Full wwPDB X-ray Structure Validation Report (i)

Feb 7, 2024 – 12:08 am GMT

PDB ID	:	2V74
Title	:	Crystal structure of coactivator-associated arginine methyltransferase 1 (CARM1), in complex with S-adenosyl-homocysteine
Authors	:	Yue, W.W.; Hassler, M.; Roe, S.M.; Thompson-Vale, V.; Pearl, L.H.
Deposited on	:	2007-07-26
Resolution	:	2.70 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:

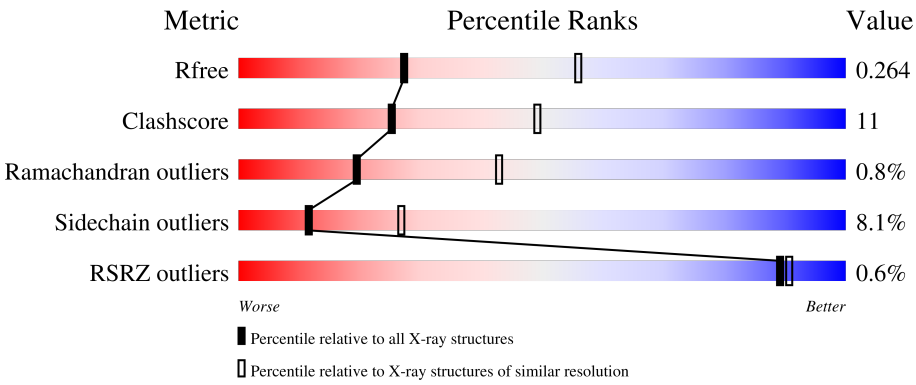
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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

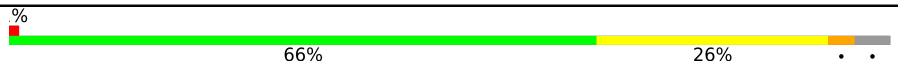
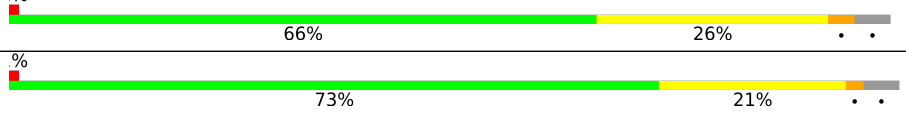
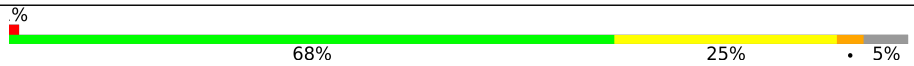
The reported resolution of this entry is 2.70 Å.

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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	B	346	
1	D	346	
1	F	346	
1	H	346	

2 Entry composition (i)

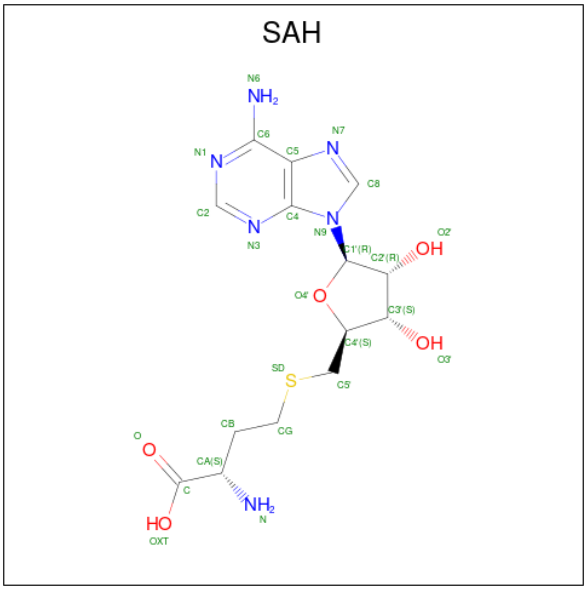
There are 3 unique types of molecules in this entry. The entry contains 10832 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HISTONE-ARGININE METHYLTRANSFERASE CARM1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	331	2600	1685	422	479	14	0	0	0
1	D	333	2630	1701	434	482	13	0	0	1
1	F	332	2614	1693	425	482	14	0	0	0
1	H	330	2623	1701	431	477	14	0	0	0

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	F	1	26	14	6	5	1	0	0
			Total	C	N	O	S		
2	H	1	26	14	6	5	1	0	0

- Molecule 3 is water.

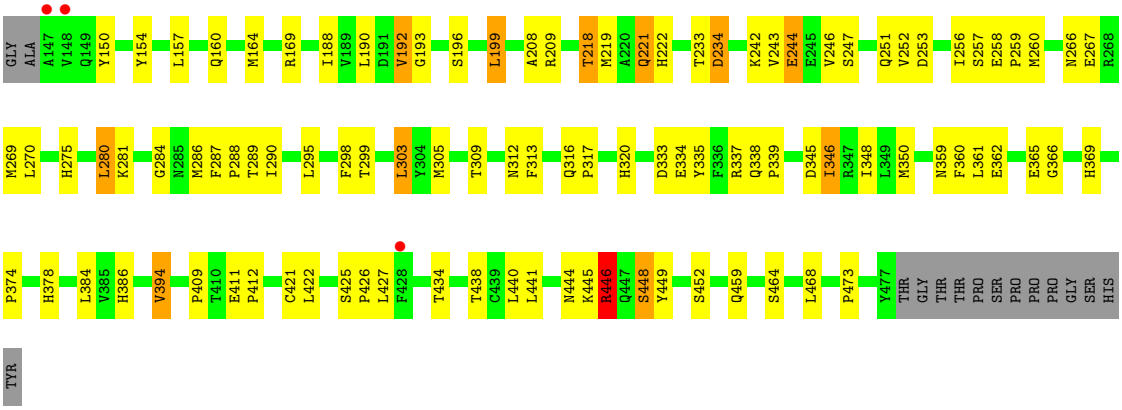
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	B	54	54	54	0	0
			Total	O		
3	D	67	67	67	0	0
			Total	O		
3	F	81	81	81	0	0
			Total	O		
3	H	59	59	59	0	0

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.

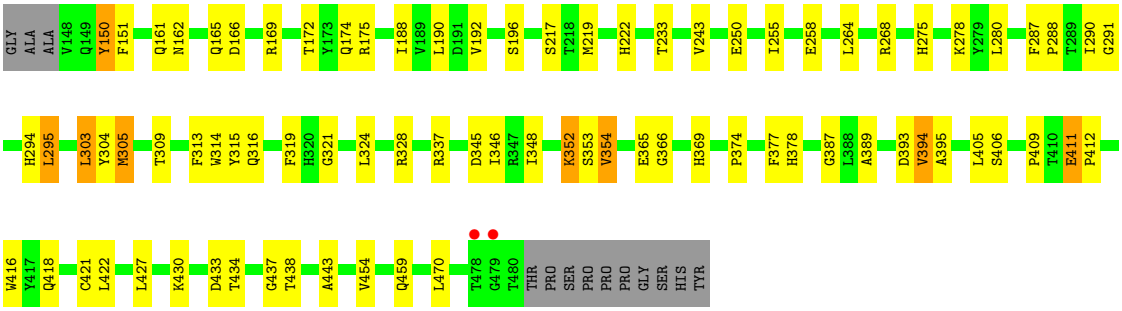
• Molecule 1: HISTONE-ARGININE METHYLTRANSFERASE CARM1

