Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 07:46 PM JST

PDB ID	:	5ZZW
Title	:	Proteobacterial origin of protein arginine methylation and regulation of Complex I assembly by MidA
Authors	:	Arold, S.T.; Swaminathan, K.; Hameed, U.F.S.
Deposited on	:	2018-06-04
Resolution	:	2.60 Å(reported)

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

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

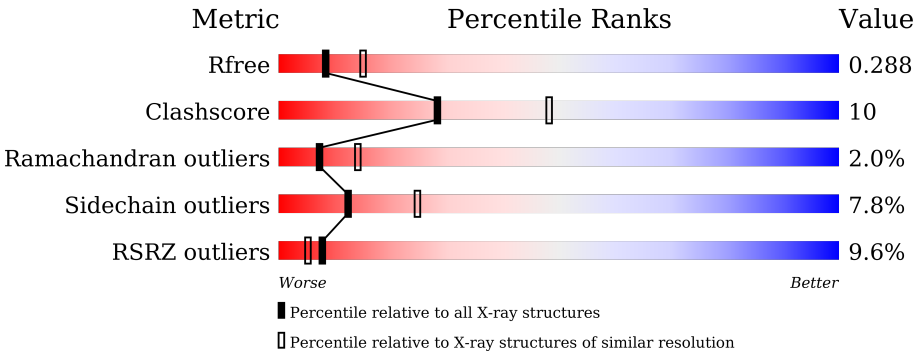
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	414	12% 74% 19%
1	B	414	6% 77% 16%
1	C	414	10% 78% 14%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9697 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.

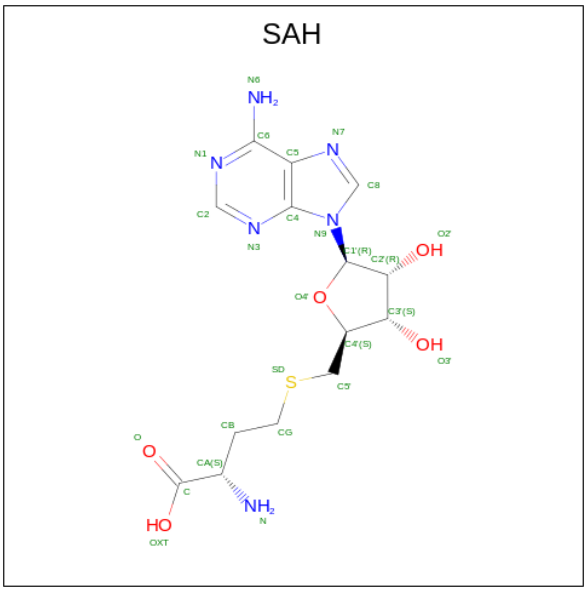
- Molecule 1 is a protein called Protein arginine methyltransferase NDUFAF7 homolog, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	400	Total	C	N	O	S	0	0	0
			3193	2062	519	599	13			
1	A	400	Total	C	N	O	S	0	0	0
			3193	2062	519	599	13			
1	C	400	Total	C	N	O	S	0	0	0
			3193	2062	519	599	13			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	71	GLY	-	expression tag	UNP Q54S83
B	72	PRO	-	expression tag	UNP Q54S83
B	73	LEU	-	expression tag	UNP Q54S83
B	74	GLY	-	expression tag	UNP Q54S83
B	75	SER	-	expression tag	UNP Q54S83
A	71	GLY	-	expression tag	UNP Q54S83
A	72	PRO	-	expression tag	UNP Q54S83
A	73	LEU	-	expression tag	UNP Q54S83
A	74	GLY	-	expression tag	UNP Q54S83
A	75	SER	-	expression tag	UNP Q54S83
C	71	GLY	-	expression tag	UNP Q54S83
C	72	PRO	-	expression tag	UNP Q54S83
C	73	LEU	-	expression tag	UNP Q54S83
C	74	GLY	-	expression tag	UNP Q54S83
C	75	SER	-	expression tag	UNP Q54S83

- 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
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 3 is water.

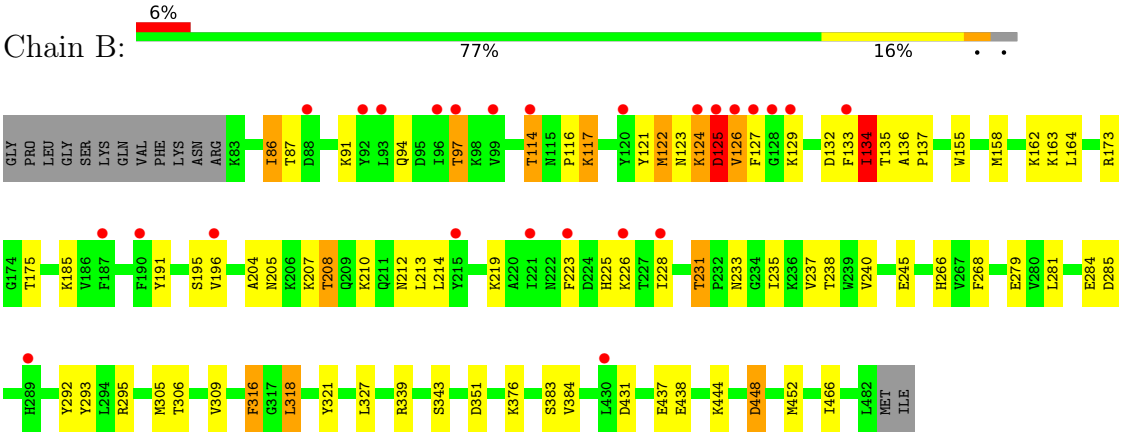
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	15	Total	O	0	0
			15	15		
3	A	12	Total	O	0	0
			12	12		
3	C	13	Total	O	0	0
			13	13		

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.

