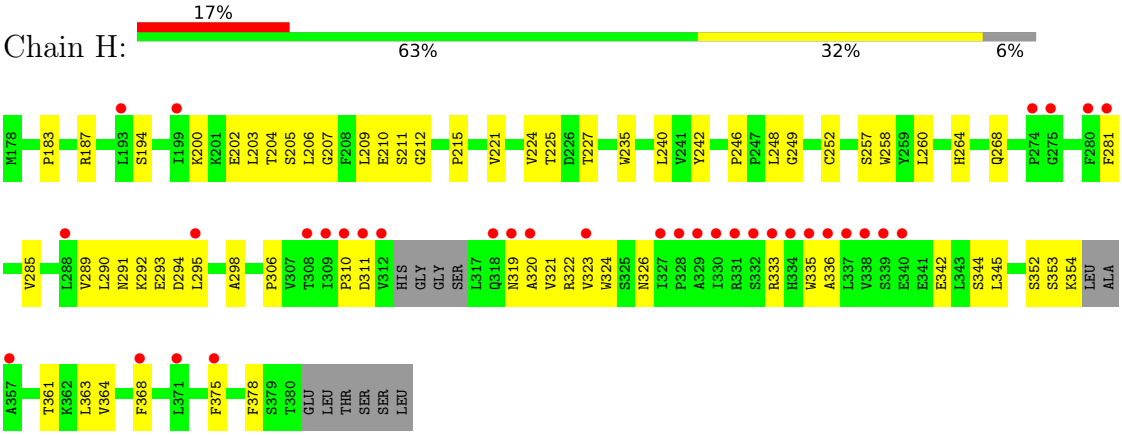
• Molecule 2: DNA (cytosine-5)-methyltransferase 3-like

Chain C:



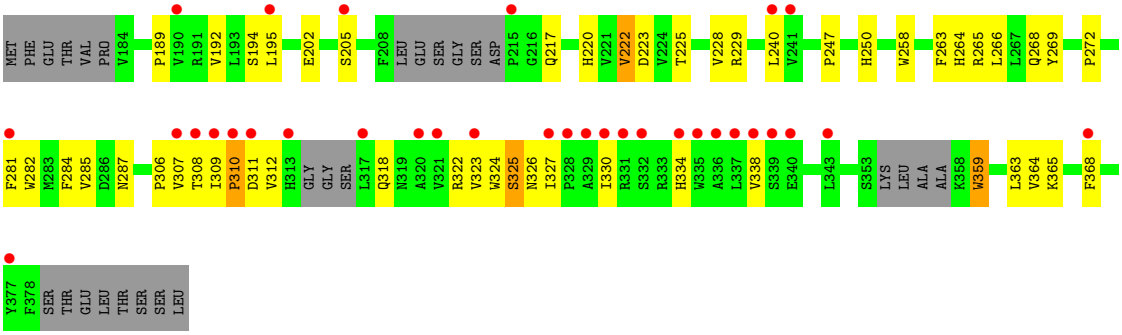
• Molecule 2: DNA (cytosine-5)-methyltransferase 3-like

Chain H:

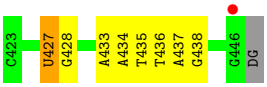


• Molecule 2: DNA (cytosine-5)-methyltransferase 3-like

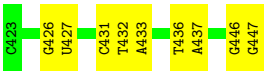
Chain I:



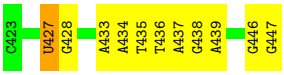
• Molecule 3: CGA DNA (25-MER)



• Molecule 3: CGA DNA (25-MER)



• Molecule 3: CGA DNA (25-MER)



• Molecule 3: CGA DNA (25-MER)

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	187.56Å 187.56Å 82.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	37.72 – 2.50 39.53 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (37.72-2.50) 98.5 (39.53-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.196 , 0.240 0.199 , 0.241	Depositor DCC
R_{free} test set	2014 reflections (1.82%)	wwPDB-VP
Wilson B-factor (Å^2)	56.2	Xtriage
Anisotropy	0.729	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 58.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.487 for -h,-k,l 0.023 for h,-h-k,-l 0.023 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17145	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PYO, SAH, CIT

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	0.40	0/2342	0.54	0/3168
1	D	0.37	0/2364	0.52	0/3193
1	G	0.35	0/2353	0.50	0/3180
1	J	0.37	0/2372	0.51	0/3204
2	B	0.34	0/1508	0.53	0/2071
2	C	0.37	0/1311	0.54	0/1802
2	H	0.41	0/1523	0.58	0/2093
2	I	0.36	0/1352	0.55	0/1859
3	E	0.64	0/526	0.98	0/808
3	F	0.68	0/550	0.98	0/846
3	K	0.64	0/550	1.00	0/846
3	L	0.66	0/550	0.98	0/846
All	All	0.42	0/17301	0.62	0/23916