Chain B:



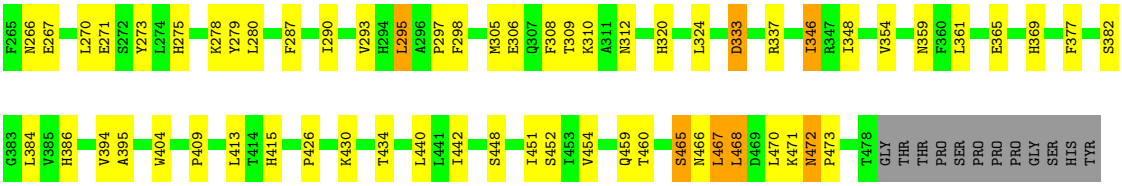
• Molecule 1: HISTONE-ARGININE METHYLTRANSFERASE CARM1

Chain D:



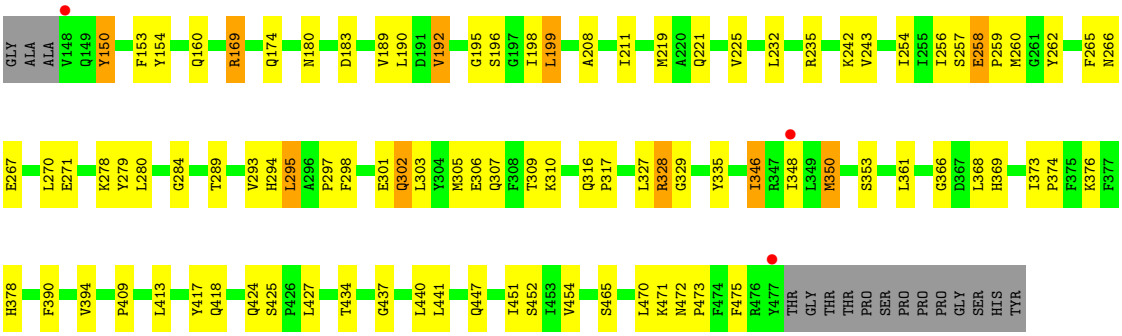
• Molecule 1: HISTONE-ARGININE METHYLTRANSFERASE CARM1

Chain F:



• Molecule 1: HISTONE-ARGININE METHYLTRANSFERASE CARM1

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	74.88Å 98.69Å 207.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.70 74.88 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-2.70) 99.0 (74.88-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.65 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.223 , 0.273 0.217 , 0.264	Depositor DCC
R_{free} test set	2144 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	53.4	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 50.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10832	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.49 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.7133e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: SAH

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	B	0.49	0/2668	0.60	0/3628
1	D	0.49	0/2698	0.61	0/3665
1	F	0.45	0/2683	0.59	0/3650
1	H	0.46	0/2692	0.62	1/3655 (0.0%)
All	All	0.47	0/10741	0.60	1/14598 (0.0%)

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	1	3
1	F	0	1
1	H	0	1
All	All	1	5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	329	GLY	N-CA-C	-5.88	98.39	113.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	449	TYR	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	233	THR	Peptide
1	B	446	ARG	Peptide
1	B	448	SER	Peptide
1	F	232	LEU	Peptide
1	H	328	ARG	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	B	2600	0	2503	56	0
1	D	2630	0	2555	51	0
1	F	2614	0	2507	65	0
1	H	2623	0	2555	52	0
2	B	26	0	19	5	0
2	D	26	0	19	0	0
2	F	26	0	19	5	0
2	H	26	0	19	3	0
3	B	54	0	0	4	0
3	D	67	0	0	5	0
3	F	81	0	0	2	0
3	H	59	0	0	4	0
All	All	10832	0	10196	223	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 11.