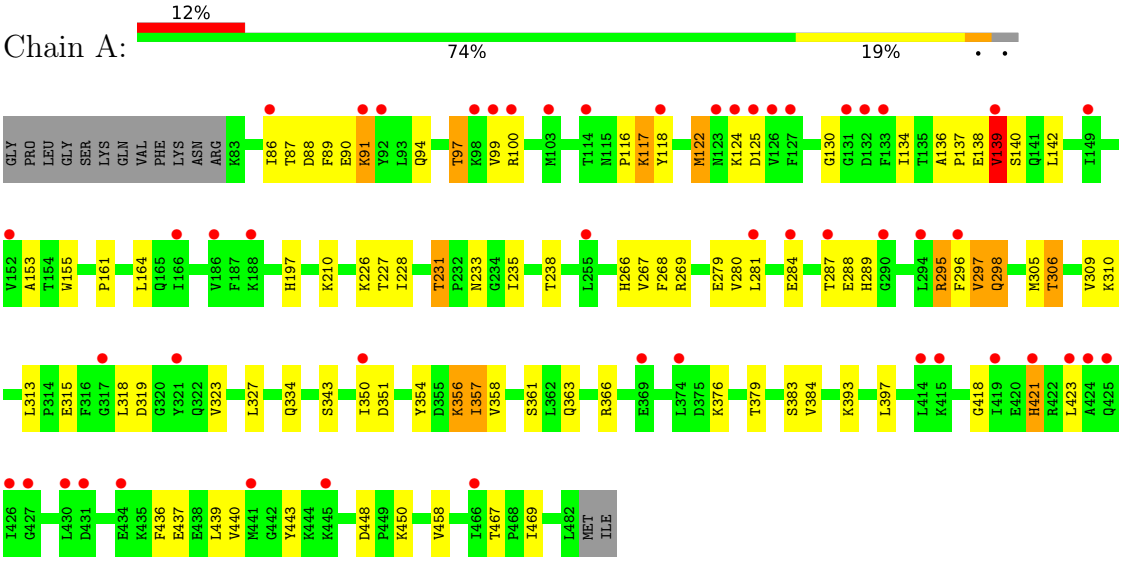
• Molecule 1: Protein arginine methyltransferase NDUFAF7 homolog, mitochondrial

Chain B:



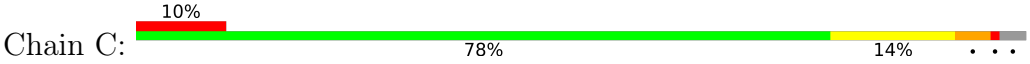
• Molecule 1: Protein arginine methyltransferase NDUFAF7 homolog, mitochondrial

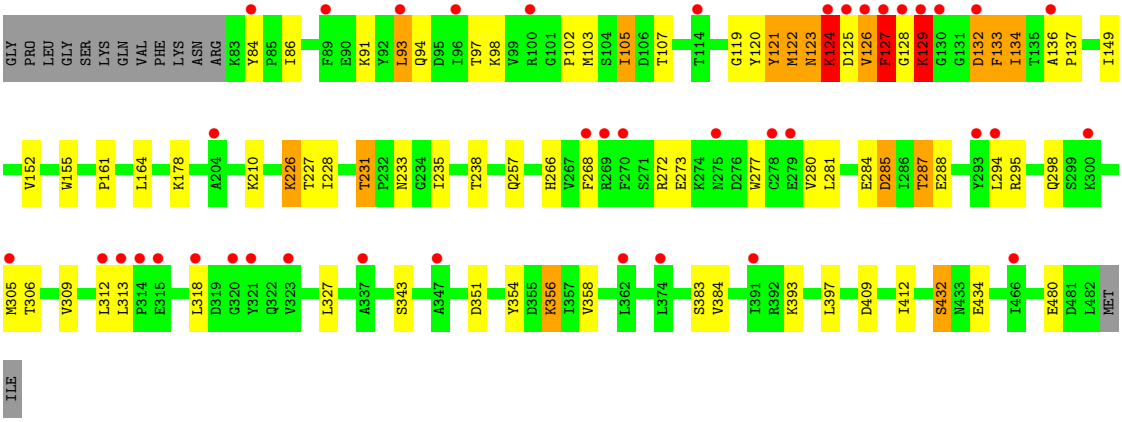
Chain A:



• Molecule 1: Protein arginine methyltransferase NDUFAF7 homolog, mitochondrial

Chain C:




GLY PRO LEU GLY SER LYS GLN VAL PHE LYS ASN ARG K83 Y84 P85 I86 F89 E90 K91 Y92 L93 Q94 D95 I96 T97 K98 V99 R100 G101 P102 M103 S104 I105 D106 T107 T114 G119 Y120 Y121 M122 N123 K124 D125 V126 F127 G128 K129 G130 G131 D132 F133 I134 T135 A136 P137 I149
V152 W155 P161 L164 K178 A204 K210 K226 T227 I228 T231 P232 N233 G234 I235 T238 Q257 H266 V267 F268 R269 F270 S271 R272 E273 K274 N275 D276 W277 C278 E279 V280 L281 E284 D285 I286 T287 E288 Y293 L294 R295 Q298 S299 K300
M305 T306 V309 L312 L313 P314 E315 L318 D319 G320 Y321 Q322 V323 L327 A337 S343 A347 D351 Y354 D355 K356 I357 V358 L362 L374 S383 V384 I391 R392 K393 L397 D409 I412 S432 N433 E434 I466 E480 D481 L482 MET
ILE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.95Å 103.54Å 192.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.54 – 2.60 54.54 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (54.54-2.60) 99.7 (54.54-2.60)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0216	Depositor
R, R_{free}	0.248 , 0.280 0.251 , 0.288	Depositor DCC
R_{free} test set	2280 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	69.9	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 53.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9697	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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: 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	A	0.39	0/3262	0.63	0/4404
1	B	0.42	0/3262	0.63	0/4404
1	C	0.41	0/3262	0.63	1/4404 (0.0%)
All	All	0.40	0/9786	0.63	1/13212 (0.0%)

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	C	121	TYR	N-CA-C	-6.54	93.34	111.00

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	3193	0	3225	71	0
1	B	3193	0	3225	53	0
1	C	3193	0	3225	67	0
2	A	26	0	19	0	0
2	B	26	0	19	0	0
2	C	26	0	19	0	0
3	A	12	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	15	0	0	1	0
3	C	13	0	0	1	0
All	All	9697	0	9732	189	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 10.