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2284	0	2230	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2300	0	2281	22	0
1	G	2289	0	2255	27	0
1	J	2308	0	2283	30	0
2	B	1464	0	1289	34	0
2	C	1275	0	1069	40	0
2	H	1477	0	1309	37	0
2	I	1314	0	1127	39	0
3	E	489	0	271	11	0
3	F	510	0	279	5	0
3	K	510	0	279	13	0
3	L	510	0	279	10	0
4	A	13	0	5	1	0
4	D	13	0	5	3	0
4	G	13	0	5	0	0
4	J	13	0	5	1	0
5	A	26	0	19	0	0
5	D	26	0	19	0	0
5	G	26	0	19	1	0
5	J	26	0	19	1	0
6	A	69	0	0	10	0
6	B	12	0	0	2	0
6	C	3	0	0	0	0
6	D	41	0	0	2	0
6	E	2	0	0	1	0
6	F	2	0	0	0	0
6	G	56	0	0	3	0
6	H	4	0	0	0	0
6	I	7	0	0	1	0
6	J	51	0	0	6	0
6	K	5	0	0	3	0
6	L	7	0	0	0	0
All	All	17145	0	15047	283	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (283) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:TYR:HA	6:A:1105:HOH:O	1.57	1.03
2:H:285:VAL:HG12	2:H:323:VAL:HG22	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:281:PHE:HD2	2:C:327:ILE:HG12	1.33	0.91
2:C:285:VAL:HG23	2:C:323:VAL:HG22	1.50	0.91
1:A:636:VAL:HB	6:A:1105:HOH:O	1.74	0.87
1:A:649:VAL:HG11	6:A:1117:HOH:O	1.73	0.86
5:G:1002:SAH:SD	6:G:1156:HOH:O	2.40	0.79
5:J:1002:SAH:SD	6:J:1143:HOH:O	2.40	0.78
2:C:271:ARG:HA	2:C:280:PHE:HE2	1.50	0.75
2:C:307:VAL:HG21	2:C:330:ILE:HG22	1.69	0.75
3:E:437:DA:H8	3:E:437:DA:H5"	1.50	0.75
2:I:285:VAL:HG23	2:I:323:VAL:HG22	1.68	0.74
2:I:222:VAL:HG23	2:I:223:ASP:H	1.53	0.74
2:C:241:VAL:HG21	2:C:267:LEU:HD23	1.69	0.73
2:I:308:THR:HG22	2:I:322:ARG:HG2	1.69	0.73
1:A:808:THR:HG23	1:A:810:ASN:OD1	1.87	0.73
3:E:433:DA:H8	3:E:433:DA:H5"	1.54	0.72
1:A:808:THR:CG2	1:A:810:ASN:OD1	2.37	0.71
2:C:260:LEU:HD11	2:C:298:ALA:HA	1.72	0.71
2:I:247:PRO:HA	2:I:287:ASN:HD22	1.55	0.71
2:H:225:THR:HG22	2:H:258:TRP:HZ2	1.55	0.70
1:A:862:THR:HG23	6:A:1103:HOH:O	1.91	0.70
1:J:774:GLU:OE1	2:I:229:ARG:NH1	2.25	0.69
3:E:437:DA:H5"	3:E:437:DA:C8	2.27	0.69
1:A:882:HIS:ND1	6:A:1101:HOH:O	2.26	0.69
3:E:438:DG:H1'	6:E:501:HOH:O	1.92	0.68
1:J:666:CYS:SG	6:J:1151:HOH:O	2.51	0.68
2:C:281:PHE:CD2	2:C:327:ILE:HG12	2.24	0.68
3:K:437:DA:H5"	3:K:437:DA:H8	1.59	0.68
2:C:222:VAL:HG23	2:C:223:ASP:H	1.59	0.68
3:K:446:DG:H2"	3:K:447:DG:O4'	1.94	0.67
1:D:790:ARG:NH2	1:D:833:ILE:O	2.28	0.66
2:C:285:VAL:CG2	2:C:323:VAL:HG22	2.23	0.66
3:K:438:DG:N3	6:K:501:HOH:O	2.29	0.66
2:C:373:GLU:N	2:C:373:GLU:OE1	2.28	0.65
1:A:885:ARG:NH1	6:A:1103:HOH:O	2.28	0.65
2:B:225:THR:HG22	2:B:258:TRP:HZ2	1.61	0.65
1:G:885:ARG:NH2	1:J:876:ASP:OD1	2.31	0.64
1:A:790:ARG:NH2	1:A:833:ILE:O	2.30	0.64
2:B:281:PHE:HA	2:B:326:ASN:HD21	1.63	0.64
2:H:321:VAL:HG22	2:H:363:LEU:HD23	1.78	0.64
2:C:271:ARG:HA	2:C:280:PHE:CE2	2.33	0.63
2:I:285:VAL:CG2	2:I:323:VAL:HG22	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:291:ASN:OD1	2:H:293:GLU:HG2	1.98	0.63
1:J:785:VAL:HG11	1:J:805:LEU:HD22	1.80	0.63
2:H:361:THR:HA	2:H:364:VAL:HG12	1.82	0.62
2:I:281:PHE:HA	2:I:326:ASN:HD21	1.64	0.62
1:A:659:ARG:NH1	6:A:1104:HOH:O	2.29	0.62
3:K:433:DA:H2'	3:K:434:DA:C8	2.35	0.62
2:I:265:ARG:HG2	2:I:269:TYR:HE2	1.64	0.61
1:D:831[B]:ARG:HD3	1:D:842:GLN:HA	1.82	0.61
2:I:189:PRO:HB2	2:I:217:GLN:HE22	1.64	0.61
2:C:308:THR:HG22	2:C:322:ARG:HG2	1.83	0.61
2:B:224:VAL:HA	2:B:227:THR:HG23	1.83	0.61
3:K:437:DA:H5"	3:K:437:DA:C8	2.35	0.61
3:L:436:DT:H2"	3:L:437:DA:C8	2.36	0.60
2:B:245:THR:HG22	2:B:286:ASP:HA	1.84	0.60
1:A:876:ASP:OD1	1:D:885:ARG:NH2	2.30	0.60
1:A:883:LEU:HD12	3:E:437:DA:H5'	1.84	0.60
1:G:883:LEU:HD12	3:K:437:DA:H5'	1.84	0.60
2:H:202:GLU:O	2:H:206:LEU:HD12	2.01	0.59
2:H:344:SER:OG	2:H:345:LEU:N	2.35	0.59
2:I:282:TRP:O	2:I:325:SER:HB2	2.02	0.59
2:I:266:LEU:HA	2:I:269:TYR:HD2	1.68	0.59
3:E:433:DA:H5"	3:E:433:DA:C8	2.37	0.59
2:I:240:LEU:HA	2:I:281:PHE:O	2.02	0.59
2:C:361:THR:HG22	2:C:363:LEU:N	2.18	0.59
1:G:790:ARG:NH1	1:G:892:SER:O	2.35	0.59
2:C:361:THR:HG22	2:C:363:LEU:H	1.68	0.58
3:K:439:DA:H5'	6:K:501:HOH:O	2.03	0.58
1:D:803:ARG:HH21	4:D:1001:CIT:H22	1.68	0.58
2:B:240:LEU:HA	2:B:281:PHE:O	2.04	0.58
2:I:307:VAL:HG21	2:I:330:ILE:HG22	1.84	0.58
2:H:224:VAL:HA	2:H:227:THR:HG23	1.86	0.58
2:C:311:ASP:O	2:C:318:GLN:N	2.37	0.58
1:J:891:ARG:HD3	6:J:1120:HOH:O	2.03	0.58
2:I:330:ILE:HD12	2:I:330:ILE:H	1.68	0.58
2:H:187:ARG:HD3	2:H:375:PHE:O	2.04	0.57
1:J:836:ARG:NH2	6:J:1103:HOH:O	2.38	0.57
2:B:200:LYS:O	2:B:204:THR:HG23	2.04	0.57
1:G:891:ARG:HD3	6:G:1128:HOH:O	2.03	0.57
2:H:281:PHE:HA	2:H:326:ASN:HD21	1.68	0.57
2:B:260:LEU:HD21	2:B:298:ALA:HA	1.86	0.57
2:C:225:THR:HG22	2:C:258:TRP:HZ2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:312:VAL:HG22	2:I:318:GLN:H	1.70	0.57