All (223) 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:F:233:THR:HG22	3:F:2016:HOH:O	1.72	0.89
1:D:352:LYS:H	1:D:352:LYS:HD3	1.37	0.89
1:F:472:ASN:H	1:F:473:PRO:HD3	1.38	0.87
1:D:352:LYS:H	1:D:352:LYS:CD	1.93	0.81
1:D:411:GLU:HG2	1:D:412:PRO:HD2	1.61	0.80
1:F:233:THR:O	1:F:234:ASP:HB3	1.83	0.78
1:B:445:LYS:O	1:B:446:ARG:CB	2.30	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304:TYR:HD1	1:D:304:TYR:O	1.70	0.75
1:B:305:MET:O	1:B:309:THR:HG22	1.87	0.74
1:D:305:MET:O	1:D:309:THR:HG23	1.86	0.74
1:H:366:GLY:HA2	1:H:369:HIS:CD2	2.22	0.74
1:F:386:HIS:CD2	1:F:426:PRO:HG3	2.24	0.73
1:D:161:GLN:O	1:D:165:GLN:HG3	1.90	0.71
1:B:266:ASN:O	3:B:2015:HOH:O	2.09	0.70
1:D:264:LEU:HD22	3:D:2031:HOH:O	1.90	0.70
1:F:434:THR:H	1:F:459:GLN:HE22	1.40	0.69
1:D:188:ILE:HG12	1:D:250:GLU:OE1	1.92	0.69
1:D:352:LYS:HD3	1:D:352:LYS:N	2.08	0.68
1:F:233:THR:O	1:F:234:ASP:CB	2.41	0.67
1:F:218:THR:O	1:F:221:GLN:HG2	1.95	0.66
1:B:253:ASP:OD1	1:B:281:LYS:HE2	1.96	0.66
1:F:305:MET:HE3	1:F:308:PHE:HB3	1.78	0.66
1:H:262:TYR:HH	1:H:475:PHE:HE2	1.42	0.66
1:H:378:HIS:HE1	3:H:2040:HOH:O	1.80	0.65
1:B:160:GLN:O	1:B:164:MET:HG3	1.97	0.65
1:D:196:SER:HA	1:D:219:MET:HE2	1.78	0.65
1:D:268:ARG:NH1	1:D:443:ALA:HB1	2.13	0.64
1:H:199:LEU:HB3	1:H:256:ILE:HD12	1.80	0.64
1:B:434:THR:H	1:B:459:GLN:HE22	1.45	0.64
1:H:366:GLY:HA2	1:H:369:HIS:HD2	1.61	0.64
1:H:440:LEU:HB3	1:H:452:SER:HB3	1.80	0.63
1:F:472:ASN:H	1:F:473:PRO:CD	2.11	0.63
1:F:451:ILE:HB	1:F:468:LEU:HB2	1.82	0.61
1:B:303:LEU:HD13	1:B:422:LEU:HD21	1.82	0.61
1:F:472:ASN:N	1:F:473:PRO:HD3	2.10	0.61
1:B:259:PRO:HD2	1:B:260:MET:SD	2.40	0.61
1:F:259:PRO:HG2	1:F:270:LEU:HD23	1.83	0.61
1:D:172:THR:HG21	1:D:405:LEU:HB2	1.82	0.60
1:D:304:TYR:O	1:D:304:TYR:CD1	2.52	0.60
1:B:320:HIS:HD2	1:D:174:GLN:NE2	1.99	0.60
1:F:320:HIS:HD2	1:H:174:GLN:NE2	2.00	0.59
1:B:290:ILE:HG22	1:B:359:ASN:HA	1.85	0.59
1:F:239:ILE:HD13	1:F:248:LEU:HD12	1.83	0.58
1:D:313:PHE:O	1:D:316:GLN:HG3	2.03	0.58
1:F:386:HIS:HD2	1:F:426:PRO:HG3	1.67	0.58
1:D:303:LEU:HD13	1:D:422:LEU:HD21	1.84	0.58
1:H:424:GLN:HG3	1:H:465:SER:O	2.04	0.58
1:B:299:THR:HB	1:B:350:MET:SD	2.43	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:440:LEU:HB3	1:F:452:SER:HB3	1.86	0.58
1:B:218:THR:O	1:B:221:GLN:HG2	2.04	0.57
1:H:189:VAL:HG13	1:H:254:ILE:HG23	1.87	0.57
1:F:168:VAL:O	1:F:172:THR:OG1	2.18	0.56
1:F:256:ILE:HG22	1:F:287:PHE:HB2	1.87	0.56
1:B:244:GLU:HA	1:B:275:HIS:CE1	2.42	0.55
1:F:290:ILE:HG22	1:F:359:ASN:HA	1.88	0.55
1:F:298:PHE:HB2	1:F:348:ILE:HD12	1.88	0.55
1:H:301:GLU:O	1:H:305:MET:HG3	2.07	0.55
1:D:169:ARG:NH1	1:D:258:GLU:OE1	2.37	0.55
1:F:471:LYS:O	1:F:472:ASN:HB2	2.07	0.54
1:D:219:MET:HE1	1:D:222:HIS:HB2	1.89	0.54
1:F:305:MET:O	1:F:309:THR:HG23	2.07	0.54
1:B:199:LEU:HD22	2:B:1478:SAH:HN2	1.71	0.54
1:B:374:PRO:HA	1:B:438:THR:HG22	1.89	0.54
1:F:466:ASN:HB3	3:F:2049:HOH:O	2.06	0.54
1:F:160:GLN:HA	1:F:163:MET:HE2	1.89	0.54
1:H:346:ILE:HG22	1:H:409:PRO:HB2	1.90	0.54
1:F:166:ASP:OD2	1:F:415:HIS:HD2	1.91	0.53
1:D:295:LEU:HA	1:D:389:ALA:O	2.08	0.53
1:F:233:THR:O	1:F:233:THR:CG2	2.56	0.53
1:D:352:LYS:NZ	1:D:378:HIS:O	2.42	0.53
1:H:265:PHE:CE1	1:H:293:VAL:HG21	2.43	0.53
1:B:221:GLN:HG3	1:B:222:HIS:N	2.23	0.53
1:H:196:SER:HA	1:H:219:MET:CE	2.38	0.53
1:H:413:LEU:HD11	1:H:417:TYR:CD2	2.44	0.53
1:D:378:HIS:ND1	1:D:434:THR:HG22	2.25	0.52
1:H:192:VAL:HG13	1:H:257:SER:HB2	1.91	0.52
1:D:290:ILE:HG13	1:D:395:ALA:HB3	1.91	0.52
1:H:208:ALA:HB3	1:H:211:ILE:HD11	1.93	0.51
1:H:242:LYS:HA	2:H:1478:SAH:N1	2.25	0.51
1:D:374:PRO:HA	1:D:438:THR:HG22	1.91	0.51
1:D:346:ILE:HG22	1:D:409:PRO:HB2	1.92	0.51
1:F:320:HIS:HD2	1:H:174:GLN:HE22	1.57	0.51
1:F:266:ASN:O	1:F:267:GLU:HB2	2.10	0.51
1:H:378:HIS:CE1	3:H:2040:HOH:O	2.61	0.51
1:B:259:PRO:HG2	1:B:270:LEU:HD23	1.93	0.50
1:D:196:SER:HA	1:D:219:MET:CE	2.41	0.50
1:H:180:ASN:O	1:H:183:ASP:HB2	2.12	0.50
1:D:275:HIS:HE1	1:D:278:LYS:NZ	2.10	0.50
1:D:291:GLY:HA3	3:D:2031:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:190:LEU:HG	1:F:248:LEU:HD21	1.94	0.50
1:H:295:LEU:HD13	1:H:390:PHE:CE2	2.47	0.50
1:B:275:HIS:HD2	1:B:365:GLU:OE1	1.95	0.49
1:F:333:ASP:O	1:F:337:ARG:HG3	2.12	0.49
1:H:376:LYS:HG2	1:H:434:THR:CG2	2.43	0.49
1:B:280:LEU:HD22	1:B:284:GLY:HA3	1.93	0.49
1:F:275:HIS:HE1	1:F:278:LYS:NZ	2.11	0.49
1:H:294:HIS:HD2	1:H:353:SER:OG	1.95	0.49
1:B:366:GLY:HA2	1:B:369:HIS:CD2	2.48	0.49
1:D:337:ARG:HD3	3:D:2040:HOH:O	2.13	0.49
1:H:195:GLY:O	1:H:219:MET:HG3	2.12	0.49
1:D:150:TYR:C	1:D:150:TYR:CD2	2.85	0.49
1:F:395:ALA:HB2	1:F:404:TRP:CZ3	2.48	0.49
1:H:160:GLN:OE1	3:H:2004:HOH:O	2.20	0.49
1:H:298:PHE:HB2	1:H:348:ILE:HD12	1.94	0.48
1:B:269:MET:O	1:B:269:MET:HG2	2.12	0.48
1:B:286:MET:O	1:B:287:PHE:HD2	1.96	0.48
1:D:387:GLY:HA3	1:D:421:CYS:O	2.12	0.48
1:H:259:PRO:HD2	1:H:260:MET:SD	2.54	0.48
1:D:393:ASP:OD1	1:D:406:SER:OG	2.22	0.48
1:F:271:GLU:HB3	1:F:365:GLU:HG3	1.94	0.48
1:D:315:TYR:HB2	1:D:328:ARG:HG3	1.95	0.48
1:B:288:PRO:HB3	1:B:394:VAL:HG13	1.96	0.48
1:B:192:VAL:HG13	1:B:257:SER:HB2	1.96	0.47
1:D:433:ASP:OD1	1:D:459:GLN:HG3	2.14	0.47
