



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:20 AM UTC

PDB ID : 5DPL / pdb_00005dpl
Title : The structure of PKMT2 from Rickettsia typhi in complex with AdoHcy
Authors : Noinaj, N.; Abeykoon, A.; He, Y.; Yang, D.C.; Buchanan, S.K.
Deposited on : 2015-09-12
Resolution : 3.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

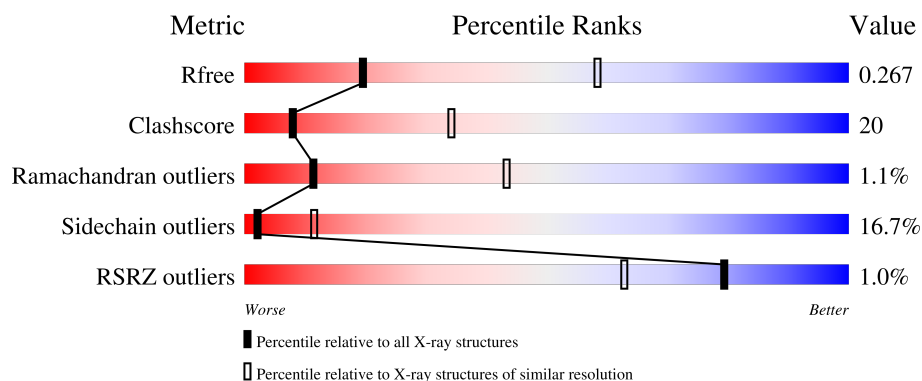
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	535	 52% 38% 7% . .
1	B	535	 52% 35% 8% .

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 8077 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.

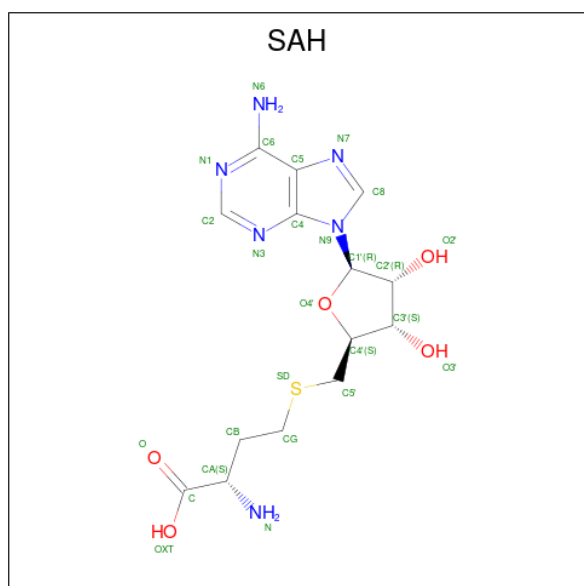
- Molecule 1 is a protein called protein lysine methyltransferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	520	Total	C	N	O	S	0	1	0
			4055	2615	659	768	13			
1	B	512	Total	C	N	O	S	0	1	0
			3970	2566	643	749	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q68XQ5
B	0	GLY	-	expression tag	UNP Q68XQ5

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



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

Continued on next page...

Continued from previous page...

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.35Å 91.03Å 105.83Å 90.00° 112.30° 90.00°	Depositor
Resolution (Å)	48.95 – 3.20 48.95 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.4 (48.95-3.20) 94.1 (48.95-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.10_2142)	Depositor
R, R_{free}	0.244 , 0.280 (Not available) , 0.267	Depositor DCC
R_{free} test set	2000 reflections (8.36%)	wwPDB-VP
Wilson B-factor (Å ²)	68.7	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 1.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.080 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8077	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.26	0/4145	0.69	3/5643 (0.1%)
1	B	0.27	0/4059	0.73	6/5530 (0.1%)
All	All	0.27	0/8204	0.71	9/11173 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	5
All	All	0	11

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	353	THR	CA-C-N	6.97	134.25	121.70
1	A	353	THR	C-N-CA	6.97	134.25	121.70
1	B	118	HIS	CA-C-N	-6.65	108.38	121.41
1	B	118	HIS	C-N-CA	-6.65	108.38	121.41
1	B	198	THR	CA-C-N	-5.86	116.08	122.59
1	B	198	THR	C-N-CA	-5.86	116.08	122.59
1	B	353	THR	CA-C-N	5.28	131.21	121.70
1	B	353	THR	C-N-CA	5.28	131.21	121.70
1	A	177	HIS	N-CA-C	5.15	121.77	110.80

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	ASP	Peptide
1	A	176	SER	Peptide
1	A	226	GLY	Peptide
1	A	299	GLN	Peptide
1	A	501	LYS	Peptide
1	A	505	VAL	Peptide
1	B	107	GLU	Peptide
1	B	119	GLY	Peptide
1	B	196	ASN	Peptide
1	B	346	LEU	Peptide
1	B	506	THR	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4055	0	3881	155	0
1	B	3970	0	3781	156	0
2	A	26	0	19	2	0
2	B	26	0	19	2	0
All	All	8077	0	7700	309	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 20.