2:C:245:THR:OG1	2:C:286:ASP:HA	2.04	0.57
1:D:831[B]:ARG:NH1	1:D:843:GLY:O	2.38	0.57
2:H:311:ASP:HB2	2:H:319:ASN:O	2.05	0.57
1:G:876:ASP:OD1	1:J:885:ARG:NH2	2.31	0.56
3:L:431:DC:H2'	3:L:432:DT:C6	2.40	0.56
2:H:240:LEU:HA	2:H:281:PHE:O	2.06	0.56
2:B:330:ILE:HA	2:B:335:TRP:HH2	1.69	0.56
2:H:187:ARG:HB3	2:H:375:PHE:O	2.06	0.56
1:D:875:THR:O	1:D:885:ARG:HD3	2.05	0.56
2:C:341:GLU:HA	2:C:344:SER:HB3	1.87	0.55
1:G:860:TRP:CE2	1:J:878:SER:HA	2.42	0.55
1:J:818:CYS:HB3	1:J:866:ARG:HB2	1.89	0.55
1:J:875:THR:O	1:J:885:ARG:HD3	2.06	0.55
1:G:875:THR:O	1:G:885:ARG:HD3	2.06	0.55
1:J:887[B]:ARG:NH1	6:J:1104:HOH:O	2.39	0.55
1:G:805:LEU:HG	1:G:900:HIS:CD2	2.41	0.55
2:H:311:ASP:CB	2:H:319:ASN:H	2.20	0.55
2:I:189:PRO:HB2	2:I:217:GLN:NE2	2.22	0.55
2:H:306:PRO:HB3	2:H:324:TRP:CE2	2.41	0.55
2:C:272:PRO:HD3	2:C:280:PHE:CD2	2.42	0.55
2:I:324:TRP:O	2:I:325:SER:HB3	2.07	0.54
1:A:831[A]:ARG:NH2	1:A:838:ASN:O	2.40	0.54
1:A:898:ILE:HG22	6:A:1117:HOH:O	2.07	0.54
2:B:347:ALA:O	2:B:351:GLN:HG3	2.08	0.53
2:H:264:HIS:O	2:H:268:GLN:HG2	2.08	0.53
2:B:245:THR:CG2	2:B:286:ASP:HA	2.39	0.53
2:B:306:PRO:HB3	2:B:324:TRP:CE2	2.43	0.53
3:F:432:DT:H2'	3:F:433:DA:C8	2.43	0.53
3:F:446:DG:H2"	3:F:447:DG:O5'	2.08	0.53
2:I:266:LEU:HA	2:I:269:TYR:CD2	2.44	0.53
3:E:435:DT:H2"	3:E:436:DT:H5"	1.90	0.53
1:A:716:VAL:HB	3:F:426:DG:H1'	1.91	0.53
1:A:823:ARG:NH2	1:A:850:VAL:HG11	2.24	0.52
1:D:904:PRO:O	1:D:907:GLU:HG2	2.09	0.52
1:G:794:PHE:HD1	6:G:1101:HOH:O	1.92	0.52
1:D:806:ALA:HB3	4:D:1001:CIT:O5	2.10	0.52
3:F:436:DT:H2"	3:F:437:DA:C8	2.45	0.52
1:D:774:GLU:OE1	2:C:229:ARG:NH2	2.43	0.52
2:C:372:ARG:HD3	2:C:377:TYR:CB	2.39	0.52
2:I:265:ARG:HG2	2:I:269:TYR:CE2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:245:THR:HG21	2:B:286:ASP:OD1	2.10	0.51
1:A:860:TRP:CZ3	1:D:877:VAL:HG13	2.46	0.51
1:A:861:CYS:SG	1:A:882:HIS:HB2	2.50	0.51
1:G:716:VAL:HB	3:L:426:DG:H1'	1.90	0.51
2:B:291:ASN:OD1	2:B:293:GLU:HG2	2.10	0.51
2:B:344:SER:OG	2:B:345:LEU:N	2.44	0.51
2:H:352:SER:OG	2:H:353:SER:N	2.44	0.51
1:J:752:PHE:HB3	1:J:798:LEU:CD2	2.40	0.51
1:A:885:ARG:NH2	1:D:876:ASP:OD1	2.40	0.51
3:K:438:DG:H1'	6:K:501:HOH:O	2.09	0.51
2:H:311:ASP:HB3	2:H:319:ASN:H	1.75	0.51
2:I:225:THR:HG22	2:I:258:TRP:HZ2	1.74	0.51
1:G:771:ARG:HG3	1:G:771:ARG:HH11	1.76	0.50
2:H:364:VAL:HG22	2:H:368:PHE:CE2	2.46	0.50
1:A:808:THR:HG21	1:A:810:ASN:OD1	2.11	0.50
2:H:203:LEU:HB2	2:H:209:LEU:HD11	1.94	0.50
2:H:207:GLY:HA3	2:H:378:PHE:O	2.12	0.50
2:B:246:PRO:O	2:B:289:VAL:HG21	2.12	0.50
2:C:202:GLU:HA	2:C:205:SER:HB2	1.94	0.50
2:I:306:PRO:HB3	2:I:324:TRP:CE2	2.46	0.50
1:A:651:LYS:NZ	6:A:1102:HOH:O	2.27	0.50
2:H:221:VAL:HG11	2:H:235:TRP:CH2	2.47	0.49
1:G:777:PRO:HB3	1:G:795:TRP:CD2	2.47	0.49
1:A:875:THR:O	1:A:885:ARG:HD3	2.13	0.49
1:G:878:SER:HA	1:J:860:TRP:CE2	2.47	0.49
3:K:428:DG:H5'	3:K:428:DG:C8	2.48	0.49
3:K:435:DT:H2"	3:K:436:DT:H5"	1.95	0.49
2:H:249:GLY:HA2	2:H:354:LYS:CB	2.43	0.48
2:B:291:ASN:ND2	2:B:294:ASP:OD1	2.46	0.48
1:D:798:LEU:O	1:D:801:MET:HG3	2.13	0.48
2:B:373:GLU:O	6:B:401:HOH:O	2.20	0.48
2:C:241:VAL:HG21	2:C:267:LEU:CD2	2.41	0.48
2:B:364:VAL:HG12	2:B:368:PHE:HE2	1.78	0.48
1:A:703:LEU:HA	1:A:752:PHE:O	2.14	0.48
1:G:778:VAL:HG13	1:G:794:PHE:HB2	1.96	0.48
1:A:777:PRO:HB3	1:A:795:TRP:CD2	2.49	0.48
3:L:432:DT:H2'	3:L:433:DA:C8	2.48	0.48
2:I:282:TRP:CZ3	2:I:325:SER:HA	2.49	0.48
2:C:263:PHE:CD2	2:C:284:PHE:HD1	2.31	0.48
2:I:263:PHE:CZ	2:I:284:PHE:HB2	2.49	0.47
3:L:446:DG:H2"	3:L:447:DG:O5'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:752:PHE:HB3	1:G:798:LEU:HD23	1.96	0.47
2:H:310:PRO:HG3	2:H:336:ALA:HB3	1.95	0.47
1:A:659:ARG:NH2	1:J:681:ILE:O	2.47	0.47
2:B:264:HIS:O	2:B:268:GLN:HG2	2.14	0.47
1:D:637:LEU:HB3	1:D:704:VAL:HG22	1.96	0.47
1:D:887[B]:ARG:NH1	6:D:1106:HOH:O	2.48	0.47
1:J:836:ARG:NH1	1:J:837:SER:H	2.11	0.47
2:I:311:ASP:CB	2:I:363:LEU:HD21	2.45	0.47
2:C:291:ASN:ND2	2:C:294:ASP:OD1	2.48	0.47
2:B:181:THR:OG1	2:B:182:VAL:N	2.48	0.47
2:C:327:ILE:HB	2:C:330:ILE:CD1	2.44	0.47
3:F:431:DC:H2'	3:F:432:DT:C6	2.50	0.47
2:H:200:LYS:O	2:H:204:THR:HG23	2.14	0.47
3:E:428:DG:C8	3:E:428:DG:H5'	2.49	0.47
1:G:826:LYS:HE3	1:G:848:PHE:O	2.14	0.47
1:G:729:ARG:NH2	2:H:257:SER:OG	2.48	0.47
2:H:290:LEU:HB3	2:H:294:ASP:HB2	1.97	0.47
2:I:307:VAL:HG21	2:I:330:ILE:CG2	2.44	0.47
2:C:197:GLU:HG3	2:C:199:ILE:HG23	1.96	0.46
2:C:224:VAL:HG21	2:C:262:GLN:HB3	1.97	0.46
1:A:898:ILE:C	6:A:1117:HOH:O	2.54	0.46
2:I:192:VAL:HG21	2:I:240:LEU:HD23	1.96	0.46
2:I:309:ILE:HG22	2:I:363:LEU:HD23	1.98	0.46
1:D:750:PRO:O	6:D:1101:HOH:O	2.20	0.46