1:B:242:LYS:O	1:B:246:VAL:HG13	2.14	0.47
1:B:313:PHE:O	1:B:316:GLN:HG3	2.14	0.47
1:D:437:GLY:HA3	1:D:454:VAL:O	2.14	0.47
1:F:257:SER:HB3	1:F:273:TYR:CE2	2.49	0.47
1:D:255:ILE:HG13	1:D:280:LEU:HD13	1.97	0.47
1:F:255:ILE:HG13	1:F:280:LEU:HD13	1.95	0.47
1:D:319:PHE:C	1:D:321:GLY:N	2.67	0.47
1:H:169:ARG:NH1	1:H:258:GLU:OE1	2.48	0.47
1:H:198:ILE:HG23	1:H:199:LEU:HD13	1.95	0.47
1:H:265:PHE:HE1	1:H:293:VAL:HG21	1.79	0.47
1:B:427:LEU:HD21	1:B:464:SER:HB2	1.97	0.47
1:B:267:GLU:HB2	3:B:2015:HOH:O	2.15	0.46
1:D:354:VAL:HG13	1:D:377:PHE:CE1	2.49	0.46
1:B:251:GLN:HB3	1:B:281:LYS:HG2	1.97	0.46
1:F:377:PHE:O	1:F:434:THR:HA	2.15	0.46
1:B:193:GLY:HA3	2:B:1478:SAH:O4'	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:192:VAL:HG13	1:F:257:SER:HB2	1.96	0.46
1:F:266:ASN:ND2	1:F:267:GLU:HG3	2.31	0.46
1:F:278:LYS:HE2	1:F:279:TYR:CE1	2.51	0.46
1:H:307:GLN:HE21	1:H:335:TYR:HB3	1.80	0.45
1:B:411:GLU:HB3	1:B:412:PRO:HD2	1.97	0.45
1:F:454:VAL:HG22	1:F:465:SER:HB3	1.98	0.45
1:H:409:PRO:HG3	1:H:418:GLN:HG2	1.98	0.45
1:B:320:HIS:CD2	1:D:174:GLN:NE2	2.83	0.45
1:B:339:PRO:HD2	1:B:473:PRO:HA	1.97	0.45
1:F:290:ILE:HG13	1:F:395:ALA:HB3	1.99	0.45
1:H:271:GLU:HG3	1:H:368:LEU:HD12	1.98	0.45
1:F:297:PRO:HD3	1:F:377:PHE:CE1	2.51	0.45
1:H:196:SER:HA	1:H:219:MET:HE2	1.97	0.45
1:B:335:TYR:O	1:B:338:GLN:HB2	2.17	0.45
1:B:378:HIS:HB3	3:B:2044:HOH:O	2.16	0.45
1:F:295:LEU:N	1:F:295:LEU:HD13	2.32	0.45
1:F:233:THR:O	1:F:234:ASP:OD2	2.35	0.45
1:F:259:PRO:HD2	1:F:260:MET:SD	2.57	0.45
1:D:275:HIS:HD2	1:D:365:GLU:OE1	1.99	0.45
1:F:188:ILE:HG22	1:F:252:VAL:HG12	1.99	0.45
1:D:314:TRP:CZ3	1:D:324:LEU:HD22	2.51	0.44
1:F:263:MET:O	1:F:264:LEU:HB3	2.18	0.44
1:H:262:TYR:OH	1:H:475:PHE:HE2	1.99	0.44
1:B:346:ILE:HG22	1:B:409:PRO:HB2	1.98	0.44
1:B:157:LEU:HD23	1:B:219:MET:HE1	1.98	0.44
1:H:150:TYR:O	1:H:153:PHE:HB3	2.18	0.44
1:B:444:ASN:CG	1:B:445:LYS:H	2.21	0.44
1:D:345:ASP:O	1:D:348:ILE:HG12	2.18	0.44
1:F:306:GLU:O	1:F:310:LYS:HG2	2.18	0.44
1:B:459:GLN:H	1:B:459:GLN:NE2	2.14	0.44
1:F:194:CYS:SG	1:F:213:ALA:HB1	2.58	0.44
1:B:298:PHE:HB2	1:B:348:ILE:HD12	2.00	0.44
1:B:316:GLN:HA	1:B:317:PRO:HD3	1.89	0.44
2:F:1479:SAH:HG2	2:F:1479:SAH:H4'	1.32	0.43
1:B:188:ILE:HG22	1:B:252:VAL:HG12	1.99	0.43
1:B:154:TYR:CD1	2:B:1478:SAH:H3'	2.54	0.43
1:D:304:TYR:CD1	1:D:304:TYR:C	2.91	0.43
2:H:1478:SAH:H8	3:H:2001:HOH:O	2.19	0.43
1:D:264:LEU:CD2	3:D:2031:HOH:O	2.58	0.43
1:F:259:PRO:HG2	1:F:270:LEU:CD2	2.47	0.43
1:H:437:GLY:HA3	1:H:454:VAL:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:393:ASP:OD1	1:D:406:SER:CB	2.67	0.43
1:F:264:LEU:HD23	1:F:293:VAL:HG22	2.00	0.43
1:B:444:ASN:HB3	1:B:448:SER:O	2.18	0.43
1:D:288:PRO:HB3	1:D:394:VAL:HG13	2.01	0.43
3:D:2006:HOH:O	1:F:460:THR:HG23	2.18	0.43
2:F:1479:SAH:HN1	2:F:1479:SAH:HG1	1.62	0.42
1:B:289:THR:O	1:B:360:PHE:HB2	2.19	0.42
1:B:345:ASP:O	1:B:348:ILE:HG12	2.19	0.42
1:F:166:ASP:OD2	1:F:415:HIS:CD2	2.71	0.42
1:F:242:LYS:HA	2:F:1479:SAH:N1	2.34	0.42
1:F:337:ARG:HG2	1:F:467:LEU:O	2.18	0.42
1:F:346:ILE:HG22	1:F:409:PRO:HB2	2.01	0.42
1:H:221:GLN:O	1:H:225:VAL:HG23	2.19	0.42
1:B:412:PRO:HD2	3:B:2040:HOH:O	2.19	0.42
1:B:196:SER:HA	1:B:219:MET:HE2	2.00	0.42
1:B:440:LEU:HB3	1:B:452:SER:HB3	2.00	0.42
1:F:154:TYR:OH	1:F:267:GLU:OE1	2.32	0.42
1:H:297:PRO:HG2	1:H:350:MET:HB2	2.00	0.42
1:H:373:ILE:HA	1:H:374:PRO:HD3	1.91	0.42
1:D:366:GLY:HA2	1:D:369:HIS:NE2	2.35	0.42
1:F:192:VAL:HB	1:F:243:VAL:HG11	2.01	0.42
1:F:309:THR:O	1:F:312:ASN:HB3	2.20	0.42
1:H:302:GLN:O	1:H:306:GLU:HB2	2.19	0.42
1:B:169:ARG:HH12	2:B:1478:SAH:C	2.33	0.42
1:B:434:THR:H	1:B:459:GLN:NE2	2.15	0.42
1:F:169:ARG:HH12	2:F:1479:SAH:C	2.32	0.41
1:B:150:TYR:OH	2:B:1478:SAH:H8	2.20	0.41
1:H:376:LYS:HG2	1:H:434:THR:HG23	2.02	0.41
1:H:154:TYR:CD1	2:H:1478:SAH:H3'	2.55	0.41
1:D:169:ARG:HG3	1:D:416:TRP:CH2	2.55	0.41
1:H:280:LEU:HD11	1:H:284:GLY:HA3	2.03	0.41
1:H:451:ILE:HD11	1:H:470:LEU:HB2	2.02	0.41
1:B:386:HIS:CD2	1:B:426:PRO:HG3	2.56	0.41
1:D:294:HIS:HD2	1:D:353:SER:OG	2.03	0.41
1:F:199:LEU:HD22	2:F:1479:SAH:HN2	1.86	0.41
1:H:278:LYS:HE3	1:H:279:TYR:CZ	2.56	0.41
1:H:301:GLU:HG3	1:H:305:MET:CE	2.51	0.41
1:B:334:GLU:HA	1:B:337:ARG:HD3	2.02	0.41
1:B:425:SER:HA	1:B:426:PRO:HD3	1.97	0.40
1:F:221:GLN:HG3	1:F:222:HIS:N	2.36	0.40
1:H:471:LYS:O	1:H:473:PRO:HD3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:433:ASP:CG	1:D:459:GLN:HG3	2.42	0.40
1:B:256:ILE:HG22	1:B:287:PHE:HB2	2.03	0.40
1:D:352:LYS:H	1:D:352:LYS:CE	2.33	0.40
1:F:204:ALA:O	1:F:235:ARG:NH2	2.54	0.40
1:H:232:LEU:HD23	1:H:235:ARG:HD3	2.02	0.40
1:H:266:ASN:O	1:H:267:GLU:CB	2.69	0.40
1:H:328:ARG:HD3	1:H:328:ARG:C	2.42	0.40
1:D:151:PHE:O	1:D:217:SER:HB2	2.21	0.40
1:F:382:SER:HA	1:F:430:LYS:HA	2.03	0.40
1:F:471:LYS:O	1:F:472:ASN:CB	2.69	0.40
1:H:316:GLN:HA	1:H:317:PRO:HD3	1.85	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	B	329/346 (95%)	303 (92%)	22 (7%)	4 (1%)	13	32
1	D	331/346 (96%)	313 (95%)	16 (5%)	2 (1%)	25	50
1	F	330/346 (95%)	299 (91%)	26 (8%)	5 (2%)	10	26
1	H	328/346 (95%)	309 (94%)	19 (6%)	0	100	100
All	All	1318/1384 (95%)	1224 (93%)	83 (6%)	11 (1%)	19	43