All (309) 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:B:320:ASN:HA	1:B:369:ILE:HD11	1.36	1.03
1:A:435:ARG:NH1	1:A:473:LEU:O	2.01	0.92
1:B:186:LEU:O	1:B:189:PHE:HB3	1.68	0.92
1:B:393:ASP:OD1	1:B:393:ASP:N	2.05	0.89
1:A:421:ILE:HG22	1:A:423:THR:H	1.42	0.84
1:A:432:GLN:OE1	1:A:435:ARG:NH2	2.12	0.83
1:B:207:ASP:O	1:B:211:LEU:HB2	1.78	0.82
1:A:441:ALA:HB1	1:A:442:HIS:HA	1.61	0.81
1:B:435:ARG:NH1	1:B:473:LEU:O	2.13	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:THR:OG1	1:A:448:ASN:N	2.12	0.80
1:A:234:PHE:O	1:A:237:PHE:N	2.15	0.78
1:A:354:THR:HG23	1:A:355:SER:H	1.46	0.78
1:A:422:ALA:O	1:A:527:ARG:NH1	2.17	0.78
1:B:103:LEU:HD11	1:B:128:VAL:HG22	1.67	0.76
1:A:421:ILE:HD12	1:A:534:GLY:HA2	1.69	0.75
1:B:242:GLN:C	1:B:244:ASN:H	1.95	0.74
1:B:40:PRO:HG3	1:B:113:ASP:HB3	1.69	0.74
1:A:353:THR:HA	1:A:354:THR:HG22	1.69	0.74
1:B:189:PHE:O	1:B:193:SER:N	2.15	0.74
1:B:158:MET:HE1	1:B:205:LEU:HD12	1.70	0.74
1:B:68:SER:O	1:B:94:ASN:ND2	2.20	0.74
1:A:283:MET:O	1:A:287:THR:OG1	2.05	0.73
1:A:299:GLN:O	1:A:301:ILE:N	2.12	0.73
1:B:422:ALA:O	1:B:527:ARG:NE	2.21	0.73
1:A:103:LEU:HD11	1:A:128:VAL:HG22	1.71	0.72
1:A:343:TYR:HB2	1:A:350:PHE:HD2	1.54	0.71
1:A:60:ASN:ND2	1:A:457:ASN:OD1	2.23	0.71
1:A:307:ILE:HG21	1:A:407:PHE:HZ	1.56	0.70
1:B:316:TYR:HB3	1:B:372:PRO:HB2	1.72	0.70
1:B:29:ARG:NH2	1:B:40:PRO:O	2.24	0.70
1:B:312:LEU:HD23	1:B:403:ILE:HD12	1.73	0.70
1:B:23:THR:HG21	1:B:57:ASN:HD21	1.58	0.69
1:B:199:THR:O	1:B:199:THR:OG1	2.09	0.69
1:B:524:GLU:OE1	1:B:527:ARG:NH1	2.25	0.69
1:B:371:ASN:HB3	1:B:422:ALA:HB2	1.75	0.68
1:A:48:LEU:HD23	1:A:115:ILE:HD12	1.76	0.68
1:A:69:GLN:NE2	1:A:94:ASN:O	2.26	0.67
1:A:49:ASP:HB2	1:A:58:LEU:HD11	1.76	0.67
1:B:307:ILE:HG12	1:B:407:PHE:HZ	1.58	0.67
1:A:256:ALA:HB1	1:A:289:ARG:HH12	1.60	0.67
1:B:102:ILE:O	1:B:131:LYS:NZ	2.29	0.66
1:B:283:MET:O	1:B:287:THR:OG1	2.12	0.66
1:A:18:PHE:CD1	1:A:459:MET:HE1	2.32	0.65
1:A:62:ALA:HB1	1:A:94:ASN:HB2	1.78	0.65
1:A:178:ASP:O	1:A:182:GLN:HG2	1.96	0.65
1:A:66:PRO:O	1:A:94:ASN:ND2	2.26	0.64
1:A:163:ARG:NH2	1:A:226:GLY:O	2.31	0.64
1:A:299:GLN:C	1:A:301:ILE:H	2.03	0.64
1:B:477:HIS:HB3	1:B:481:ASP:HB3	1.79	0.64
1:B:146:ALA:O	1:B:295:LEU:HA	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:ALA:HB1	1:B:289:ARG:HH12	1.63	0.63