2:B:224:VAL:HG21	2:B:262:GLN:HB3	1.97	0.46
2:B:306:PRO:HB2	2:B:322:ARG:HB3	1.99	0.45
2:C:306:PRO:HB3	2:C:324:TRP:CE2	2.52	0.45
1:G:703:LEU:HA	1:G:752:PHE:O	2.16	0.45
2:I:202:GLU:OE1	2:I:365:LYS:HA	2.16	0.45
1:G:798:LEU:O	1:G:801:MET:HG3	2.16	0.45
2:I:240:LEU:HD12	2:I:281:PHE:HB2	1.99	0.45
1:D:803:ARG:NH2	4:D:1001:CIT:H22	2.31	0.45
2:C:327:ILE:HG22	2:C:329:ALA:H	1.80	0.45
2:B:374:TYR:HA	6:B:401:HOH:O	2.16	0.45
1:J:777:PRO:HB3	1:J:795:TRP:CE2	2.51	0.45
2:B:240:LEU:HD12	2:B:241:VAL:N	2.32	0.45
2:H:361:THR:HA	2:H:364:VAL:CG1	2.47	0.45
1:A:735:TYR:OH	2:B:265:ARG:HA	2.17	0.44
3:E:433:DA:H2'	3:E:434:DA:C8	2.52	0.44
2:I:195:LEU:CD2	2:I:266:LEU:HD12	2.47	0.44
1:A:806:ALA:HB3	4:A:1001:CIT:O6	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:285:VAL:HG23	2:C:323:VAL:CG2	2.35	0.44
3:E:434:DA:H1'	3:E:435:DT:H5"	1.98	0.44
2:C:240:LEU:HD12	2:C:281:PHE:C	2.37	0.44
2:H:285:VAL:HA	2:H:322:ARG:O	2.18	0.44
1:J:883:LEU:HD12	3:L:436:DT:H3'	2.00	0.44
1:D:803:ARG:NH2	1:D:900:HIS:O	2.44	0.44
1:G:808:THR:HG23	1:G:810:ASN:H	1.82	0.44
2:H:246:PRO:O	2:H:289:VAL:HG21	2.17	0.44
2:C:192:VAL:HA	2:C:240:LEU:O	2.17	0.44
2:I:308:THR:CG2	2:I:322:ARG:HG2	2.45	0.44
2:C:344:SER:OG	2:C:345:LEU:N	2.50	0.44
2:I:202:GLU:O	2:I:205:SER:HB2	2.18	0.44
1:D:752:PHE:HB3	1:D:798:LEU:HD23	1.99	0.43
1:G:710:CYS:N	3:L:427:PYO:HC5	2.32	0.43
2:B:366:ASN:OD1	2:B:366:ASN:N	2.51	0.43
2:C:240:LEU:HA	2:C:281:PHE:O	2.18	0.43
1:G:826:LYS:HD3	1:G:851:PHE:CE2	2.53	0.43
1:J:883:LEU:HD23	1:J:883:LEU:HA	1.89	0.43
2:I:327:ILE:HB	2:I:330:ILE:CD1	2.48	0.43
1:A:823:ARG:HG2	1:A:852:MET:HB2	1.99	0.43
2:B:204:THR:HG22	2:B:209:LEU:HB2	2.00	0.43
2:I:247:PRO:HG3	2:I:359:TRP:CG	2.52	0.43
1:A:777:PRO:HB3	1:A:795:TRP:CE2	2.53	0.43
2:H:333:ARG:HG2	2:H:335:TRP:CZ2	2.54	0.43
2:H:319:ASN:OD1	2:H:320:ALA:N	2.47	0.43
3:K:433:DA:H2"	3:K:434:DA:O4'	2.18	0.43
3:L:435:DT:H2"	3:L:436:DT:C6	2.53	0.43
1:A:752:PHE:HB3	1:A:798:LEU:HD23	1.99	0.43
1:J:841:LYS:HD2	1:J:846:GLN:HB3	2.01	0.43
1:J:900:HIS:HD1	4:J:1001:CIT:H22	1.83	0.43
1:J:710:CYS:N	3:K:427:PYO:HC5	2.34	0.43
2:H:292:LYS:HA	2:H:295:LEU:HD12	2.01	0.42
1:A:906:LYS:HB2	1:A:911:CYS:SG	2.58	0.42
2:B:322:ARG:NE	2:B:340:GLU:OE2	2.48	0.42
1:G:704:VAL:O	1:G:753:TRP:HA	2.19	0.42
1:A:878:SER:HA	1:D:860:TRP:CE2	2.54	0.42
2:B:204:THR:HG22	2:B:209:LEU:HD12	2.01	0.42
1:J:798:LEU:O	1:J:801:MET:HG3	2.19	0.42
1:D:710:CYS:SG	3:E:427:PYO:H2'	2.59	0.42
2:H:242:TYR:OH	2:H:285:VAL:HG21	2.19	0.42
2:B:319:ASN:OD1	2:B:320:ALA:N	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:790:ARG:NH2	1:J:833:ILE:O	2.51	0.42
2:C:272:PRO:HD3	2:C:280:PHE:HD2	1.85	0.42
2:C:286:ASP:OD1	2:C:290:LEU:HG	2.19	0.42
2:I:228:VAL:HA	6:I:407:HOH:O	2.20	0.42
1:J:802:ASN:ND2	6:J:1105:HOH:O	2.40	0.42
3:K:433:DA:C2	3:L:437:DA:C2	3.08	0.42
2:H:183:PRO:O	2:H:187:ARG:HG3	2.19	0.41
1:A:693:LYS:O	1:A:697:GLU:HG3	2.20	0.41
1:A:756:GLU:OE1	1:A:893:TRP:NE1	2.51	0.41
2:C:254:ARG:HG3	2:C:258:TRP:CE3	2.55	0.41
1:G:777:PRO:HB3	1:G:795:TRP:CE2	2.56	0.41
2:B:193:LEU:HD22	2:B:238:PHE:CE2	2.55	0.41
1:G:743:PRO:HB2	1:G:747:ASP:HB3	2.02	0.41
1:A:659:ARG:NE	1:J:682:MET:SD	2.92	0.41
2:I:282:TRP:CH2	2:I:325:SER:HA	2.56	0.41
1:A:659:ARG:HH21	1:J:682:MET:HA	1.86	0.41
1:A:860:TRP:CE2	1:D:878:SER:HA	2.56	0.41
1:D:642:GLY:O	1:D:669:SER:HB3	2.21	0.41
2:C:192:VAL:O	2:C:218:LEU:HA	2.21	0.41
2:C:280:PHE:HD1	2:C:281:PHE:N	2.18	0.41
2:H:260:LEU:HD21	2:H:298:ALA:HA	2.02	0.41
2:H:364:VAL:HG22	2:H:368:PHE:HE2	1.86	0.41
1:J:661:ILE:HG12	1:J:682:MET:HB3	2.03	0.41
1:J:763:VAL:HG22	3:L:446:DG:OP1	2.21	0.41
2:I:264:HIS:O	2:I:268:GLN:HG2	2.21	0.41
1:A:820:GLU:CD	1:A:866:ARG:HH22	2.25	0.41
2:B:346:LEU:O	2:B:346:LEU:HD23	2.20	0.41
1:J:703:LEU:HA	1:J:752:PHE:O	2.20	0.41
2:I:364:VAL:O	2:I:368:PHE:HD2	2.03	0.41
1:G:885:ARG:HH22	1:J:876:ASP:CG	2.21	0.40
1:A:771:ARG:NH1	2:B:226:ASP:OD1	2.47	0.40
1:A:798:LEU:O	1:A:801:MET:HG3	2.21	0.40
2:B:310:PRO:HG3	2:B:336:ALA:HB3	2.03	0.40
1:G:887[B]:ARG:CZ	1:G:887[B]:ARG:HB2	2.51	0.40
2:I:310:PRO:HB3	2:I:338:VAL:HG21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	285/285 (100%)	279 (98%)	6 (2%)	0	100 100
1	D	286/285 (100%)	280 (98%)	6 (2%)	0	100 100
1	G	285/285 (100%)	280 (98%)	5 (2%)	0	100 100
1	J	287/285 (101%)	281 (98%)	6 (2%)	0	100 100
2	B	187/209 (90%)	174 (93%)	10 (5%)	3 (2%)	9 17
2	C	170/209 (81%)	156 (92%)	13 (8%)	1 (1%)	25 43
2	H	191/209 (91%)	171 (90%)	17 (9%)	3 (2%)	9 17
2	I	174/209 (83%)	157 (90%)	12 (7%)	5 (3%)	4 6
All	All	1865/1976 (94%)	1778 (95%)	75 (4%)	12 (1%)	25 43