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	234	ASP
1	B	446	ARG
1	F	472	ASN
1	D	305	MET

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Mol	Chain	Res	Type
1	B	218	THR
1	F	234	ASP
1	F	448	SER
1	B	208	ALA
1	F	218	THR
1	D	166	ASP
1	F	233	THR

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	B	275/298 (92%)	251 (91%)	24 (9%)	10	23
1	D	280/298 (94%)	262 (94%)	18 (6%)	17	39
1	F	276/298 (93%)	252 (91%)	24 (9%)	10	23
1	H	280/298 (94%)	256 (91%)	24 (9%)	10	24
All	All	1111/1192 (93%)	1021 (92%)	90 (8%)	11	27

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	190	LEU
1	B	192	VAL
1	B	199	LEU
1	B	209	ARG
1	B	221	GLN
1	B	234	ASP
1	B	243	VAL
1	B	244	GLU
1	B	247	SER
1	B	258	GLU
1	B	280	LEU
1	B	295	LEU
1	B	303	LEU
1	B	312	ASN

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Mol	Chain	Res	Type
1	B	333	ASP
1	B	346	ILE
1	B	361	LEU
1	B	362	GLU
1	B	384	LEU
1	B	394	VAL
1	B	421	CYS
1	B	441	LEU
1	B	449	TYR
1	B	468	LEU
1	D	150	TYR
1	D	162	ASN
1	D	175	ARG
1	D	190	LEU
1	D	192	VAL
1	D	233	THR
1	D	243	VAL
1	D	287	PHE
1	D	295	LEU
1	D	303	LEU
1	D	352	LYS
1	D	354	VAL
1	D	394	VAL
1	D	411	GLU
1	D	418	GLN
1	D	427	LEU
1	D	430	LYS
1	D	470	LEU
1	F	190	LEU
1	F	192	VAL
1	F	199	LEU
1	F	233	THR
1	F	234	ASP
1	F	243	VAL
1	F	244	GLU
1	F	248	LEU
1	F	258	GLU
1	F	295	LEU
1	F	324	LEU
1	F	333	ASP
1	F	346	ILE
1	F	354	VAL

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Mol	Chain	Res	Type
1	F	361	LEU
1	F	369	HIS
1	F	384	LEU
1	F	394	VAL
1	F	413	LEU
1	F	442	ILE
1	F	465	SER
1	F	467	LEU
1	F	468	LEU
1	F	470	LEU
1	H	150	TYR
1	H	169	ARG
1	H	190	LEU
1	H	192	VAL
1	H	199	LEU
1	H	243	VAL
1	H	258	GLU
1	H	270	LEU
1	H	289	THR
1	H	295	LEU
1	H	302	GLN
1	H	303	LEU
1	H	309	THR
1	H	310	LYS
1	H	327	LEU
1	H	346	ILE
1	H	350	MET
1	H	361	LEU
1	H	394	VAL
1	H	425	SER
1	H	427	LEU
1	H	441	LEU
1	H	447	GLN
1	H	472	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	174	GLN
1	B	179	GLN
1	B	275	HIS
1	B	294	HIS

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Mol	Chain	Res	Type
1	B	320	HIS
1	B	459	GLN
1	D	149	GLN
1	D	162	ASN
1	D	174	GLN
1	D	179	GLN
1	D	275	HIS
1	D	294	HIS
1	D	320	HIS
1	D	338	GLN
1	D	415	HIS
1	D	418	GLN
1	D	472	ASN
1	F	161	GLN
1	F	174	GLN
1	F	179	GLN
1	F	275	HIS
1	F	294	HIS
1	F	312	ASN
1	F	320	HIS
1	F	415	HIS
1	F	456	GLN
1	F	459	GLN
1	H	162	ASN
1	H	165	GLN
1	H	174	GLN
1	H	179	GLN
1	H	221	GLN
1	H	275	HIS
1	H	294	HIS
1	H	302	GLN
1	H	307	GLN
1	H	316	GLN
1	H	320	HIS
1	H	338	GLN
1	H	369	HIS
1	H	472	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
2	SAH	B	1478	-	24,28,28	1.31	3 (12%)	25,40,40	1.61	3 (12%)
2	SAH	F	1479	-	24,28,28	1.32	3 (12%)	25,40,40	1.63	3 (12%)
2	SAH	D	1480	-	24,28,28	1.19	3 (12%)	25,40,40	1.54	4 (16%)
2	SAH	H	1478	-	24,28,28	1.21	3 (12%)	25,40,40	1.65	3 (12%)

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	SAH	B	1478	-	-	0/11/31/31	0/3/3/3
2	SAH	F	1479	-	-	6/11/31/31	0/3/3/3
2	SAH	D	1480	-	-	0/11/31/31	0/3/3/3
2	SAH	H	1478	-	-	1/11/31/31	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1478	SAH	C2-N3	4.42	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1479	SAH	C2-N3	4.18	1.38	1.32
2	D	1480	SAH	C2-N3	3.81	1.38	1.32
2	H	1478	SAH	C2-N3	3.63	1.37	1.32
2	F	1479	SAH	C2-N1	2.71	1.38	1.33
2	H	1478	SAH	C2-N1	2.57	1.38	1.33
2	B	1478	SAH	C2-N1	2.56	1.38	1.33
2	D	1480	SAH	C2-N1	2.53	1.38	1.33
2	B	1478	SAH	OXT-C	-2.27	1.23	1.30
2	D	1480	SAH	OXT-C	-2.25	1.23	1.30
2	F	1479	SAH	OXT-C	-2.10	1.23	1.30
2	H	1478	SAH	OXT-C	-2.06	1.23	1.30