1:B:483:LYS:O	1:B:487:ILE:HG12	1.98	0.63
1:B:428:PRO:HB2	1:B:473:LEU:HD13	1.80	0.63
1:A:18:PHE:HD1	1:A:459:MET:HE1	1.62	0.63
1:A:282:TYR:HE1	1:B:168:PHE:HD2	1.46	0.63
1:A:310:ASP:HA	1:A:313:LYS:HD2	1.81	0.62
1:B:437:GLN:OE1	1:B:453:THR:OG1	2.17	0.62
1:A:483:LYS:HD3	1:A:516:ASP:HA	1.82	0.62
1:B:159:GLN:OE1	1:B:224:TYR:OH	2.06	0.62
1:A:223:GLU:OE2	1:A:229:ASN:ND2	2.32	0.62
1:A:343:TYR:HB2	1:A:350:PHE:CD2	2.34	0.62
1:A:117:CYS:SG	1:A:120:VAL:HG22	2.39	0.62
1:B:183:ALA:O	1:B:186:LEU:HB3	2.00	0.62
1:B:398:LEU:O	1:B:402:PHE:HB2	1.99	0.62
1:B:402:PHE:O	1:B:405:LEU:N	2.32	0.62
1:B:235:HIS:O	1:B:239:GLU:CB	2.48	0.61
1:A:106:ASP:OD1	1:A:106:ASP:N	2.33	0.61
1:B:259:ILE:HG12	1:B:260:GLY:H	1.66	0.61
1:A:364:VAL:HG12	1:A:385:LYS:HD3	1.82	0.61
1:A:343:TYR:O	1:A:346:LEU:HD13	2.01	0.60
1:B:59:LEU:HD21	1:B:87:ILE:HG12	1.82	0.60
1:A:447:THR:HG1	1:A:448:ASN:H	1.50	0.60
1:B:108:SER:CB	1:B:109:TYR:HA	2.31	0.60
1:B:450:PHE:HB2	1:B:462:ILE:HG23	1.81	0.60
1:B:120:VAL:HG12	2:B:601:SAH:H5'2	1.84	0.59
1:A:29:ARG:HG3	1:A:39:PRO:HB2	1.84	0.59
1:A:69:GLN:HE21	1:A:69:GLN:HA	1.66	0.59
1:A:323:PRO:HA	1:A:341:PHE:HD1	1.68	0.59
1:A:115:ILE:HG23	1:A:146:ALA:HA	1.85	0.59
1:B:40:PRO:CG	1:B:113:ASP:HB3	2.32	0.59
1:A:307:ILE:HG21	1:A:407:PHE:CZ	2.38	0.58
1:B:390:ARG:HB3	1:B:393:ASP:OD1	2.03	0.58
1:A:19:THR:H	1:A:459:MET:HE2	1.69	0.58
1:A:450:PHE:O	1:A:461:GLY:HA2	2.03	0.58
1:A:354:THR:CG2	1:A:355:SER:H	2.15	0.58
1:B:235:HIS:O	1:B:239:GLU:HB3	2.04	0.57
1:A:209:ALA:HA	1:A:212:ILE:HD12	1.86	0.57
1:A:324:ILE:HG13	1:A:325:SER:N	2.19	0.57
1:A:402:PHE:O	1:A:405:LEU:N	2.36	0.57
1:A:353:THR:HG22	1:A:354:THR:HG22	1.86	0.57
1:B:430:THR:HG22	1:B:431:SER:H	1.68	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:GLN:NE2	1:A:208:GLU:OE2	2.38	0.57
1:A:354:THR:HG23	1:A:355:SER:N	2.17	0.57
1:A:466:GLU:HG2	1:A:522:SER:HB3	1.87	0.57
1:A:194:LEU:HD11	1:B:286:ILE:HG23	1.87	0.57
1:A:235:HIS:O	1:A:239:GLU:CB	2.52	0.57
1:A:415:GLU:O	1:A:416:THR:OG1	2.20	0.56
1:B:338:ASN:OD1	1:B:352:SER:HB3	2.04	0.56
1:A:142:PRO:HA	1:A:298:HIS:ND1	2.21	0.56
1:A:386:LEU:O	1:A:386:LEU:HD12	2.06	0.56
1:B:487:ILE:O	1:B:491:ASN:HB2	2.05	0.56
1:A:318:THR:HG23	1:A:412:LYS:HB2	1.86	0.56
1:B:466:GLU:HG2	1:B:522:SER:HB3	1.88	0.55