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	222	VAL
2	C	222	VAL
2	H	212	GLY
2	H	215	PRO
2	I	222	VAL
2	B	248	LEU
2	H	248	LEU
2	I	250	HIS
2	I	310	PRO
2	I	334	HIS
2	I	272	PRO
2	B	228	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	240/250 (96%)	239 (100%)	1 (0%)	91 97
1	D	246/250 (98%)	245 (100%)	1 (0%)	91 97
1	G	243/250 (97%)	239 (98%)	4 (2%)	62 84
1	J	246/250 (98%)	245 (100%)	1 (0%)	91 97
2	B	140/191 (73%)	138 (99%)	2 (1%)	67 86
2	C	110/191 (58%)	107 (97%)	3 (3%)	44 71
2	H	139/191 (73%)	133 (96%)	6 (4%)	29 53
2	I	119/191 (62%)	115 (97%)	4 (3%)	37 63
All	All	1483/1764 (84%)	1461 (98%)	22 (2%)	65 85

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	764	SER
2	B	194	SER
2	B	342	GLU
1	D	855	LYS
2	C	194	SER
2	C	280	PHE
2	C	339	SER
1	G	663	SER
1	G	735	TYR
1	G	764	SER
1	G	861	CYS
2	H	194	SER
2	H	205	SER
2	H	210	GLU
2	H	211	SER
2	H	252	CYS
2	H	342	GLU
1	J	861	CYS
2	I	194	SER
2	I	220	HIS
2	I	325	SER
2	I	359	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	810	ASN
1	G	900	HIS
2	I	217	GLN
2	I	287	ASN
2	I	319	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)

4 non-standard protein/DNA/RNA residues 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	PYO	F	427	1,3	16,20,21	1.99	4 (25%)	22,28,31	1.14	1 (4%)
3	PYO	E	427	1,3	16,20,21	1.96	4 (25%)	22,28,31	1.16	1 (4%)
3	PYO	K	427	1,3	16,20,21	2.00	4 (25%)	22,28,31	1.04	1 (4%)
3	PYO	L	427	1,3	16,20,21	2.02	4 (25%)	22,28,31	1.03	1 (4%)

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	PYO	F	427	1,3	-	4/7/25/26	0/2/2/2
3	PYO	E	427	1,3	-	4/7/25/26	0/2/2/2
3	PYO	K	427	1,3	-	4/7/25/26	0/2/2/2
3	PYO	L	427	1,3	-	4/7/25/26	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	427	PYO	C6-C5	6.34	1.49	1.35
3	E	427	PYO	C6-C5	6.33	1.49	1.35
3	L	427	PYO	C6-C5	6.19	1.49	1.35
3	F	427	PYO	C6-C5	6.12	1.49	1.35
3	L	427	PYO	C2-N1	2.91	1.46	1.40
3	F	427	PYO	C2-N1	2.86	1.46	1.40
3	L	427	PYO	C5-C4	2.67	1.45	1.40
3	F	427	PYO	C5-C4	2.59	1.45	1.40
3	K	427	PYO	C2-N1	2.58	1.45	1.40
3	K	427	PYO	C5-C4	2.49	1.45	1.40
3	E	427	PYO	C2-N1	2.41	1.45	1.40
3	E	427	PYO	C5-C4	2.38	1.45	1.40
3	L	427	PYO	C4-N3	2.32	1.42	1.33
3	E	427	PYO	C4-N3	2.31	1.42	1.33
3	K	427	PYO	C4-N3	2.29	1.42	1.33
3	F	427	PYO	C4-N3	2.26	1.42	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	427	PYO	C5-C4-N3	-4.72	118.50	124.29
3	F	427	PYO	C5-C4-N3	-4.37	118.93	124.29
3	K	427	PYO	C5-C4-N3	-4.17	119.17	124.29
3	L	427	PYO	C5-C4-N3	-3.70	119.75	124.29