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1478	SAH	N3-C2-N1	-5.92	119.42	128.68
2	F	1479	SAH	N3-C2-N1	-5.86	119.52	128.68
2	H	1478	SAH	N3-C2-N1	-5.81	119.60	128.68
2	D	1480	SAH	N3-C2-N1	-5.51	120.06	128.68
2	H	1478	SAH	C5'-SD-CG	-2.96	93.38	102.27
2	F	1479	SAH	C5'-SD-CG	-2.92	93.52	102.27
2	B	1478	SAH	C5'-SD-CG	-2.86	93.67	102.27
2	B	1478	SAH	OXT-C-O	-2.81	117.71	124.09
2	D	1480	SAH	C5'-SD-CG	-2.55	94.62	102.27
2	D	1480	SAH	OXT-C-O	-2.48	118.46	124.09
2	D	1480	SAH	OXT-C-CA	2.19	120.86	113.38
2	F	1479	SAH	OXT-C-O	-2.03	119.47	124.09
2	H	1478	SAH	OXT-C-CA	2.00	120.20	113.38

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	1479	SAH	N-CA-CB-CG
2	F	1479	SAH	CA-CB-CG-SD
2	F	1479	SAH	C4'-C5'-SD-CG
2	F	1479	SAH	O4'-C4'-C5'-SD
2	F	1479	SAH	C3'-C4'-C5'-SD
2	F	1479	SAH	C-CA-CB-CG
2	H	1478	SAH	C-CA-CB-CG

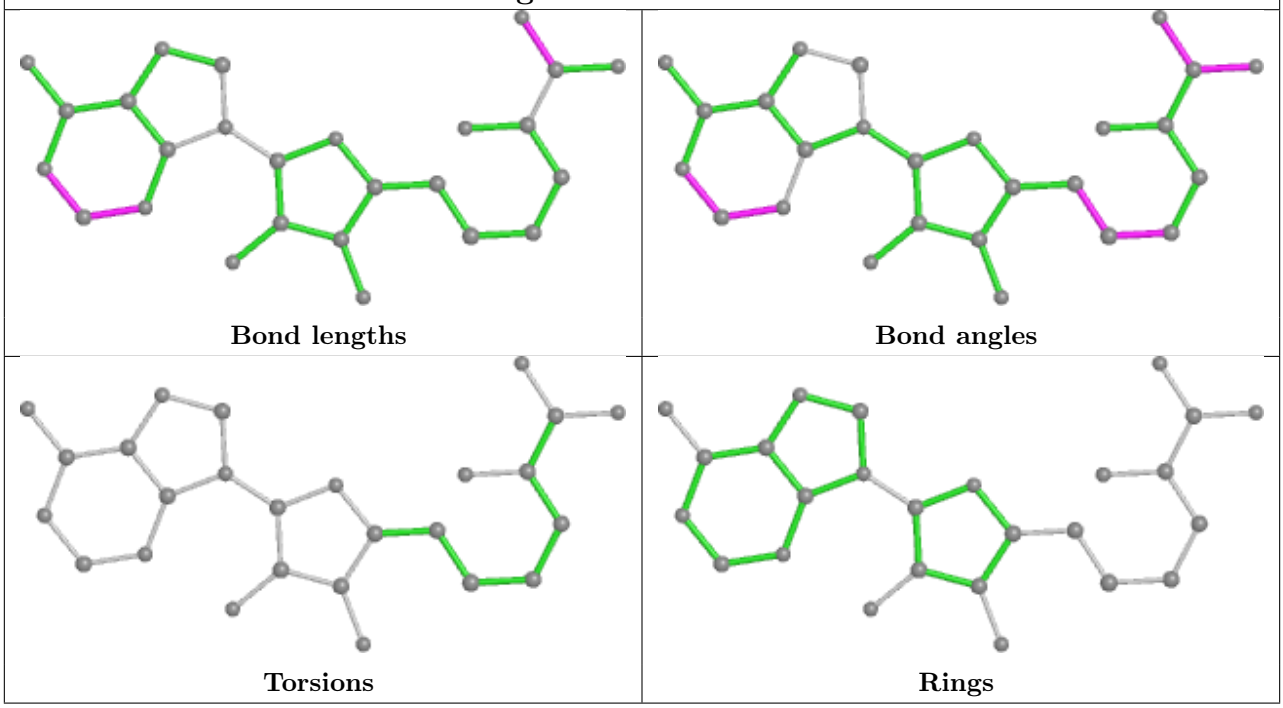
There are no ring outliers.

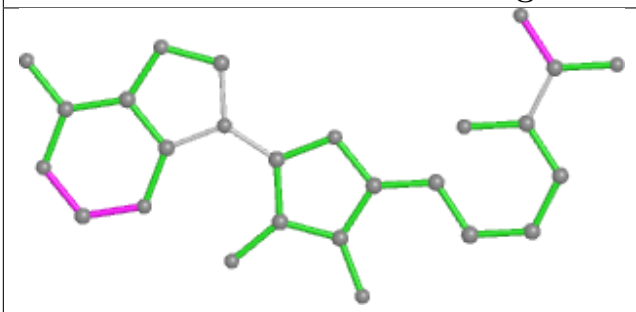
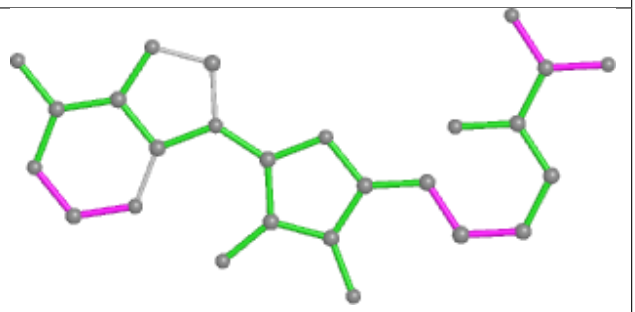
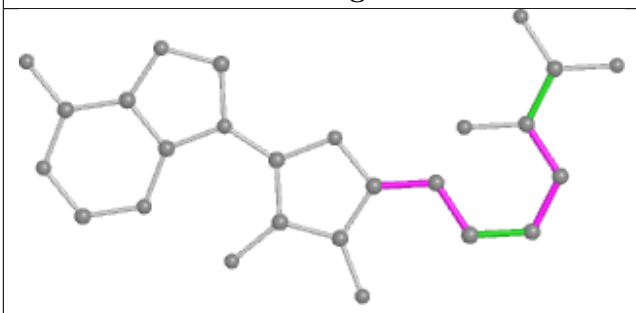
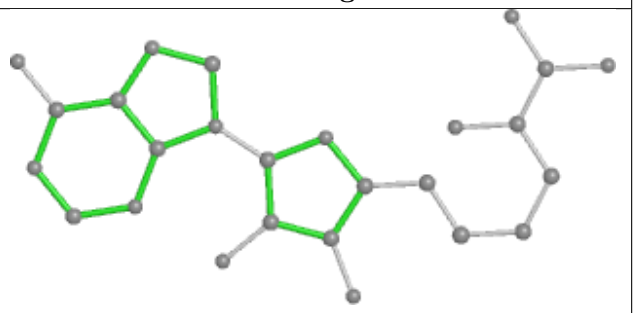
3 monomers are involved in 13 short contacts:

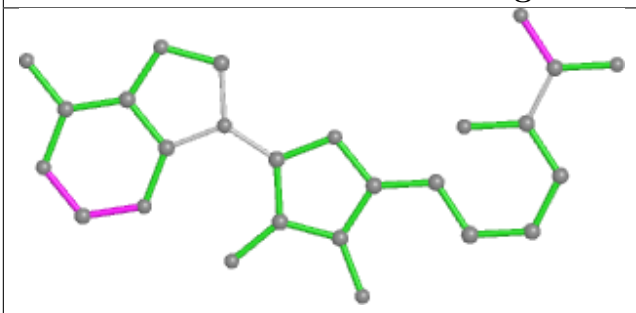
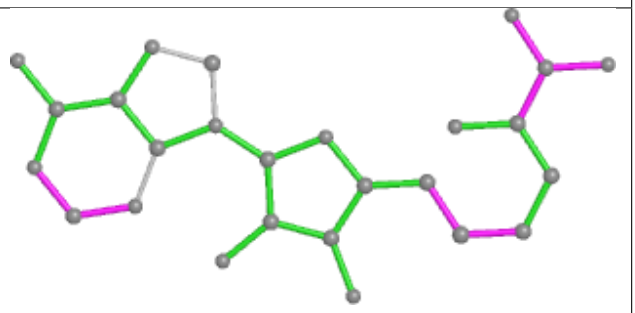
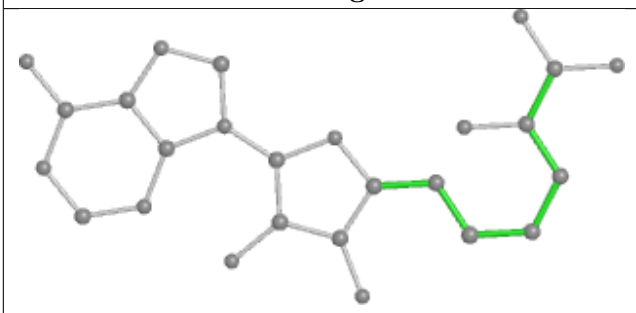
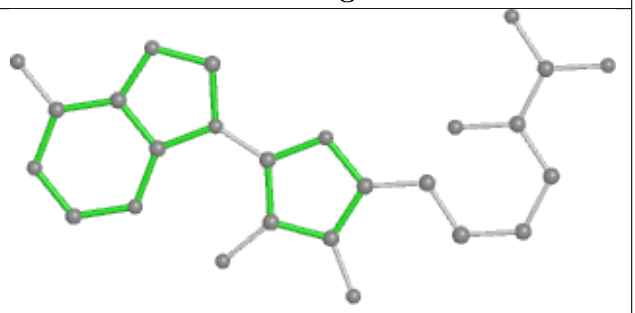
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1478	SAH	5	0
2	F	1479	SAH	5	0
2	H	1478	SAH	3	0

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

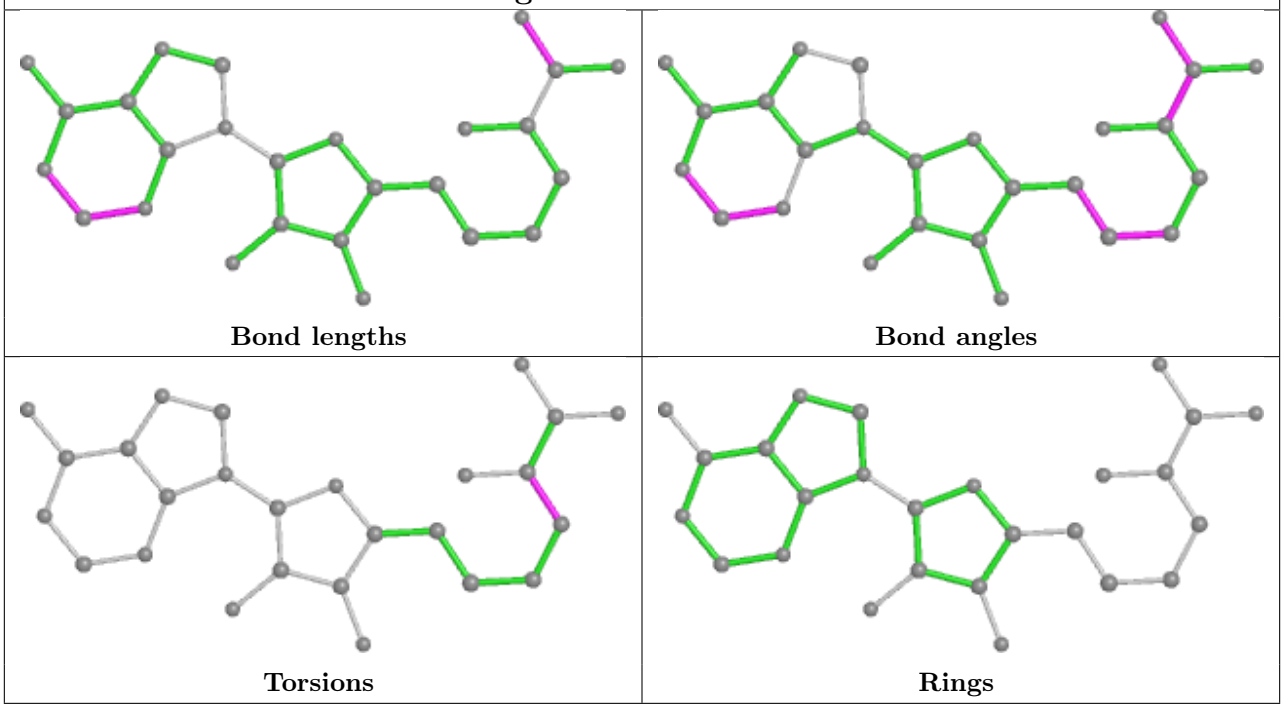
Ligand SAH B 1478



Ligand SAH F 1479	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SAH D 1480	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SAH H 1478



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	B	331/346 (95%)	0.04	3 (0%) 84 85	35, 49, 58, 78	0
1	D	333/346 (96%)	-0.02	2 (0%) 89 91	26, 45, 59, 75	0
1	F	332/346 (95%)	0.05	0 100 100	37, 48, 63, 71	0
1	H	330/346 (95%)	0.00	3 (0%) 84 85	34, 49, 61, 82	0
All	All	1326/1384 (95%)	0.02	8 (0%) 89 91	26, 48, 61, 82	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	348	ILE	3.5
1	H	148	VAL	3.3
1	D	479	GLY	2.7
1	D	478	THR	2.6
1	H	477	TYR	2.5
1	B	148	VAL	2.4
1	B	147	ALA	2.3
1	B	428	PHE	2.3