1:A:396:ALA:O	1:A:399:GLU:N	2.40	0.55
1:B:348:GLU:HB3	1:B:349:PRO:HD2	1.86	0.55
1:B:515:VAL:HA	1:B:518:VAL:HG12	1.88	0.55
1:A:146:ALA:O	1:A:295:LEU:HA	2.07	0.55
1:A:525:LYS:O	1:A:529:ASN:ND2	2.33	0.55
1:B:480:ASP:OD1	1:B:481:ASP:N	2.41	0.54
1:B:430:THR:HG23	1:B:531:LEU:O	2.06	0.54
1:A:324:ILE:HG21	1:A:340:SER:HB2	1.89	0.54
1:A:77:LYS:O	1:A:81:GLU:HG2	2.08	0.54
1:B:478:ASN:ND2	1:B:480:ASP:OD1	2.41	0.54
1:B:115:ILE:HG13	1:B:146:ALA:HA	1.90	0.53
1:B:284:ASP:OD1	1:B:292:ARG:NH2	2.27	0.53
1:A:186:LEU:O	1:A:190:ILE:HG12	2.08	0.53
1:B:142:PRO:HA	1:B:298:HIS:ND1	2.24	0.53
1:B:361:ILE:O	1:B:364:VAL:HG12	2.09	0.53
1:A:83:GLY:HA2	1:A:86:THR:HG22	1.91	0.53
1:B:137:ASN:ND2	1:B:244:ASN:O	2.41	0.53
1:A:398:LEU:O	1:A:402:PHE:HB2	2.10	0.52
1:B:204:PHE:C	1:B:206:ARG:H	2.16	0.52
1:B:350:PHE:CD1	1:B:351:ILE:HG13	2.44	0.52
1:B:355:SER:OG	1:B:357:ILE:HG22	2.09	0.52
1:B:392:GLN:OE1	1:B:392:GLN:N	2.35	0.52
1:A:445:ASN:HA	1:A:448:ASN:O	2.08	0.52
1:B:304:ASN:HD21	1:B:306:LYS:HE3	1.74	0.52
1:B:313:LYS:HA	1:B:375:LEU:HB3	1.92	0.52
1:A:472:MET:HE3	1:A:482:ILE:HD13	1.91	0.52
1:A:120:VAL:HG12	2:A:601:SAH:H5'2	1.91	0.52
1:B:107:GLU:HA	1:B:108:SER:O	2.10	0.52
1:A:392:GLN:OE1	1:A:392:GLN:N	2.37	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:THR:OG1	1:A:431:SER:N	2.41	0.52
1:B:518:VAL:O	1:B:522:SER:OG	2.19	0.51
1:A:131:LYS:HA	1:A:134:GLU:CD	2.36	0.51
1:B:118:HIS:O	1:B:120:VAL:N	2.43	0.51
1:A:478:ASN:O	1:A:482:ILE:HG12	2.10	0.51
1:A:212:ILE:HG12	1:A:224:TYR:HE2	1.75	0.51
1:A:217:ASP:O	1:A:221:LEU:HB2	2.10	0.51
1:B:132:ILE:O	1:B:135:VAL:HG22	2.10	0.51
1:B:259:ILE:HG12	1:B:260:GLY:N	2.25	0.51
1:B:242:GLN:C	1:B:244:ASN:N	2.65	0.51
1:A:346:LEU:HD23	1:A:348:GLU:HB2	1.91	0.51
1:B:274:ASN:O	1:B:274:ASN:ND2	2.44	0.51
1:B:499:ASP:H	1:B:504:VAL:CB	2.23	0.51
1:A:479:ILE:HG12	1:A:483:LYS:HE2	1.93	0.50
1:A:421:ILE:N	1:A:532:LEU:O	2.44	0.50
1:A:512:LYS:O	1:A:515:VAL:HG12	2.10	0.50
1:B:238:ILE:HG21	1:B:248:TYR:HB2	1.93	0.50
1:A:102:ILE:HG21	1:A:132:ILE:HD13	1.92	0.50
1:B:405:LEU:HB3	1:B:411:LEU:HD13	1.94	0.50
1:B:425:THR:HG21	1:B:534:GLY:O	2.12	0.50
1:A:136:LEU:HD23	1:A:146:ALA:HB1	1.93	0.49
1:B:131:LYS:O	1:B:135:VAL:HG13	2.12	0.49
1:B:325:SER:O	1:B:363:TYR:OH	2.24	0.49
1:A:426:GLU:O	1:A:426:GLU:HG2	2.12	0.49