All (189) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:ASP:OD1	1:C:126:VAL:N	1.91	1.03
1:C:133:PHE:HD1	1:C:134:ILE:H	1.14	0.95
1:C:133:PHE:O	1:C:134:ILE:HB	1.75	0.86
1:C:285:ASP:HB2	1:C:295:ARG:HD3	1.57	0.85
1:B:86:ILE:HD12	1:B:91:LYS:HG3	1.59	0.85
1:C:285:ASP:CB	1:C:295:ARG:HD3	2.06	0.84
1:C:121:TYR:C	1:C:122:MET:HG2	1.98	0.82
1:C:309:VAL:HG23	1:C:312:LEU:HD12	1.60	0.81
1:A:153:ALA:HB1	1:A:469:ILE:HD13	1.63	0.80
1:A:296:PHE:CG	1:A:296:PHE:O	2.31	0.80
1:B:285:ASP:N	1:B:293:TYR:O	2.17	0.78
1:A:423:LEU:HD12	1:A:439:LEU:HD22	1.67	0.76
1:C:125:ASP:OD1	1:C:126:VAL:HG23	1.88	0.73
1:C:133:PHE:HD1	1:C:134:ILE:N	1.88	0.72
1:C:178:LYS:NZ	3:C:601:HOH:O	2.22	0.71
1:B:339:ARG:NH1	3:B:601:HOH:O	2.20	0.70
1:A:350:ILE:HD13	1:A:458:VAL:HG13	1.74	0.69
1:B:214:LEU:HD21	1:B:237:VAL:HG21	1.75	0.69
1:C:133:PHE:CD1	1:C:134:ILE:N	2.61	0.69
1:B:214:LEU:HD21	1:B:237:VAL:CG2	2.23	0.69
1:A:88:ASP:O	1:A:91:LYS:HG3	1.93	0.68
1:C:354:TYR:HB3	1:C:356:LYS:HD2	1.78	0.66
1:A:296:PHE:O	1:A:296:PHE:CD2	2.49	0.65
1:B:163:LYS:NZ	1:B:195:SER:OG	2.29	0.65
1:A:153:ALA:CB	1:A:469:ILE:HD13	2.27	0.65
1:B:94:GLN:O	1:B:97:THR:HG22	1.98	0.64
1:A:297:VAL:HG23	1:A:298:GLN:H	1.63	0.64
1:C:94:GLN:O	1:C:97:THR:HG22	1.98	0.64
1:C:309:VAL:CG2	1:C:312:LEU:HD12	2.28	0.64
1:B:136:ALA:HB2	1:B:452:MET:HE1	1.81	0.62
1:A:94:GLN:O	1:A:97:THR:HG22	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:THR:HG23	1:B:233:ASN:H	1.65	0.62
1:C:126:VAL:O	1:C:126:VAL:HG12	1.99	0.62
1:C:231:THR:HG23	1:C:233:ASN:H	1.65	0.62
1:A:231:THR:HG23	1:A:233:ASN:H	1.65	0.62
1:A:423:LEU:CD1	1:A:439:LEU:HD22	2.30	0.61
1:B:266:HIS:HD2	1:B:279:GLU:OE2	1.84	0.60
1:B:155:TRP:HA	1:B:158:MET:HE3	1.83	0.60
1:B:117:LYS:HG2	1:A:318:LEU:HD21	1.83	0.60
1:A:99:VAL:HG23	1:A:100:ARG:HG3	1.83	0.60
1:C:119:GLY:O	1:C:121:TYR:O	2.19	0.60
1:A:87:THR:HG22	1:A:90:GLU:OE1	2.02	0.59
1:B:173:ARG:HB2	1:B:175:THR:HG23	1.84	0.59
1:A:323:VAL:HG23	1:A:357:ILE:HG23	1.84	0.59
1:A:418:GLY:O	1:A:421:HIS:ND1	2.28	0.59
1:A:295:ARG:HH11	1:A:297:VAL:HG12	1.68	0.58
1:A:361:SER:O	1:A:363:GLN:HG2	2.03	0.58
1:B:129:LYS:HB2	1:B:173:ARG:HD2	1.86	0.58
1:C:285:ASP:HB2	1:C:295:ARG:CD	2.30	0.58
1:A:268:PHE:CD1	1:A:306:THR:HG23	2.39	0.57
1:C:93:LEU:HD11	1:C:294:LEU:CD1	2.34	0.57
1:C:125:ASP:CG	1:C:126:VAL:HG23	2.24	0.57
1:A:266:HIS:HD2	1:A:279:GLU:OE2	1.88	0.57
1:C:93:LEU:HD11	1:C:294:LEU:HD13	1.85	0.57
1:B:228:ILE:HG12	1:B:238:THR:HG23	1.87	0.56
1:A:313:LEU:HD22	1:A:323:VAL:HG11	1.87	0.56
1:C:133:PHE:CD1	1:C:133:PHE:N	2.72	0.56
1:A:350:ILE:HD13	1:A:458:VAL:HG22	1.88	0.55
1:C:120:TYR:C	1:C:121:TYR:O	2.37	0.55
1:C:266:HIS:CD2	1:C:327:LEU:HD22	2.42	0.55
1:A:423:LEU:HD12	1:A:439:LEU:CD2	2.35	0.55
1:A:228:ILE:HG23	1:A:238:THR:HG22	1.88	0.55
1:A:439:LEU:O	1:A:439:LEU:HD23	2.07	0.55
1:A:138:GLU:O	1:A:139:VAL:HG12	2.08	0.54
1:A:437:GLU:HA	1:A:440:VAL:HG22	1.88	0.54
1:A:423:LEU:CD1	1:A:439:LEU:CD2	2.85	0.54
1:B:114:THR:O	1:B:114:THR:HG23	2.07	0.54
1:A:295:ARG:HD3	1:A:297:VAL:CG1	2.38	0.54
1:C:228:ILE:HG12	1:C:238:THR:HG23	1.88	0.54
1:B:121:TYR:O	1:B:122:MET:HG2	2.08	0.54
1:A:210:LYS:NZ	1:A:226:LYS:O	2.24	0.53
1:A:287:THR:HG22	1:A:288:GLU:N	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:PHE:CD1	1:C:128:GLY:N	2.73	0.53
1:A:197:HIS:CD2	1:A:238:THR:OG1	2.61	0.53
1:C:97:THR:CG2	1:C:284:GLU:HG3	2.39	0.53
1:B:305:MET:O	1:B:309:VAL:HG22	2.09	0.53
1:A:297:VAL:O	1:A:298:GLN:CB	2.57	0.53
1:B:285:ASP:HB3	1:B:293:TYR:O	2.09	0.53
1:B:210:LYS:O	1:B:212:ASN:O	2.27	0.53
1:C:155:TRP:CD1	1:C:161:PRO:HD2	2.44	0.53
1:B:134:ILE:O	1:B:134:ILE:HG23	2.09	0.52
1:C:268:PHE:CD1	1:C:306:THR:HG22	2.43	0.52
1:A:297:VAL:O	1:A:298:GLN:HB2	2.10	0.52
1:C:91:LYS:HA	1:C:94:GLN:HG2	1.91	0.52
1:C:309:VAL:HG22	1:C:312:LEU:HB2	1.91	0.52
1:A:142:LEU:HD11	1:A:439:LEU:HD21	1.92	0.52
1:A:155:TRP:CD1	1:A:161:PRO:HD2	2.45	0.52
1:A:268:PHE:C	3:A:601:HOH:O	2.47	0.52
1:C:121:TYR:O	1:C:122:MET:HG2	2.09	0.51
1:C:125:ASP:CG	1:C:126:VAL:N	2.64	0.51
1:C:210:LYS:NZ	1:C:226:LYS:O	2.26	0.51
1:C:231:THR:HG22	1:C:235:ILE:H	1.75	0.51
1:C:354:TYR:HD2	1:C:358:VAL:HG22	1.76	0.51
1:B:466:ILE:HD12	1:B:466:ILE:N	2.25	0.51
1:B:285:ASP:CB	1:B:293:TYR:O	2.59	0.51
1:A:231:THR:HG22	1:A:235:ILE:H	1.74	0.51
1:C:98:LYS:NZ	1:C:284:GLU:OE2	2.38	0.50