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	427	PYO	C2'-C1'-N1-C6
3	E	427	PYO	C2'-C1'-N1-C2
3	K	427	PYO	C2'-C1'-N1-C6
3	F	427	PYO	C2'-C1'-N1-C6
3	L	427	PYO	C2'-C1'-N1-C6
3	K	427	PYO	C2'-C1'-N1-C2
3	L	427	PYO	C2'-C1'-N1-C2
3	F	427	PYO	C2'-C1'-N1-C2
3	F	427	PYO	O4'-C1'-N1-C2
3	L	427	PYO	O4'-C1'-N1-C2
3	K	427	PYO	O4'-C1'-N1-C6
3	L	427	PYO	O4'-C1'-N1-C6

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Mol	Chain	Res	Type	Atoms
3	E	427	PYO	O4'-C1'-N1-C6
3	F	427	PYO	O4'-C1'-N1-C6
3	K	427	PYO	O4'-C1'-N1-C2
3	E	427	PYO	O4'-C1'-N1-C2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	427	PYO	1	0
3	K	427	PYO	1	0
3	L	427	PYO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

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	$\#\|Z\| > 2$
4	CIT	A	1001	-	12,12,12	1.08	0	17,17,17	1.62	3 (17%)
4	CIT	D	1001	-	12,12,12	1.15	0	17,17,17	1.85	4 (23%)
4	CIT	G	1001	-	12,12,12	1.00	0	17,17,17	1.45	2 (11%)
5	SAH	A	1002	-	24,28,28	1.18	2 (8%)	25,40,40	1.78	5 (20%)
5	SAH	J	1002	-	24,28,28	1.24	2 (8%)	25,40,40	1.73	6 (24%)
5	SAH	G	1002	-	24,28,28	1.18	3 (12%)	25,40,40	1.66	5 (20%)
4	CIT	J	1001	-	12,12,12	1.00	0	17,17,17	7.66	9 (52%)
5	SAH	D	1002	-	24,28,28	1.27	2 (8%)	25,40,40	1.67	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
4	CIT	A	1001	-	-	2/16/16/16	-
4	CIT	D	1001	-	-	3/16/16/16	-
4	CIT	G	1001	-	-	3/16/16/16	-
5	SAH	A	1002	-	-	2/11/31/31	0/3/3/3
5	SAH	J	1002	-	-	5/11/31/31	0/3/3/3
5	SAH	G	1002	-	-	3/11/31/31	0/3/3/3
4	CIT	J	1001	-	-	6/16/16/16	-
5	SAH	D	1002	-	-	5/11/31/31	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1002	SAH	C2-N3	4.16	1.38	1.32
5	A	1002	SAH	C2-N3	4.02	1.38	1.32
5	J	1002	SAH	C2-N3	4.00	1.38	1.32
5	G	1002	SAH	C2-N3	3.92	1.38	1.32
5	D	1002	SAH	C2-N1	2.80	1.39	1.33
5	J	1002	SAH	C2-N1	2.60	1.38	1.33
5	A	1002	SAH	C2-N1	2.35	1.38	1.33
5	G	1002	SAH	C2-N1	2.30	1.38	1.33
5	G	1002	SAH	OXT-C	-2.02	1.23	1.30

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	J	1001	CIT	O7-C3-C6	13.31	127.56	108.86
4	J	1001	CIT	O7-C3-C2	-13.27	78.35	109.40
4	J	1001	CIT	O7-C3-C4	-13.26	78.38	109.40
4	J	1001	CIT	C4-C3-C6	-13.06	82.04	110.11
4	J	1001	CIT	C2-C3-C6	-12.21	83.86	110.11
4	J	1001	CIT	C4-C3-C2	10.52	136.60	109.16
5	A	1002	SAH	N3-C2-N1	-5.60	119.92	128.68
5	D	1002	SAH	N3-C2-N1	-5.48	120.11	128.68
5	J	1002	SAH	N3-C2-N1	-5.48	120.11	128.68
5	G	1002	SAH	N3-C2-N1	-5.35	120.32	128.68
4	D	1001	CIT	O6-C6-C3	4.73	121.27	113.05
4	J	1001	CIT	O6-C6-C3	4.04	120.06	113.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1001	CIT	O6-C6-C3	3.77	119.60	113.05
5	D	1002	SAH	OXT-C-O	-3.75	115.58	124.09
5	J	1002	SAH	OXT-C-O	-3.71	115.66	124.09
5	A	1002	SAH	OXT-C-O	-3.57	115.99	124.09
4	G	1001	CIT	O6-C6-C3	3.54	119.20	113.05
5	G	1002	SAH	OXT-C-O	-3.29	116.61	124.09
5	G	1002	SAH	C5'-SD-CG	-2.86	93.68	102.27
4	D	1001	CIT	O5-C6-C3	-2.83	118.25	122.25
5	A	1002	SAH	OXT-C-CA	2.78	122.86	113.38
5	A	1002	SAH	O3'-C3'-C4'	-2.69	103.27	111.05
4	A	1001	CIT	C2-C3-C6	-2.48	104.77	110.11
5	J	1002	SAH	OXT-C-CA	2.47	121.80	113.38
5	G	1002	SAH	OXT-C-CA	2.34	121.37	113.38
4	D	1001	CIT	O4-C5-O3	-2.29	117.60	123.30
4	J	1001	CIT	O4-C5-O3	-2.27	117.64	123.30
5	J	1002	SAH	O3'-C3'-C4'	-2.27	104.49	111.05
4	G	1001	CIT	O4-C5-C4	2.26	121.61	114.35
5	D	1002	SAH	O4'-C1'-C2'	-2.26	103.63	106.93
5	A	1002	SAH	C5'-SD-CG	-2.25	95.50	102.27
4	A	1001	CIT	O4-C5-O3	-2.22	117.76	123.30
5	J	1002	SAH	C5'-SD-CG	-2.22	95.60	102.27
4	D	1001	CIT	C2-C3-C6	-2.21	105.36	110.11
5	D	1002	SAH	O3'-C3'-C4'	-2.19	104.72	111.05
5	D	1002	SAH	OXT-C-CA	2.12	120.60	113.38
5	J	1002	SAH	O4'-C1'-C2'	-2.05	103.92	106.93
4	J	1001	CIT	O4-C5-C4	2.02	120.83	114.35
5	G	1002	SAH	O3'-C3'-C4'	-2.00	105.26	111.05

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1001	CIT	O7-C3-C4-C5
4	D	1001	CIT	C6-C3-C4-C5
4	J	1001	CIT	C1-C2-C3-O7
4	J	1001	CIT	O7-C3-C4-C5
4	J	1001	CIT	C6-C3-C4-C5
5	A	1002	SAH	N-CA-CB-CG
5	D	1002	SAH	N-CA-CB-CG
5	G	1002	SAH	N-CA-CB-CG
5	J	1002	SAH	N-CA-CB-CG
4	D	1001	CIT	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
4	G	1001	CIT	C2-C3-C4-C5
4	G	1001	CIT	O7-C3-C4-C5
4	G	1001	CIT	C6-C3-C4-C5
4	J	1001	CIT	C1-C2-C3-C6
4	J	1001	CIT	C4-C3-C6-O6
5	D	1002	SAH	OXT-C-CA-CB
5	J	1002	SAH	CB-CG-SD-C5'
4	J	1001	CIT	C4-C3-C6-O5
5	J	1002	SAH	OXT-C-CA-CB
5	D	1002	SAH	O-C-CA-CB
5	J	1002	SAH	O-C-CA-CB
5	G	1002	SAH	CB-CG-SD-C5'
4	A	1001	CIT	C2-C3-C6-O6
5	A	1002	SAH	C-CA-CB-CG
5	D	1002	SAH	C-CA-CB-CG
5	G	1002	SAH	C-CA-CB-CG
5	J	1002	SAH	C-CA-CB-CG
5	D	1002	SAH	CB-CG-SD-C5'
4	A	1001	CIT	C4-C3-C6-O6

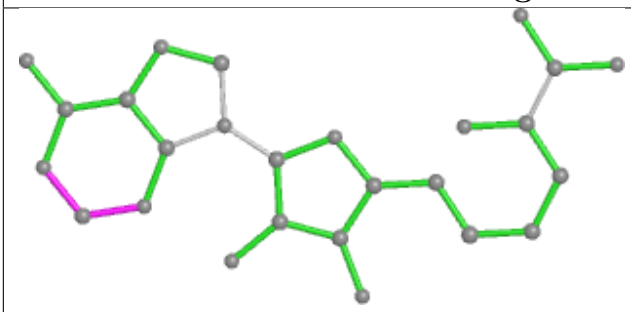
There are no ring outliers.