1:A:428:PRO:HB2	1:A:473:LEU:HD13	1.94	0.49
1:B:370:SER:OG	1:B:528:ILE:O	2.24	0.49
1:A:137:ASN:HD21	1:A:245:HIS:HB2	1.78	0.49
1:B:469:ILE:HG23	1:B:482:ILE:HD13	1.94	0.49
1:B:406:ILE:HG22	1:B:411:LEU:HD22	1.93	0.49
1:A:319:PHE:CE2	1:A:321:ILE:HD11	2.48	0.49
1:B:320:ASN:OD1	1:B:344:GLU:HG2	2.12	0.49
1:B:465:HIS:O	1:B:469:ILE:HG13	2.13	0.49
1:B:152:THR:HA	1:B:232:THR:O	2.13	0.49
1:B:321:ILE:HA	1:B:342:TYR:O	2.13	0.49
1:B:351:ILE:HG22	1:B:352:SER:H	1.78	0.48
1:A:403:ILE:HA	1:A:406:ILE:HG23	1.95	0.48
1:A:235:HIS:O	1:A:239:GLU:HB2	2.12	0.48
1:B:345:ASN:O	1:B:346:LEU:HB2	2.12	0.48
1:B:482:ILE:HG13	1:B:483:LYS:N	2.29	0.48
1:B:74:ASP:OD1	1:B:75:LEU:N	2.45	0.48
1:A:469:ILE:HD11	1:A:519:VAL:HG22	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:SER:OG	1:B:352:SER:OG	2.29	0.48
1:A:339:ILE:HD13	1:A:341:PHE:CE2	2.47	0.48
1:B:347:PRO:HB2	1:B:348:GLU:HA	1.95	0.48
1:B:472:MET:HE3	1:B:472:MET:HB2	1.69	0.48
1:A:235:HIS:O	1:A:239:GLU:HB3	2.12	0.48
1:A:245:HIS:HA	1:A:299:GLN:NE2	2.28	0.47
1:A:137:ASN:ND2	1:A:244:ASN:O	2.47	0.47
1:B:479:ILE:O	1:B:483:LYS:HG3	2.14	0.47
1:B:48:LEU:HA	1:B:71:LEU:O	2.15	0.47
1:A:63:GLU:OE1	1:A:433:PHE:HB2	2.15	0.47
1:B:179:LYS:H	1:B:180:LEU:HA	1.79	0.47
1:B:425:THR:C	1:B:427:LYS:H	2.22	0.47
1:A:102:ILE:HA	1:A:105:LEU:HD12	1.97	0.47
1:B:419:HIS:O	1:B:455:ARG:HG3	2.15	0.47
1:B:188:LYS:O	1:B:192:ASP:HB2	2.15	0.46
1:A:74:ASP:OD1	2:A:601:SAH:O2'	2.22	0.46
1:A:87:ILE:HG13	1:A:88:SER:N	2.30	0.46
1:B:59:LEU:HD23	1:B:95:VAL:HG11	1.96	0.46
1:B:123:TRP:CE3	1:B:229:ASN:HB3	2.49	0.46
1:B:105:LEU:HG	1:B:139:LEU:HD11	1.97	0.46
1:A:273:ILE:H	1:A:273:ILE:HG13	1.51	0.46
1:A:309:PHE:O	1:A:313:LYS:HG3	2.16	0.46
1:B:235:HIS:O	1:B:239:GLU:HB2	2.14	0.46
1:A:48:LEU:HD13	1:A:71:LEU:HD23	1.98	0.46
1:A:47:VAL:HG22	1:A:70:SER:HB3	1.98	0.46
1:B:389:TYR:N	1:B:389:TYR:CD1	2.84	0.46
1:B:389:TYR:N	1:B:389:TYR:HD1	2.14	0.46
1:A:162:ILE:O	1:A:166:MET:HG3	2.16	0.46
1:A:275:ASP:O	1:A:279:THR:OG1	2.34	0.46
1:B:527:ARG:HA	1:B:532:LEU:HD12	1.97	0.46
1:A:147:PHE:CZ	1:A:293:SER:HB3	2.51	0.46
1:A:361:ILE:O	1:A:364:VAL:HG22	2.16	0.45
1:A:25:PRO:HB2	1:A:26:PRO:HD3	1.98	0.45
1:B:375:LEU:HD11	1:B:398:LEU:HD11	1.98	0.45
1:A:69:GLN:HG3	1:A:70:SER:N	2.32	0.45
1:B:436:TYR:O	1:B:439:LYS:HB2	2.16	0.45