1:A:305:MET:O	1:A:309:VAL:HG22	2.11	0.50
1:B:231:THR:HG22	1:B:235:ILE:H	1.75	0.50
1:B:240:VAL:HG11	1:B:245:GLU:HB2	1.94	0.50
1:B:240:VAL:CG1	1:B:245:GLU:HB2	2.42	0.49
1:B:114:THR:O	1:B:114:THR:CG2	2.60	0.49
1:B:285:ASP:HB3	1:B:293:TYR:C	2.32	0.49
1:B:292:TYR:O	1:B:293:TYR:HB2	2.13	0.49
1:A:423:LEU:HD11	1:A:440:VAL:HG12	1.94	0.49
1:C:128:GLY:O	1:C:129:LYS:HB2	2.13	0.49
1:C:105:ILE:HD13	1:C:280:VAL:O	2.12	0.49
1:C:136:ALA:HB3	1:C:137:PRO:HD3	1.94	0.49
1:C:285:ASP:HB2	1:C:295:ARG:HB3	1.95	0.49
1:B:204:ALA:O	1:B:208:THR:HG22	2.12	0.49
1:B:207:LYS:HG3	1:B:208:THR:N	2.28	0.48
1:A:122:MET:N	1:A:122:MET:SD	2.86	0.48
1:C:134:ILE:HG22	1:C:134:ILE:O	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:ASP:OD2	1:C:295:ARG:HD3	2.13	0.48
1:A:88:ASP:O	1:A:91:LYS:HE3	2.13	0.48
1:A:318:LEU:HD23	1:A:319:ASP:O	2.13	0.48
1:B:124:LYS:O	1:B:125:ASP:OD1	2.31	0.48
1:A:356:LYS:CD	1:A:357:ILE:O	2.62	0.48
1:A:87:THR:HG23	1:A:90:GLU:H	1.78	0.48
1:A:439:LEU:HD23	1:A:439:LEU:C	2.34	0.47
1:A:138:GLU:O	1:A:139:VAL:CB	2.62	0.47
1:A:116:PRO:O	1:A:117:LYS:CB	2.61	0.47
1:A:267:VAL:HG12	3:A:601:HOH:O	2.13	0.47
1:A:155:TRP:CD1	1:A:164:LEU:HD22	2.50	0.47
1:A:323:VAL:HG23	1:A:357:ILE:CG2	2.45	0.47
1:C:285:ASP:CG	1:C:295:ARG:HD3	2.35	0.47
1:C:309:VAL:HG22	1:C:309:VAL:O	2.14	0.47
1:C:432:SER:OG	1:C:434:GLU:HG2	2.15	0.47
1:B:155:TRP:CD1	1:B:164:LEU:HD22	2.50	0.47
1:C:309:VAL:HG13	1:C:313:LEU:CD1	2.45	0.47
1:A:284:GLU:O	1:A:295:ARG:NE	2.48	0.47
1:B:133:PHE:O	1:B:135:THR:N	2.49	0.46
1:C:155:TRP:CD1	1:C:164:LEU:HD22	2.50	0.46
1:B:136:ALA:HB3	1:B:137:PRO:HD3	1.98	0.46
1:C:133:PHE:O	1:C:134:ILE:CB	2.55	0.45
1:A:116:PRO:O	1:A:117:LYS:HB2	2.15	0.45
1:C:124:LYS:HA	1:C:124:LYS:HD2	1.69	0.45
1:B:204:ALA:HA	1:B:207:LYS:HG2	1.98	0.45
1:B:316:PHE:CD1	1:B:316:PHE:O	2.69	0.45
1:B:205:ASN:HA	1:B:208:THR:CG2	2.46	0.45
1:C:149:ILE:O	1:C:152:VAL:HG12	2.17	0.45
1:B:185:LYS:HD3	1:B:191:TYR:CE2	2.52	0.45
1:C:412:ILE:HD12	1:C:412:ILE:N	2.32	0.45
1:B:205:ASN:HA	1:B:208:THR:HG22	1.99	0.45
1:C:119:GLY:O	1:C:123:ASN:ND2	2.50	0.45
1:C:277:TRP:CD2	1:C:313:LEU:HD23	2.52	0.45
1:B:284:GLU:O	1:B:295:ARG:NH1	2.46	0.44
1:C:393:LYS:O	1:C:397:LEU:HD23	2.18	0.44
1:C:103:MET:HE2	1:C:107:THR:HG22	2.00	0.44
1:B:124:LYS:O	1:B:126:VAL:HG22	2.18	0.44
1:A:136:ALA:HB3	1:A:137:PRO:HD3	1.98	0.44
1:A:280:VAL:HG23	3:A:601:HOH:O	2.17	0.43
1:A:350:ILE:CD1	1:A:458:VAL:HG13	2.46	0.43
1:C:409:ASP:HB2	1:C:412:ILE:HD13	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:HIS:CD2	1:A:238:THR:HG1	2.37	0.43
1:A:356:LYS:HD2	1:A:357:ILE:O	2.19	0.43
1:C:354:TYR:HB3	1:C:356:LYS:CD	2.47	0.43
1:B:237:VAL:O	1:B:237:VAL:HG23	2.19	0.42
1:B:292:TYR:O	1:B:293:TYR:CB	2.68	0.42
1:A:350:ILE:HD13	1:A:458:VAL:CG1	2.47	0.42
1:A:393:LYS:O	1:A:397:LEU:HD23	2.19	0.42
1:B:134:ILE:C	1:B:134:ILE:HD13	2.40	0.42
1:A:266:HIS:ND1	1:A:327:LEU:HD12	2.35	0.42
1:A:268:PHE:HD1	1:A:306:THR:HG23	1.84	0.42
1:C:305:MET:O	1:C:309:VAL:HG12	2.19	0.42
1:B:268:PHE:CD1	1:B:306:THR:HG22	2.54	0.42
1:C:285:ASP:HB2	1:C:295:ARG:CG	2.49	0.42
1:A:226:LYS:HE3	1:A:226:LYS:HB3	1.92	0.42
1:A:269:ARG:HD2	1:A:298:GLN:HE22	1.84	0.42
1:C:285:ASP:CA	1:C:295:ARG:HD3	2.50	0.42
1:C:133:PHE:HD1	1:C:133:PHE:H	1.66	0.41
1:B:86:ILE:HD13	1:B:87:THR:N	2.35	0.41
1:B:318:LEU:HG	1:B:321:TYR:HB2	2.01	0.41
1:A:269:ARG:HB2	3:A:601:HOH:O	2.20	0.41
1:A:138:GLU:O	1:A:139:VAL:HB	2.19	0.41
1:B:196:VAL:HB	1:B:237:VAL:HG12	2.02	0.41
1:B:266:HIS:CE1	1:B:327:LEU:HD22	2.55	0.41
1:C:124:LYS:O	1:C:125:ASP:HB2	2.20	0.41
1:C:98:LYS:HE2	1:C:284:GLU:OE2	2.20	0.41
1:B:444:LYS:O	1:B:448:ASP:HB2	2.20	0.41
1:A:356:LYS:HD3	1:A:357:ILE:O	2.20	0.41
1:C:125:ASP:OD1	1:C:126:VAL:CG2	2.65	0.41
1:B:117:LYS:CG	1:A:318:LEU:HD21	2.51	0.40
1:A:354:TYR:HD2	1:A:358:VAL:HG22	1.85	0.40
1:A:366:ARG:NE	1:A:379:THR:HG23	2.35	0.40
1:B:126:VAL:HG23	1:B:127:PHE:H	1.86	0.40
1:A:89:PHE:HB2	1:A:118:TYR:CD2	2.57	0.40
1:C:98:LYS:CE	1:C:284:GLU:OE2	2.70	0.40
1:C:102:PRO:HB2	1:C:281:LEU:HD13	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	398/414 (96%)	370 (93%)	21 (5%)	7 (2%)	8 16
1	B	398/414 (96%)	366 (92%)	25 (6%)	7 (2%)	8 16
1	C	398/414 (96%)	371 (93%)	17 (4%)	10 (2%)	5 9
All	All	1194/1242 (96%)	1107 (93%)	63 (5%)	24 (2%)	7 14