5 monomers are involved in 7 short contacts:

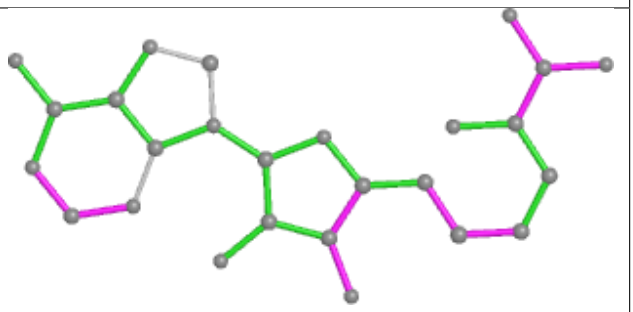
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1001	CIT	1	0
4	D	1001	CIT	3	0
5	J	1002	SAH	1	0
5	G	1002	SAH	1	0
4	J	1001	CIT	1	0

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.

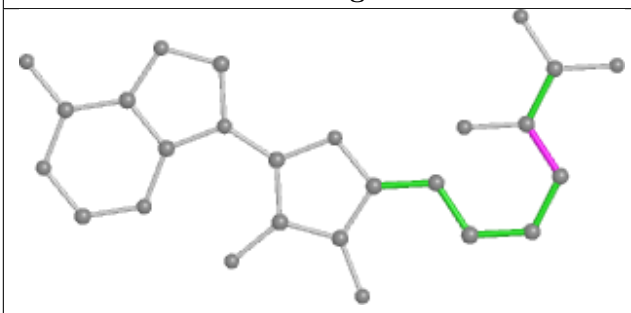
Ligand SAH A 1002



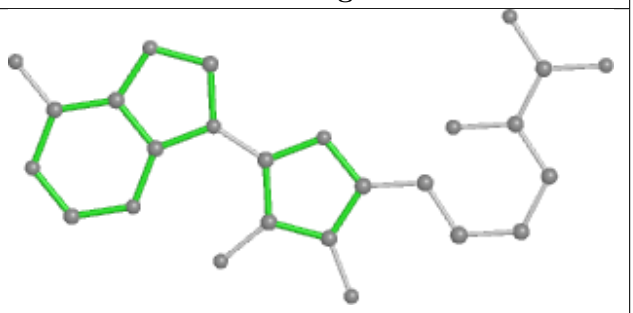
Bond lengths



Bond angles

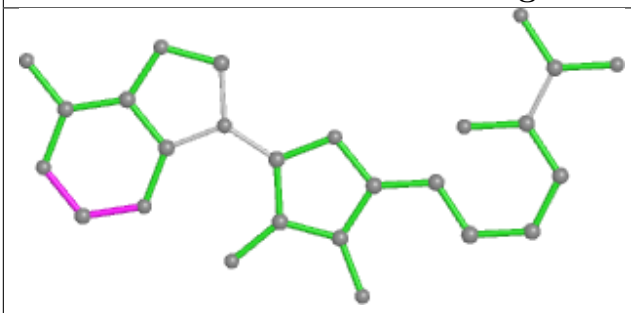


Torsions

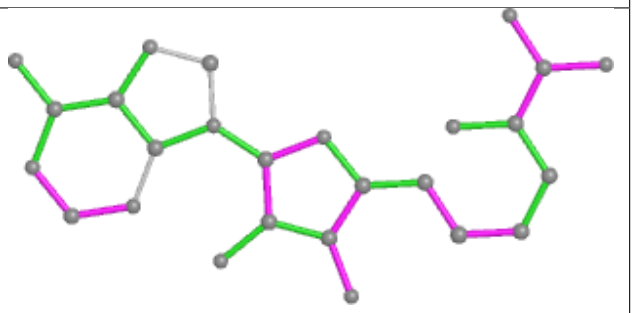


Rings

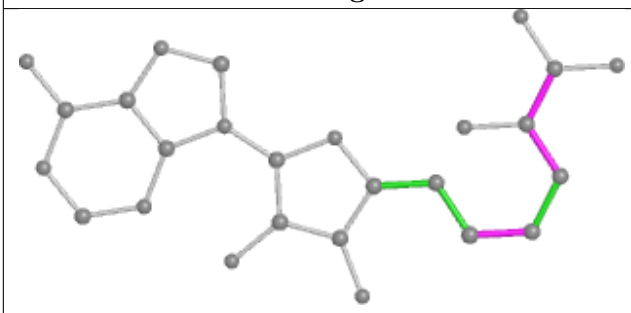
Ligand SAH J 1002



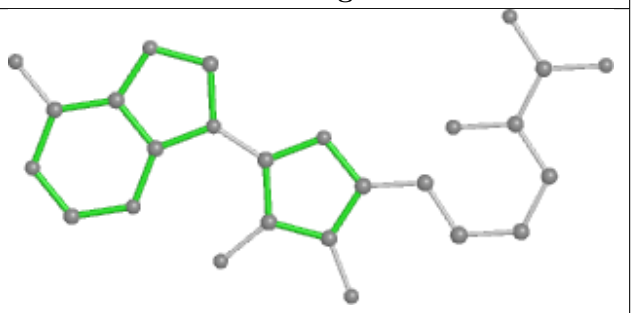
Bond lengths



Bond angles

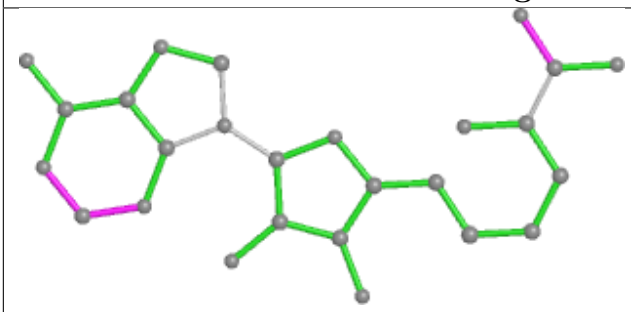


Torsions

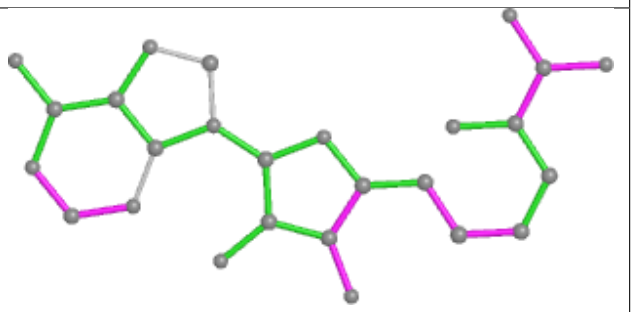


Rings

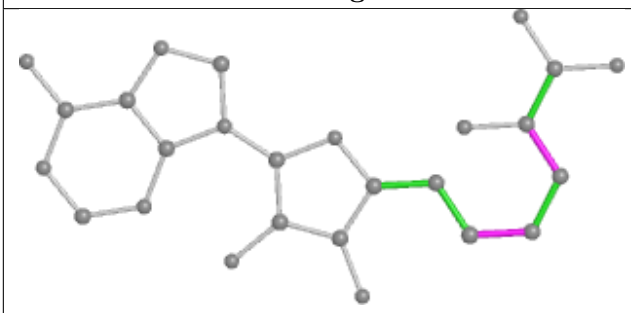
Ligand SAH G 1002



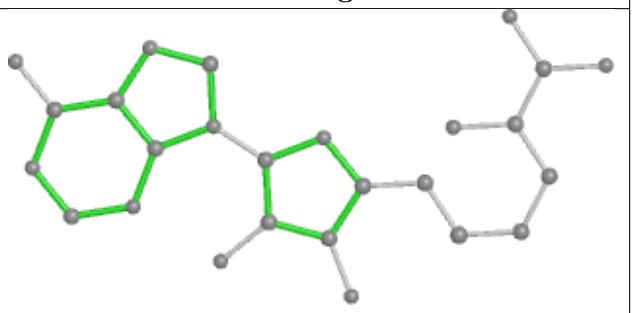
Bond lengths



Bond angles

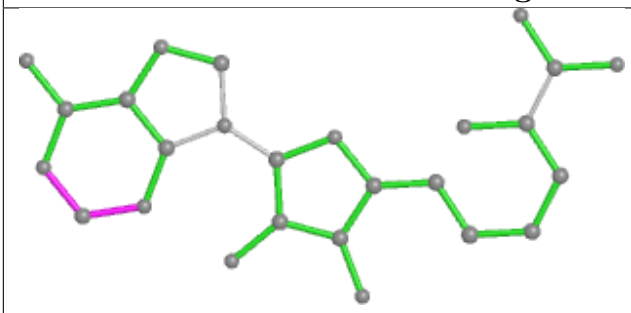


Torsions

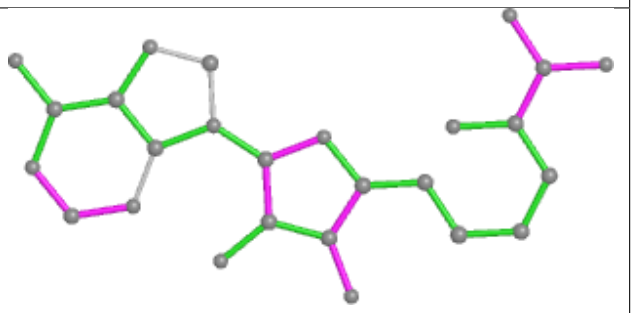


Rings

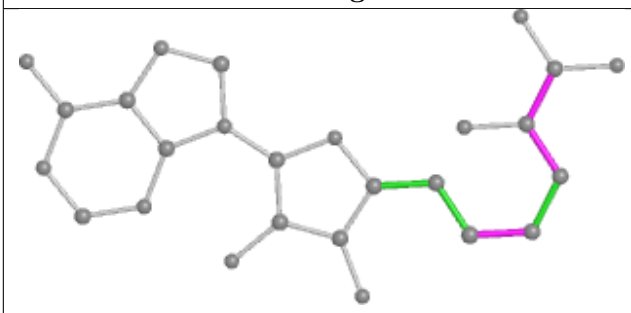
Ligand SAH D 1002



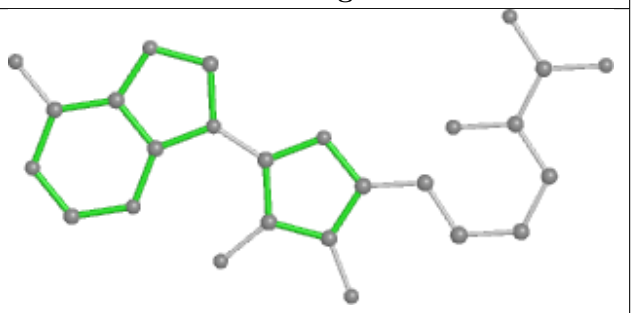
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	285/285 (100%)	-0.02	1 (0%) 92 93	44, 63, 94, 159	0
1	D	285/285 (100%)	-0.08	2 (0%) 87 89	42, 61, 93, 137	0
1	G	284/285 (99%)	-0.05	1 (0%) 92 93	44, 63, 90, 133	0
1	J	285/285 (100%)	-0.09	2 (0%) 87 89	42, 61, 91, 148	0
2	B	194/209 (92%)	0.63	27 (13%) 2 2	68, 109, 172, 198	0
2	C	178/209 (85%)	0.55	24 (13%) 3 2	72, 135, 188, 200	0
2	H	197/209 (94%)	0.74	35 (17%) 1 1	30, 111, 176, 196	0
2	I	182/209 (87%)	0.87	33 (18%) 1 1	73, 140, 189, 205	0
3	E	23/25 (92%)	-0.46	1 (4%) 35 38	67, 124, 147, 154	0
3	F	24/25 (96%)	-0.66	0 100 100	84, 118, 159, 166	0
3	K	24/25 (96%)	-0.58	0 100 100	70, 127, 144, 187	0
3	L	24/25 (96%)	-0.61	0 100 100	81, 118, 155, 165	0
All	All	1985/2076 (95%)	0.20	126 (6%) 20 21	30, 80, 171, 205	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	337	LEU	20.0
2	I	338	VAL	14.3
2	H	332	SER	10.3
2	H	338	VAL	10.0
2	B	339	SER	9.1
2	I	310	PRO	8.6
2	C	338	VAL	8.1
2	B	338	VAL	7.5
2	H	335	TRP	7.4
2	B	337	LEU	7.3
2	I	332	SER	7.2

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Mol	Chain	Res	Type	RSRZ
2	H	331	ARG	7.2
2	C	332	SER	7.0
2	I	309	ILE	7.0
2	B	336	ALA	6.6
2	B	331	ARG	6.6
2	B	332	SER	6.3
2	C	337	LEU	6.2
2	C	310	PRO	6.1
1	J	628	ALA	6.1
2	I	330	ILE	6.1
2	H	357	ALA	5.7
2	C	330	ILE	5.7
2	H	336	ALA	5.6
2	I	336	ALA	5.5
2	H	337	LEU	5.5
2	H	310	PRO	5.3
2	C	309	ILE	5.3
2	I	329	ALA	5.1
2	C	313	HIS	5.1
2	I	327	ILE	5.1
2	I	320	ALA	5.1
2	C	320	ALA	4.9
2	C	328	PRO	4.7
2	H	311	ASP	4.7
2	H	274	PRO	4.6
2	B	335	TRP	4.5
2	B	330	ILE	4.5
2	C	336	ALA	4.5
2	H	330	ILE	4.3
1	D	912	VAL	4.2
2	H	308	THR	4.2
2	C	329	ALA	4.1
2	B	274	PRO	4.0
2	I	340	GLU	4.0
2	H	312	VAL	3.9
1	D	628	ALA	3.9
2	H	329	ALA	3.8
2	B	360	PRO	3.8
2	B	368	PHE	3.7
2	H	318	GLN	3.7
2	H	339	SER	3.7
2	B	340	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
2	I	328	PRO	3.6
2	C	327	ILE	3.6
2	I	368	PHE	3.6
2	H	371	LEU	3.6
2	B	328	PRO	3.6
2	H	309	ILE	3.6
2	H	328	PRO	3.5
2	I	311	ASP	3.5
2	I	240	LEU	3.5
2	H	199	ILE	3.5
2	I	313	HIS	3.4
1	G	912	VAL	3.4
2	B	308	THR	3.4
2	I	190	VAL	3.4
2	H	334	HIS	3.4
2	H	375	PHE	3.3
2	H	340	GLU	3.3
2	C	241	VAL	3.3
1	A	912	VAL	3.2
2	I	339	SER	3.2
2	I	334	HIS	3.2
2	I	307	VAL	3.2
2	C	307	VAL	3.1
2	H	319	ASN	3.0
2	B	334	HIS	2.9
2	C	281	PHE	2.9
2	I	331	ARG	2.9
2	C	216	GLY	2.9
3	E	446	DG	2.9
2	I	281	PHE	2.9
2	C	280	PHE	2.8
2	C	311	ASP	2.8
2	H	275	GLY	2.8
2	B	333	ARG	2.8
2	I	317	LEU	2.8
2	H	368	PHE	2.7
2	C	333	ARG	2.7
2	I	377	TYR	2.7
2	B	281	PHE	2.6
2	B	310	PRO	2.6
2	H	295	LEU	2.5
2	I	321	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	329	ALA	2.5
2	H	288	LEU	2.5
2	B	309	ILE	2.5
2	H	320	ALA	2.5
2	B	240	LEU	2.4
2	H	333	ARG	2.4
2	H	280	PHE	2.4
2	B	346	LEU	2.4
2	H	327	ILE	2.4
2	B	371	LEU	2.4
2	I	215	PRO	2.4
2	C	195	LEU	2.4
2	B	288	LEU	2.3
2	H	193	LEU	2.3
2	I	335	TRP	2.3
2	I	323	VAL	2.3
2	I	205	SER	2.3
2	C	240	LEU	2.3
2	B	185	TRP	2.3
2	C	193	LEU	2.2
1	J	912	VAL	2.2
2	I	195	LEU	2.2
2	I	343	LEU	2.2
2	H	323	VAL	2.2
2	B	199	ILE	2.1
2	C	335	TRP	2.1
2	B	318	GLN	2.1
2	H	281	PHE	2.1
2	I	241	VAL	2.1
2	I	308	THR	2.1
2	C	318	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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	PYO	L	427	19/20	0.98	0.12	61,70,82,84	0
3	PYO	F	427	19/20	0.99	0.14	66,77,82,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PYO	K	427	19/20	0.99	0.14	51,65,74,77	0
3	PYO	E	427	19/20	0.99	0.14	54,66,73,77	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