1:A:358:MET:HE3	1:A:358:MET:HA	1.97	0.45
1:A:419:HIS:O	1:A:455:ARG:HG3	2.17	0.45
1:A:40:PRO:HG2	1:A:113:ASP:HB3	1.99	0.45
1:A:69:GLN:HG3	1:A:70:SER:H	1.80	0.45
1:A:507:ASP:O	1:A:511:LEU:HB2	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:LEU:O	1:B:273:ILE:HG22	2.17	0.45
1:B:338:ASN:HA	1:B:354:THR:H	1.82	0.45
1:A:300:ASN:OD1	1:A:300:ASN:N	2.50	0.45
1:B:163:ARG:O	1:B:167:MET:CB	2.65	0.45
1:B:108:SER:HB3	1:B:109:TYR:CD1	2.51	0.45
1:A:358:MET:HE1	1:A:402:PHE:HE2	1.81	0.44
1:B:157:ASN:O	1:B:161:THR:HG23	2.16	0.44
1:B:492:SER:OG	1:B:493:LYS:N	2.50	0.44
1:B:330:ILE:HD12	1:B:330:ILE:HA	1.66	0.44
1:A:152:THR:HG23	1:A:289:ARG:O	2.18	0.44
1:A:374:ARG:O	1:A:378:VAL:HG23	2.18	0.44
1:A:377:GLN:NE2	1:A:381:GLU:OE2	2.50	0.44
1:B:167:MET:O	1:B:167:MET:HG3	2.17	0.44
1:A:425:THR:C	1:A:427:LYS:H	2.25	0.44
1:A:143:ASN:OD1	1:A:143:ASN:N	2.35	0.44
1:B:479:ILE:HG12	1:B:483:LYS:HE3	1.98	0.44
1:A:238:ILE:HD12	1:A:248:TYR:HB2	1.99	0.44
1:B:25:PRO:HB2	1:B:26:PRO:HD3	1.99	0.44
1:B:159:GLN:H	1:B:159:GLN:HG2	1.65	0.44
1:B:167:MET:HE2	1:B:167:MET:HB2	1.82	0.44
1:B:369:ILE:HD12	1:B:369:ILE:HA	1.45	0.44
1:B:425:THR:O	1:B:426:GLU:HG2	2.18	0.44
1:A:425:THR:O	1:A:426:GLU:HB3	2.18	0.43
1:B:482:ILE:HG13	1:B:483:LYS:H	1.83	0.43
1:A:29:ARG:HD2	1:A:114:TYR:OH	2.18	0.43
1:B:80:ILE:HG13	1:B:99:ALA:HB2	1.99	0.43
1:B:221:LEU:O	1:B:225:LEU:HB2	2.18	0.43
1:A:360:ALA:O	1:A:364:VAL:HG13	2.18	0.43
1:A:490:ILE:HG21	1:A:511:LEU:HD21	1.99	0.43
1:B:305:ARG:O	1:B:307:ILE:HD12	2.18	0.43
1:A:321:ILE:HG23	1:A:341:PHE:HB3	2.01	0.43
1:A:398:LEU:HA	1:A:402:PHE:HD2	1.84	0.43
1:B:135:VAL:O	1:B:139:LEU:HB2	2.18	0.43
1:A:489:LYS:O	1:A:494:LEU:HA	2.18	0.43
1:B:102:ILE:HG13	2:B:601:SAH:N1	2.33	0.43
1:A:80:ILE:HG22	1:A:84:LYS:HE3	1.99	0.43
1:B:135:VAL:HB	1:B:139:LEU:HD12	1.99	0.43
1:A:398:LEU:HA	1:A:402:PHE:CD2	2.54	0.43
1:B:179:LYS:CB	1:B:182:GLN:H	2.31	0.43
1:B:358:MET:HE3	1:B:358:MET:HA	2.01	0.43
1:A:135:VAL:HG13	1:A:139:LEU:CD1	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:SER:OG	1:A:357:ILE:HG22	2.19	0.42
1:A:354:THR:CG2	1:A:355:SER:N	2.80	0.42
1:A:425:THR:OG1	1:A:534:GLY:O	2.18	0.42
1:B:63:GLU:OE1	1:B:433:PHE:HB2	2.19	0.42
1:B:152:THR:N	1:B:290:LYS:O	2.34	0.42
1:A:417:LYS:HG3	1:A:418:PRO:HD2	2.02	0.42