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	431	ASP
1	A	139	VAL
1	A	298	GLN
1	C	129	LYS
1	B	126	VAL
1	B	134	ILE
1	A	117	LYS
1	C	127	PHE
1	C	132	ASP
1	C	134	ILE
1	B	132	ASP
1	B	219	LYS
1	A	289	HIS
1	C	84	TYR
1	C	123	ASN
1	C	124	LYS
1	C	285	ASP
1	B	125	ASP
1	C	287	THR
1	A	124	LYS
1	B	124	LYS
1	A	130	GLY
1	A	297	VAL
1	C	126	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	351/363 (97%)	322 (92%)	29 (8%)	11	22
1	B	351/363 (97%)	324 (92%)	27 (8%)	13	25
1	C	351/363 (97%)	325 (93%)	26 (7%)	13	28
All	All	1053/1089 (97%)	971 (92%)	82 (8%)	12	25

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	86	ILE
1	B	97	THR
1	B	114	THR
1	B	116	PRO
1	B	117	LYS
1	B	122	MET
1	B	123	ASN
1	B	125	ASP
1	B	134	ILE
1	B	162	LYS
1	B	208	THR
1	B	213	LEU
1	B	223	PHE
1	B	225	HIS
1	B	226	LYS
1	B	231	THR
1	B	281	LEU
1	B	316	PHE
1	B	318	LEU
1	B	343	SER
1	B	351	ASP
1	B	376	LYS
1	B	383	SER
1	B	384	VAL
1	B	437	GLU
1	B	438	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	448	ASP
1	A	86	ILE
1	A	91	LYS
1	A	97	THR
1	A	122	MET
1	A	125	ASP
1	A	134	ILE
1	A	139	VAL
1	A	140	SER
1	A	227	THR
1	A	231	THR
1	A	281	LEU
1	A	295	ARG
1	A	306	THR
1	A	310	LYS
1	A	315	GLU
1	A	334	GLN
1	A	343	SER
1	A	351	ASP
1	A	356	LYS
1	A	357	ILE
1	A	376	LYS
1	A	383	SER
1	A	384	VAL
1	A	421	HIS
1	A	436	PHE
1	A	443	TYR
1	A	448	ASP
1	A	450	LYS
1	A	467	THR
1	C	86	ILE
1	C	93	LEU
1	C	105	ILE
1	C	122	MET
1	C	124	LYS
1	C	127	PHE
1	C	129	LYS
1	C	132	ASP
1	C	133	PHE
1	C	226	LYS
1	C	227	THR
1	C	231	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	257	GLN
1	C	272	ARG
1	C	273	GLU
1	C	287	THR
1	C	288	GLU
1	C	298	GLN
1	C	318	LEU
1	C	343	SER
1	C	351	ASP
1	C	356	LYS
1	C	383	SER
1	C	384	VAL
1	C	432	SER
1	C	480	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	141	GLN
1	B	205	ASN
1	B	266	HIS
1	A	205	ASN
1	A	266	HIS
1	A	298	GLN
1	C	257	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SAH	A	501	-	24,28,28	1.19	3 (12%)	25,40,40	1.47	5 (20%)
2	SAH	B	501	-	24,28,28	1.20	4 (16%)	25,40,40	1.39	4 (16%)
2	SAH	C	501	-	24,28,28	1.19	4 (16%)	25,40,40	1.39	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
2	SAH	A	501	-	-	4/11/31/31	0/3/3/3
2	SAH	B	501	-	-	3/11/31/31	0/3/3/3
2	SAH	C	501	-	-	2/11/31/31	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	SAH	C5-C4	2.81	1.48	1.40
2	B	501	SAH	C5-C4	2.73	1.48	1.40
2	C	501	SAH	C5-C4	2.68	1.48	1.40
2	B	501	SAH	O4'-C1'	2.47	1.44	1.41
2	C	501	SAH	OXT-C	-2.39	1.22	1.30
2	A	501	SAH	OXT-C	-2.34	1.22	1.30
2	C	501	SAH	O4'-C1'	2.27	1.44	1.41
2	B	501	SAH	OXT-C	-2.18	1.23	1.30
2	C	501	SAH	C2-N3	2.17	1.35	1.32
2	A	501	SAH	C2-N3	2.12	1.35	1.32
2	B	501	SAH	C2-N3	2.01	1.35	1.32

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	SAH	N3-C2-N1	-3.51	123.19	128.68
2	A	501	SAH	N3-C2-N1	-3.41	123.35	128.68
2	B	501	SAH	N3-C2-N1	-3.41	123.36	128.68
2	A	501	SAH	OXT-C-O	-2.92	117.45	124.09
2	B	501	SAH	OXT-C-O	-2.65	118.08	124.09
2	A	501	SAH	CB-CG-SD	-2.55	107.59	113.31
2	C	501	SAH	OXT-C-O	-2.55	118.30	124.09
2	B	501	SAH	C4-C5-N7	-2.30	107.00	109.40
2	A	501	SAH	C4-C5-N7	-2.28	107.02	109.40
2	A	501	SAH	OXT-C-CA	2.23	120.99	113.38
2	C	501	SAH	OXT-C-CA	2.22	120.95	113.38
2	C	501	SAH	C4-C5-N7	-2.19	107.12	109.40
2	B	501	SAH	OXT-C-CA	2.18	120.82	113.38
2	C	501	SAH	CB-CG-SD	-2.05	108.71	113.31