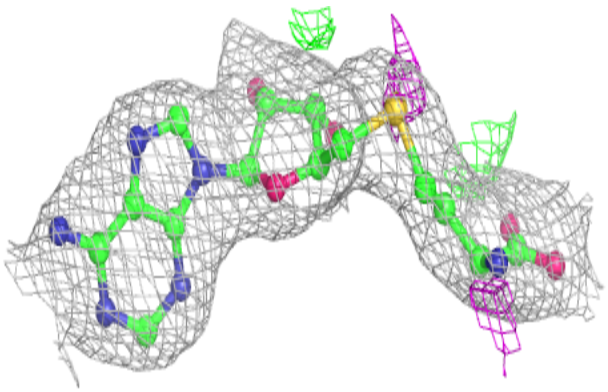
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

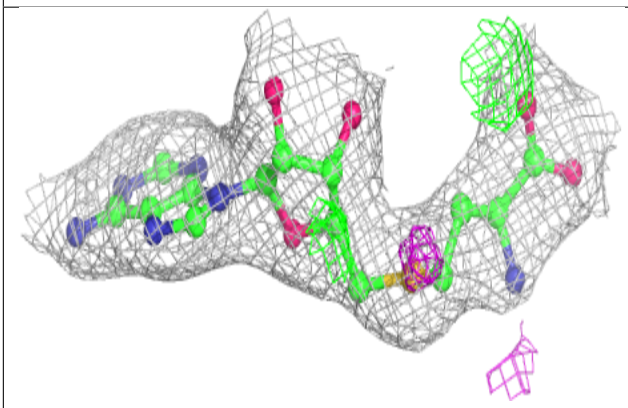
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CIT	A	1001	13/13	0.78	0.19	83,94,106,107	0
4	CIT	D	1001	13/13	0.85	0.19	97,103,112,120	0
4	CIT	J	1001	13/13	0.85	0.18	87,104,109,109	0
4	CIT	G	1001	13/13	0.88	0.23	86,103,107,110	0
5	SAH	A	1002	26/26	0.97	0.12	45,63,67,72	0
5	SAH	G	1002	26/26	0.97	0.11	48,61,70,73	0
5	SAH	J	1002	26/26	0.97	0.13	44,59,66,72	0
5	SAH	D	1002	26/26	0.98	0.13	44,58,64,69	0

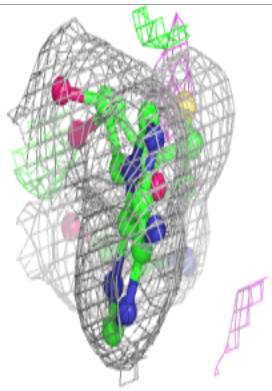
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAH A 1002:

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

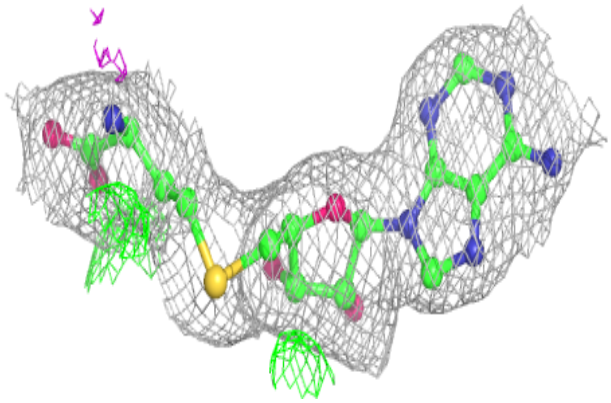


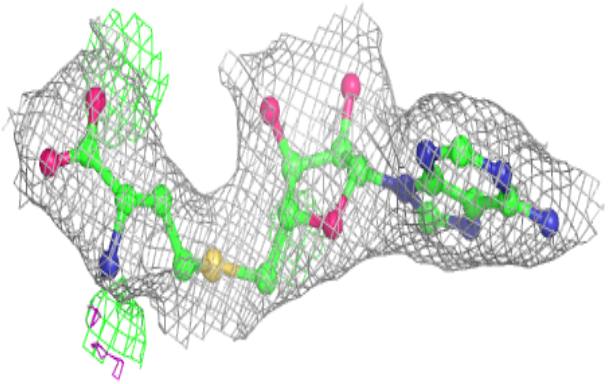


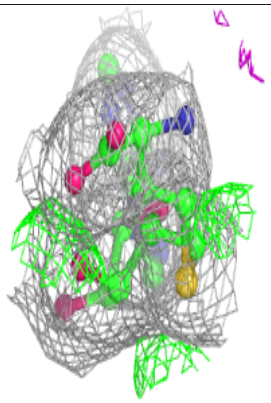


Electron density around SAH G 1002:

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

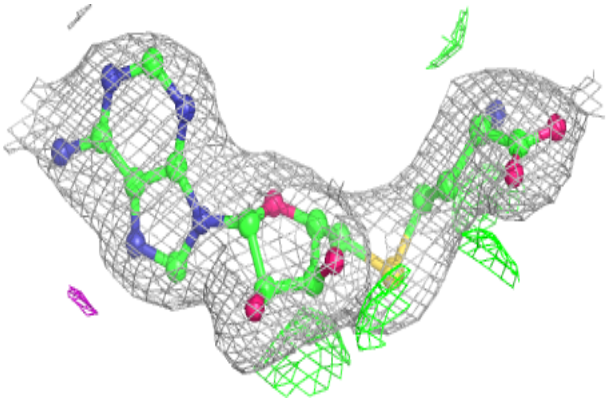


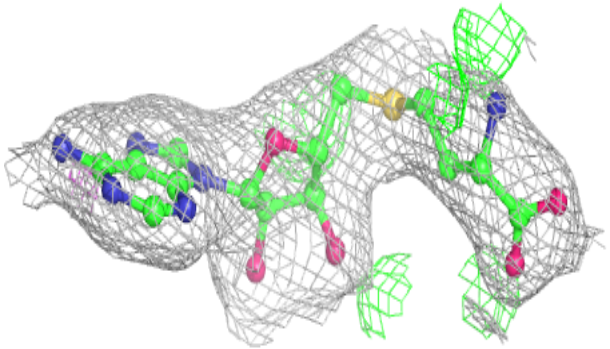


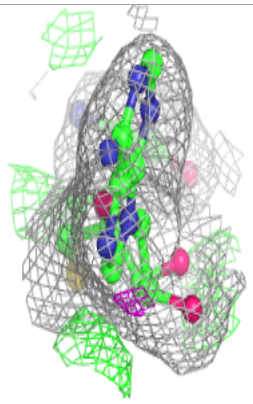


Electron density around SAH J 1002:

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

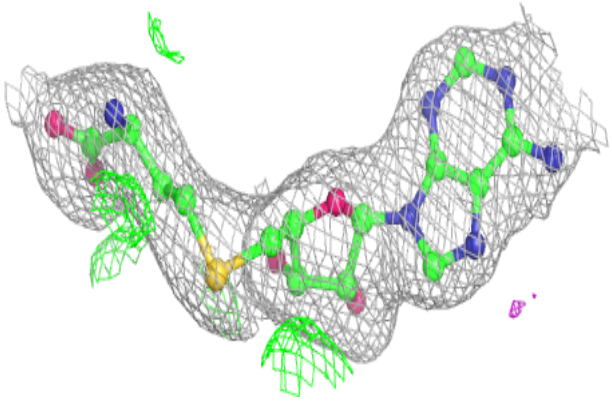


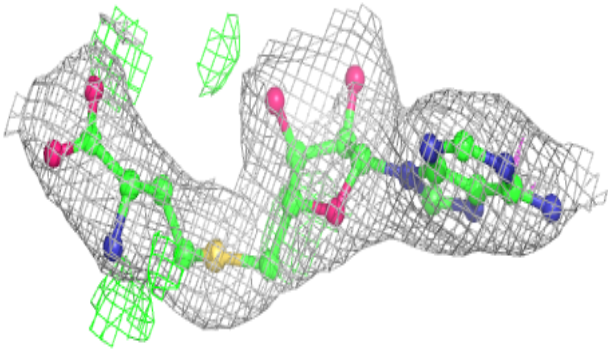


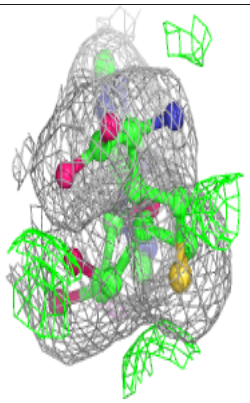


Electron density around SAH D 1002:

$2mF_o$-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.