1:B:437:GLN:OE1	1:B:453:THR:N	2.51	0.42
1:A:73:VAL:HA	1:A:98:LYS:O	2.18	0.42
1:A:327:GLU:OE1	1:A:385:LYS:NZ	2.51	0.42
1:B:23:THR:OG1	1:B:116:VAL:HG11	2.20	0.42
1:B:404:THR:O	1:B:408:GLN:HG3	2.19	0.42
1:A:340:SER:HB3	1:A:349:PRO:HB3	2.02	0.42
1:B:47:VAL:HA	1:B:114:TYR:O	2.19	0.42
1:A:21:SER:HA	1:A:457:ASN:HB3	2.02	0.42
1:A:175:THR:HA	1:A:176:SER:CB	2.49	0.42
1:A:332:LEU:HD12	1:A:332:LEU:HA	1.65	0.42
1:A:444:ASN:H	1:A:447:THR:HG23	1.83	0.42
1:B:343:TYR:C	1:B:345:ASN:H	2.28	0.42
1:B:532:LEU:HD23	1:B:532:LEU:HA	1.94	0.42
1:B:238:ILE:H	1:B:238:ILE:HG13	1.43	0.42
1:B:346:LEU:HB3	1:B:347:PRO:C	2.44	0.42
1:B:465:HIS:CE1	1:B:466:GLU:HG3	2.55	0.42
1:A:128:VAL:O	1:A:132:ILE:HG12	2.20	0.42
1:B:105:LEU:HD13	1:B:105:LEU:HA	1.91	0.41
1:B:364:VAL:HG22	1:B:368:ASN:ND2	2.34	0.41
1:A:492:SER:O	1:A:494:LEU:N	2.53	0.41
1:B:203:ASN:OD1	1:B:204:PHE:N	2.53	0.41
1:A:518:VAL:O	1:A:522:SER:OG	2.27	0.41
1:B:307:ILE:HG12	1:B:407:PHE:CZ	2.46	0.41
1:B:487:ILE:HD12	1:B:511:LEU:CD1	2.51	0.41
1:A:62:ALA:HB1	1:A:94:ASN:CB	2.46	0.41
1:B:119:GLY:N	1:B:149:SER:OG	2.53	0.41
1:A:404:THR:O	1:A:408:GLN:HG3	2.19	0.41
1:B:321:ILE:HG22	1:B:342:TYR:O	2.20	0.41
1:A:194:LEU:HD21	1:A:202:ALA:HB1	2.03	0.41
1:B:221:LEU:HA	1:B:225:LEU:HD12	2.02	0.41
1:A:329:LYS:HD2	1:A:329:LYS:N	2.35	0.41
1:A:474:ASP:OD1	1:A:476:THR:OG1	2.30	0.41
1:A:352:SER:O	1:A:353:THR:HG23	2.21	0.41
1:B:163:ARG:O	1:B:167:MET:HB3	2.21	0.41
1:B:183:ALA:O	1:B:186:LEU:CB	2.67	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:LYS:O	1:A:487:ILE:HG13	2.21	0.40
1:A:357:ILE:HG13	1:A:394:PHE:CE1	2.56	0.40
1:B:20:PHE:HB2	1:B:23:THR:HG22	2.03	0.40
1:B:200:PRO:HG2	1:B:201:TYR:H	1.87	0.40
1:A:280:GLU:O	1:A:283:MET:HB2	2.21	0.40
1:A:307:ILE:HD13	1:A:407:PHE:CE2	2.56	0.40
1:A:318:THR:CG2	1:A:412:LYS:HB2	2.50	0.40
1:B:128:VAL:O	1:B:132:ILE:HG13	2.21	0.40
1:B:187:LEU:HD11	1:B:212:ILE:HD11	2.03	0.40
1:B:330:ILE:HD11	1:B:337:GLU:OE2	2.22	0.40
1:B:518:VAL:HA	1:B:521:VAL:HG22	2.04	0.40
1:A:119:GLY:N	1:A:149:SER:OG	2.42	0.40
1:B:130:ASP:OD1	1:B:130:ASP:N	2.54	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	517/535 (97%)	445 (86%)	67 (13%)	5 (1%)	12	45
1	B	507/535 (95%)	443 (87%)	58 (11%)	6 (1%)	10	42
All	All	1024/1070 (96%)	888 (87%)	125 (12%)	11 (1%)	11	43