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	SAH	C-CA-CB-CG
2	A	501	SAH	C-CA-CB-CG
2	C	501	SAH	C-CA-CB-CG
2	A	501	SAH	OXT-C-CA-CB
2	B	501	SAH	OXT-C-CA-CB
2	A	501	SAH	O-C-CA-CB
2	A	501	SAH	N-CA-CB-CG
2	B	501	SAH	O-C-CA-CB
2	C	501	SAH	OXT-C-CA-CB

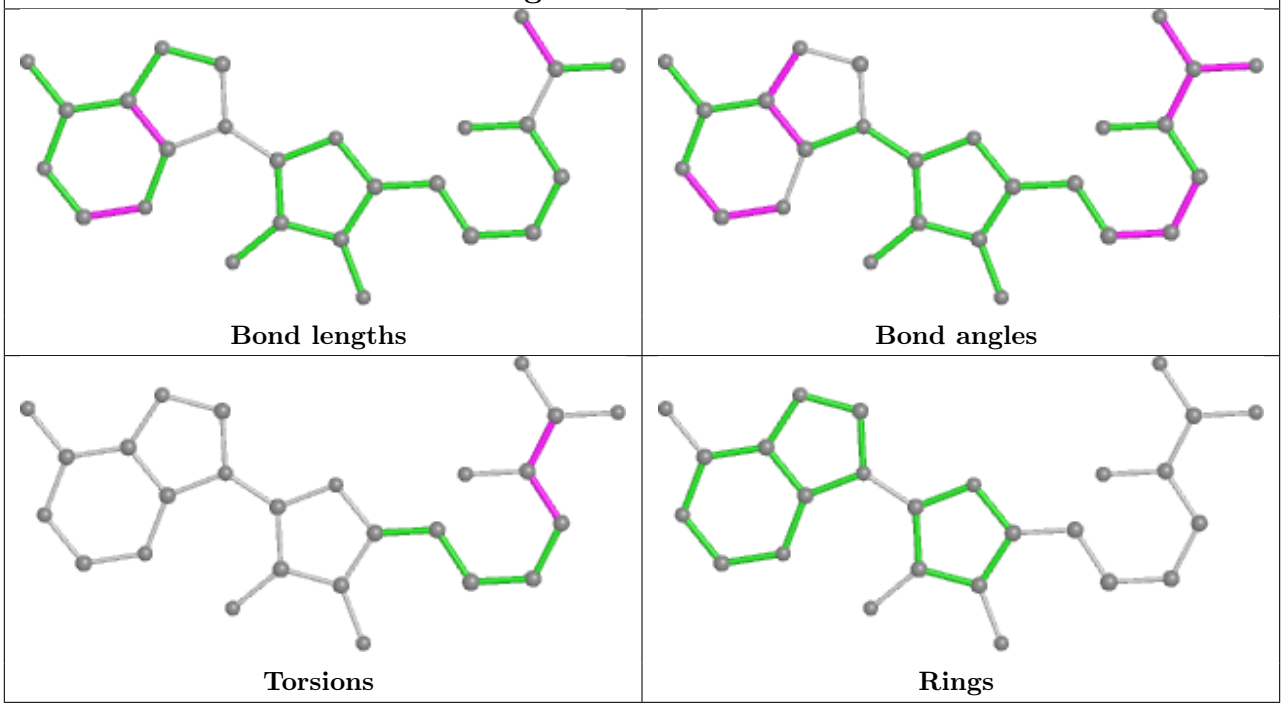
There are no ring outliers.

No monomer is involved in short contacts.

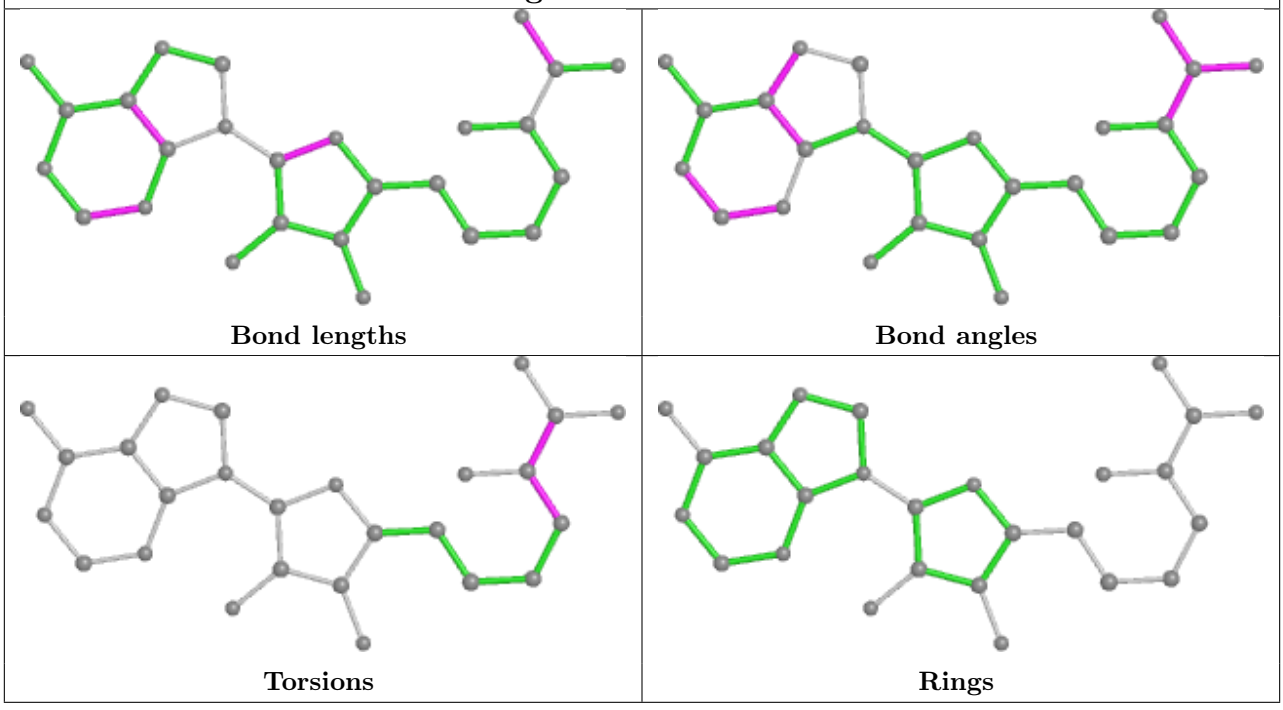
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