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

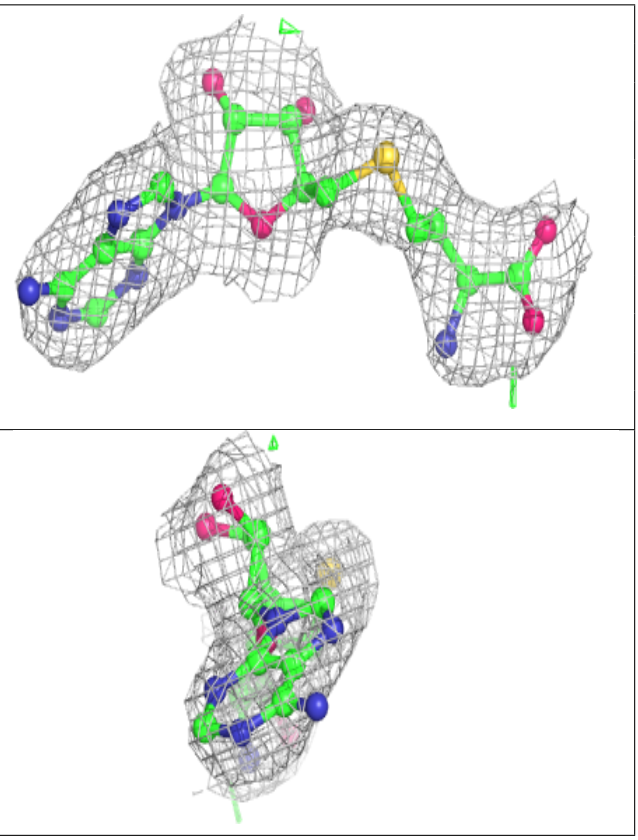
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SAH	B	1478	26/26	0.95	0.16	47,49,51,52	0
2	SAH	D	1480	26/26	0.96	0.17	26,32,40,40	0
2	SAH	F	1479	26/26	0.96	0.20	43,45,46,46	0
2	SAH	H	1478	26/26	0.97	0.16	38,40,43,43	0

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

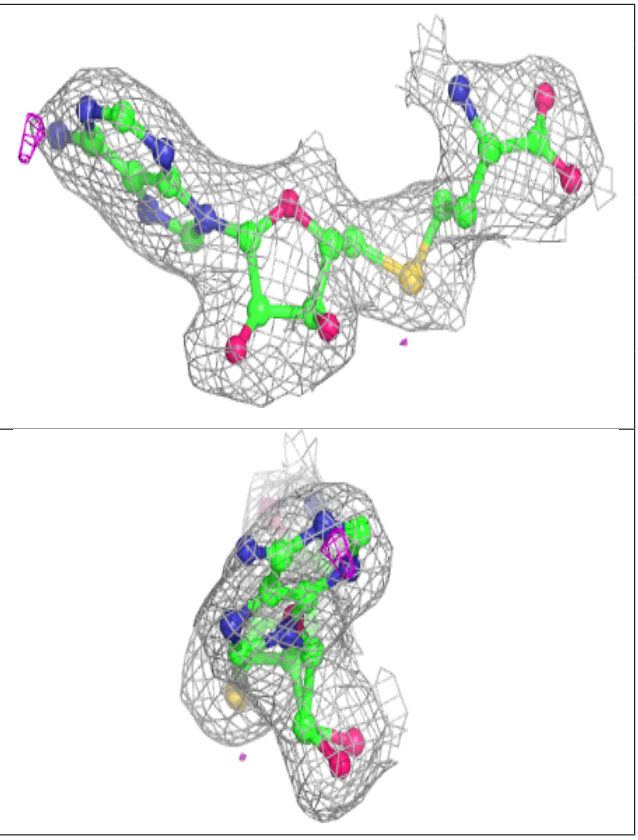
Electron density around SAH B 1478:

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



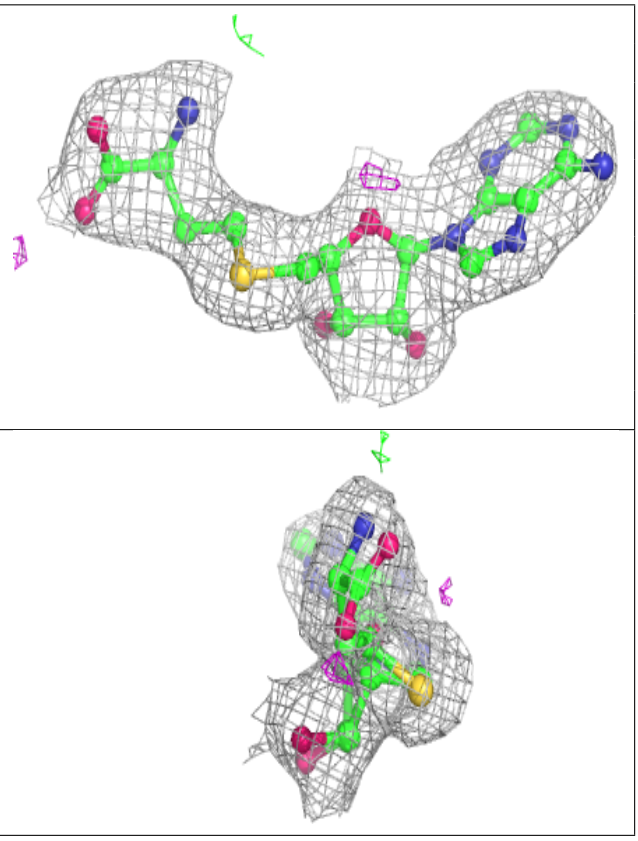
Electron density around SAH D 1480:

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



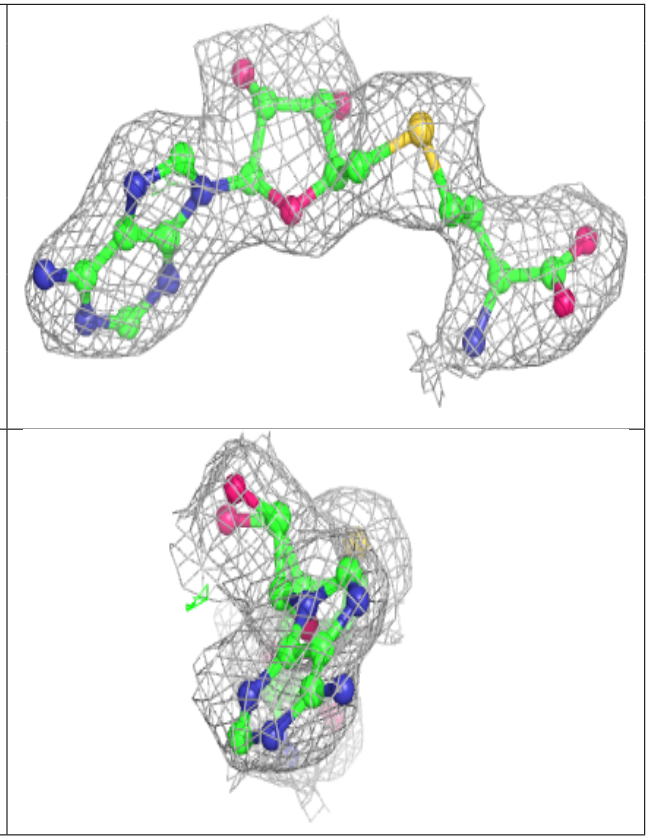
Electron density around SAH F 1479:

$2mF_o$-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 H 1478:

$2mF_o$-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.