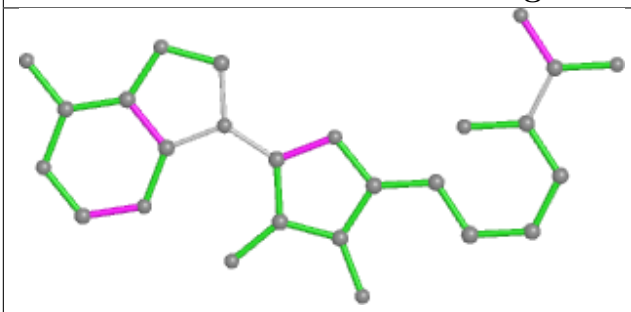
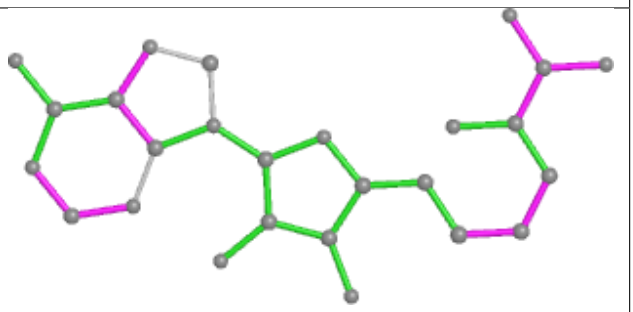
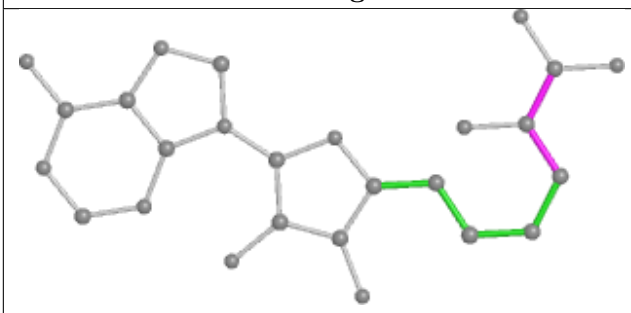
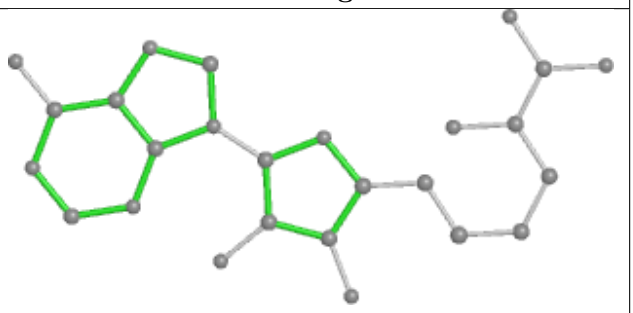
equivalents in the CSD to analyse the geometry.

Ligand SAH A 501



Ligand SAH B 501



Ligand SAH C 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	400/414 (96%)	0.74	50 (12%) 3 2	54, 83, 139, 160	0
1	B	400/414 (96%)	0.65	25 (6%) 20 15	50, 73, 130, 170	0
1	C	400/414 (96%)	0.71	40 (10%) 7 4	30, 79, 125, 144	0
All	All	1200/1242 (96%)	0.70	115 (9%) 8 5	30, 78, 133, 170	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	128	GLY	21.1
1	A	131	GLY	11.3
1	B	127	PHE	9.1
1	A	133	PHE	8.5
1	A	124	LYS	8.2
1	C	130	GLY	8.1
1	B	125	ASP	7.4
1	A	427	GLY	7.0
1	A	132	ASP	6.9
1	C	127	PHE	6.9
1	C	320	GLY	6.7
1	A	125	ASP	6.7
1	A	424	ALA	6.5
1	B	126	VAL	6.2
1	B	196	VAL	5.5
1	C	126	VAL	5.0
1	C	128	GLY	5.0
1	C	374	LEU	5.0
1	C	93	LEU	4.9
1	C	314	PRO	4.6
1	C	312	LEU	4.6
1	C	268	PHE	4.5
1	B	129	LYS	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	426	ILE	4.3
1	A	317	GLY	4.2
1	A	123	ASN	4.2
1	C	124	LYS	4.0
1	C	96	ILE	4.0
1	A	186	VAL	4.0
1	B	120	TYR	4.0
1	B	215	TYR	4.0
1	A	287	THR	3.9
1	A	99	VAL	3.8
1	C	318	LEU	3.7
1	B	124	LYS	3.4
1	B	88	ASP	3.4
1	A	103	MET	3.4
1	B	289	HIS	3.2
1	B	223	PHE	3.2
1	A	414	LEU	3.2
1	B	97	THR	3.2
1	B	187	PHE	3.2
1	B	96	ILE	3.2
1	A	284	GLU	3.1
1	A	421	HIS	3.1
1	B	190	PHE	3.1
1	C	315	GLU	3.0
1	A	86	ILE	3.0
1	A	296	PHE	3.0
1	C	129	LYS	3.0
1	A	100	ARG	3.0
1	A	152	VAL	2.9
1	A	294	LEU	2.9
1	A	419	ILE	2.9
1	A	255	LEU	2.8
1	C	100	ARG	2.8
1	A	139	VAL	2.8
1	A	118	TYR	2.8
1	C	313	LEU	2.8
1	A	290	GLY	2.8
1	C	391	ILE	2.8
1	A	98	LYS	2.8
1	C	125	ASP	2.8
1	C	294	LEU	2.7
1	A	415	LYS	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	92	TYR	2.7
1	B	133	PHE	2.7
1	A	92	TYR	2.7
1	A	425	GLN	2.6
1	A	466	ILE	2.6
1	C	321	TYR	2.6
1	B	99	VAL	2.6
1	A	374	LEU	2.6
1	A	430	LEU	2.6
1	A	445	LYS	2.6
1	C	114	THR	2.5
1	C	269	ARG	2.5
1	A	281	LEU	2.5
1	A	127	PHE	2.5
1	A	166	ILE	2.5
1	A	321	TYR	2.4
1	C	300	LYS	2.4
1	A	434	GLU	2.4
1	B	114	THR	2.4
1	C	323	VAL	2.4
1	C	275	ASN	2.4
1	C	347	ALA	2.4
1	C	84	TYR	2.4
1	C	132	ASP	2.3
1	C	278	CYS	2.3
1	A	441	MET	2.3
1	B	228	ILE	2.3
1	C	362	LEU	2.3
1	B	93	LEU	2.2
1	C	293	TYR	2.2
1	C	270	PHE	2.2
1	B	226	LYS	2.2
1	A	423	LEU	2.2
1	B	221	ILE	2.2
1	A	369	GLU	2.2
1	A	126	VAL	2.2
1	A	114	THR	2.2
1	A	91	LYS	2.1
1	C	279	GLU	2.1
1	A	149	ILE	2.1
1	A	431	ASP	2.1
1	A	188	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	466	ILE	2.1
1	A	350	ILE	2.1
1	C	204	ALA	2.1
1	C	89	PHE	2.1
1	C	337	ALA	2.1
1	C	305	MET	2.1
1	B	430	LEU	2.0
1	C	136	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

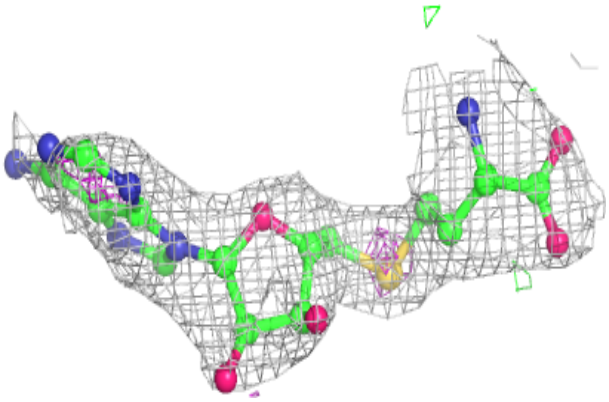
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

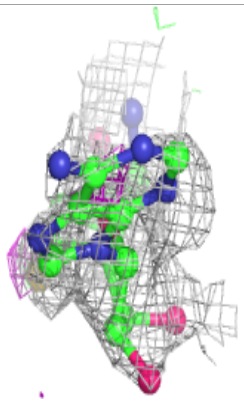
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SAH	A	501	26/26	0.75	0.31	74,77,78,80	0
2	SAH	C	501	26/26	0.79	0.25	105,113,116,116	0
2	SAH	B	501	26/26	0.88	0.25	83,90,92,93	0

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 501:

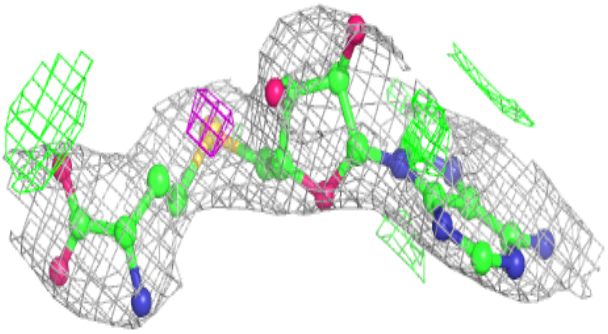
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

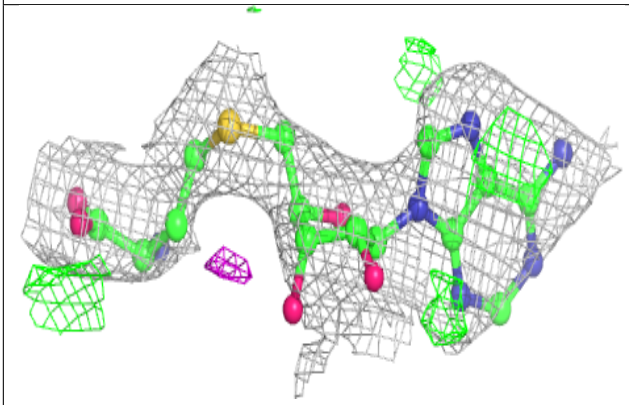


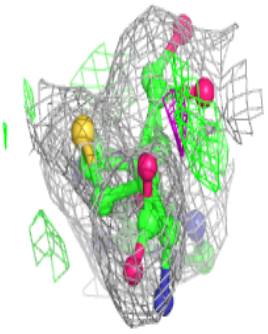


Electron density around SAH C 501:

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

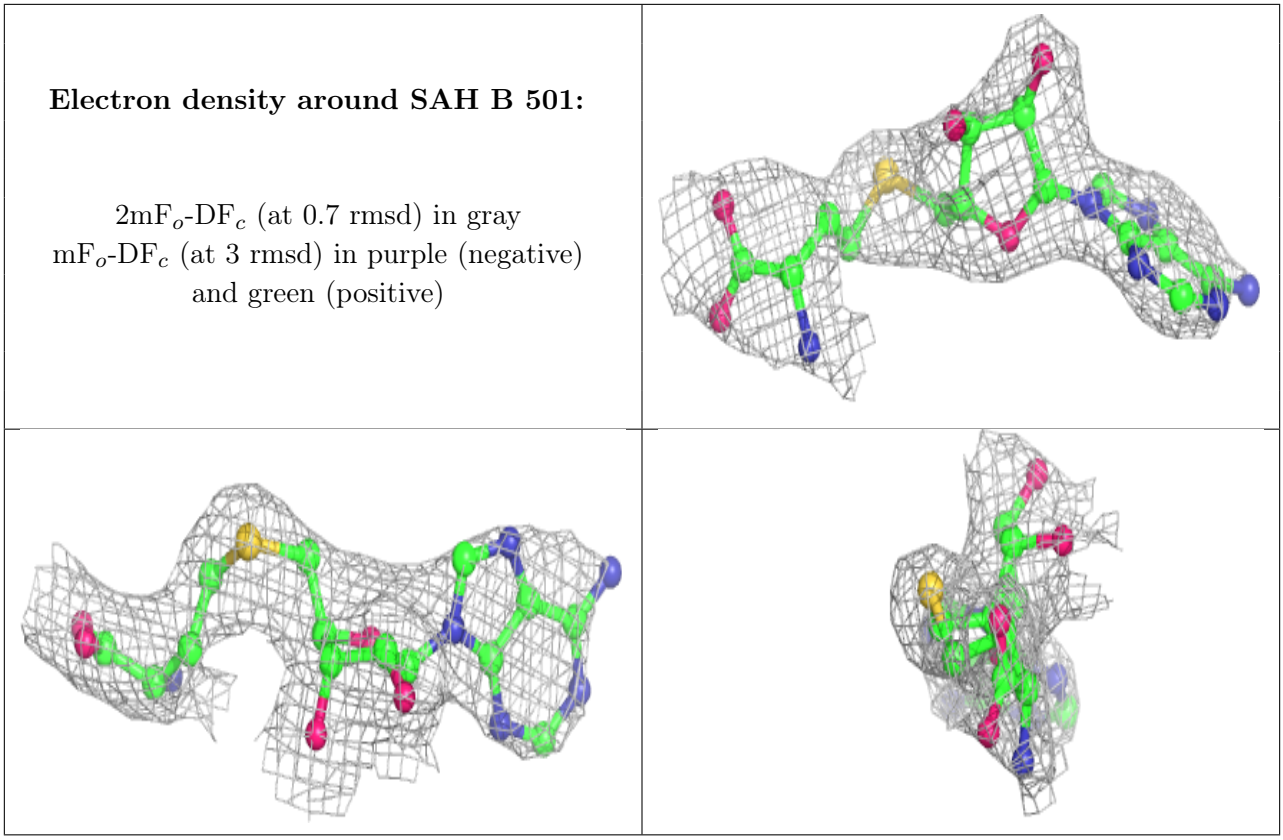






Electron density around SAH B 501:

$2mF_o$-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.