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	300	ASN
1	A	504	VAL
1	B	505	VAL
1	A	299	GLN
1	B	200	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	493	LYS
1	B	198	THR
1	B	504	VAL
1	B	400	GLN
1	A	200	PRO
1	B	346	LEU

5.3.2 Protein sidechains ⓘ

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	426/484 (88%)	357 (84%)	69 (16%)	2	12
1	B	414/484 (86%)	343 (83%)	71 (17%)	2	11
All	All	840/968 (87%)	700 (83%)	140 (17%)	2	11

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	47	VAL
1	A	58	LEU
1	A	69	GLN
1	A	71	LEU
1	A	76	SER
1	A	82	LEU
1	A	88	SER
1	A	91	LYS
1	A	95	VAL
1	A	98	LYS
1	A	106	ASP
1	A	115	ILE
1	A	120	VAL
1	A	131	LYS
1	A	134	GLU
1	A	135	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	139	LEU
1	A	143	ASN
1	A	158	MET
1	A	163	ARG
1	A	201	TYR
1	A	205	LEU
1	A	214	THR
1	A	216	ASP
1	A	221	LEU
1	A	225	LEU
1	A	227	GLU
1	A	233	TYR
1	A	262	LEU
1	A	264	THR
1	A	273	ILE
1	A	277	VAL
1	A	278	CYS
1	A	279	THR
1	A	291	PHE
1	A	293	SER
1	A	295	LEU
1	A	296	LEU
1	A	299	GLN
1	A	300	ASN
1	A	307	ILE
1	A	313	LYS
1	A	330	ILE
1	A	332	LEU
1	A	346	LEU
1	A	351	ILE
1	A	353	THR
1	A	354	THR
1	A	364	VAL
1	A	365	TYR
1	A	374	ARG
1	A	375	LEU
1	A	381	GLU
1	A	393	ASP
1	A	405	LEU
1	A	406	ILE
1	A	411	LEU
1	A	425	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	430	THR
1	A	447	THR
1	A	452	ILE
1	A	453	THR
1	A	464	ILE
1	A	474	ASP
1	A	482	ILE
1	A	498	CYS
1	A	506	THR
1	A	528	ILE
1	B	21	SER
1	B	43	GLU
1	B	47	VAL
1	B	52	CYS
1	B	58	LEU
1	B	78	THR
1	B	92	ILE
1	B	95	VAL
1	B	100	LEU
1	B	105	LEU
1	B	108	SER
1	B	118	HIS
1	B	120	VAL
1	B	124	VAL
1	B	130	ASP
1	B	143	ASN
1	B	158	MET
1	B	167	MET
1	B	170	SER
1	B	180	LEU
1	B	186	LEU
1	B	194	LEU
1	B	199	THR
1	B	201	TYR
1	B	206	ARG
1	B	207	ASP
1	B	208	GLU
1	B	211	LEU
1	B	212	ILE
1	B	214	THR
1	B	238	ILE
1	B	242	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	245	HIS
1	B	253	SER
1	B	262	LEU
1	B	287	THR
1	B	289	ARG
1	B	295	LEU
1	B	296	LEU
1	B	307	ILE
1	B	321	ILE
1	B	325	SER
1	B	330	ILE
1	B	332	LEU
1	B	333	ASN
1	B	340	SER
1	B	351	ILE
1	B	353	THR
1	B	357	ILE
1	B	365	TYR
1	B	369	ILE
1	B	386	LEU
1	B	389	TYR
1	B	393	ASP
1	B	401	HIS
1	B	405	LEU
1	B	406	ILE
1	B	416	THR
1	B	421	ILE
1	B	425	THR
1	B	431	SER
1	B	439	LYS
1	B	453	THR
1	B	462	ILE
1	B	464	ILE
1	B	474	ASP
1	B	488	GLU
1	B	495	LEU
1	B	509	LYS
1	B	510	LEU
1	B	513	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	137	ASN
1	A	222	HIS
1	A	408	GLN
1	B	304	ASN
1	B	368	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	601	-	27,28,28	1.09	4 (14%)	36,40,40	2.11	10 (27%)
2	SAH	B	601	-	27,28,28	1.10	4 (14%)	36,40,40	2.11	10 (27%)

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	601	-	-	3/15/31/31	0/3/3/3
2	SAH	B	601	-	-	6/15/31/31	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	SAH	C2-N3	2.61	1.38	1.33
2	A	601	SAH	C2-N3	2.61	1.38	1.33
2	A	601	SAH	C2-N1	2.55	1.38	1.33
2	B	601	SAH	C2-N1	2.51	1.38	1.33
2	B	601	SAH	C8-N7	2.20	1.35	1.31
2	B	601	SAH	OXT-C	-2.19	1.23	1.30
2	A	601	SAH	OXT-C	-2.16	1.23	1.30
2	A	601	SAH	C8-N7	2.12	1.35	1.31

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	SAH	N3-C2-N1	-5.48	120.29	128.58
2	A	601	SAH	N3-C2-N1	-5.41	120.39	128.58
2	B	601	SAH	C5-C4-N3	-4.81	120.09	126.72
2	A	601	SAH	C5-C4-N3	-4.69	120.26	126.72
2	B	601	SAH	C5'-SD-CG	-4.37	89.29	102.26
2	A	601	SAH	N9-C8-N7	-3.90	108.40	113.94
2	B	601	SAH	N9-C8-N7	-3.78	108.57	113.94
2	A	601	SAH	C5'-SD-CG	-3.72	91.22	102.26
2	B	601	SAH	C2-N3-C4	3.53	120.45	111.83
2	B	601	SAH	C5-N7-C8	3.47	108.91	103.45
2	A	601	SAH	C5-N7-C8	3.45	108.87	103.45
2	A	601	SAH	C2-N3-C4	3.45	120.25	111.83
2	A	601	SAH	N3-C4-N9	3.11	132.45	127.17
2	B	601	SAH	N3-C4-N9	3.09	132.42	127.17
2	A	601	SAH	O4'-C1'-N9	2.86	113.58	108.09
2	A	601	SAH	OXT-C-O	-2.68	117.99	124.08
2	B	601	SAH	C4-C5-N7	-2.53	107.69	110.58
2	B	601	SAH	OXT-C-O	-2.49	118.43	124.08
2	B	601	SAH	O4'-C1'-N9	2.41	112.72	108.09
2	A	601	SAH	C4-C5-N7	-2.39	107.86	110.58

There are no chirality outliers.

All (9) torsion outliers are listed below:

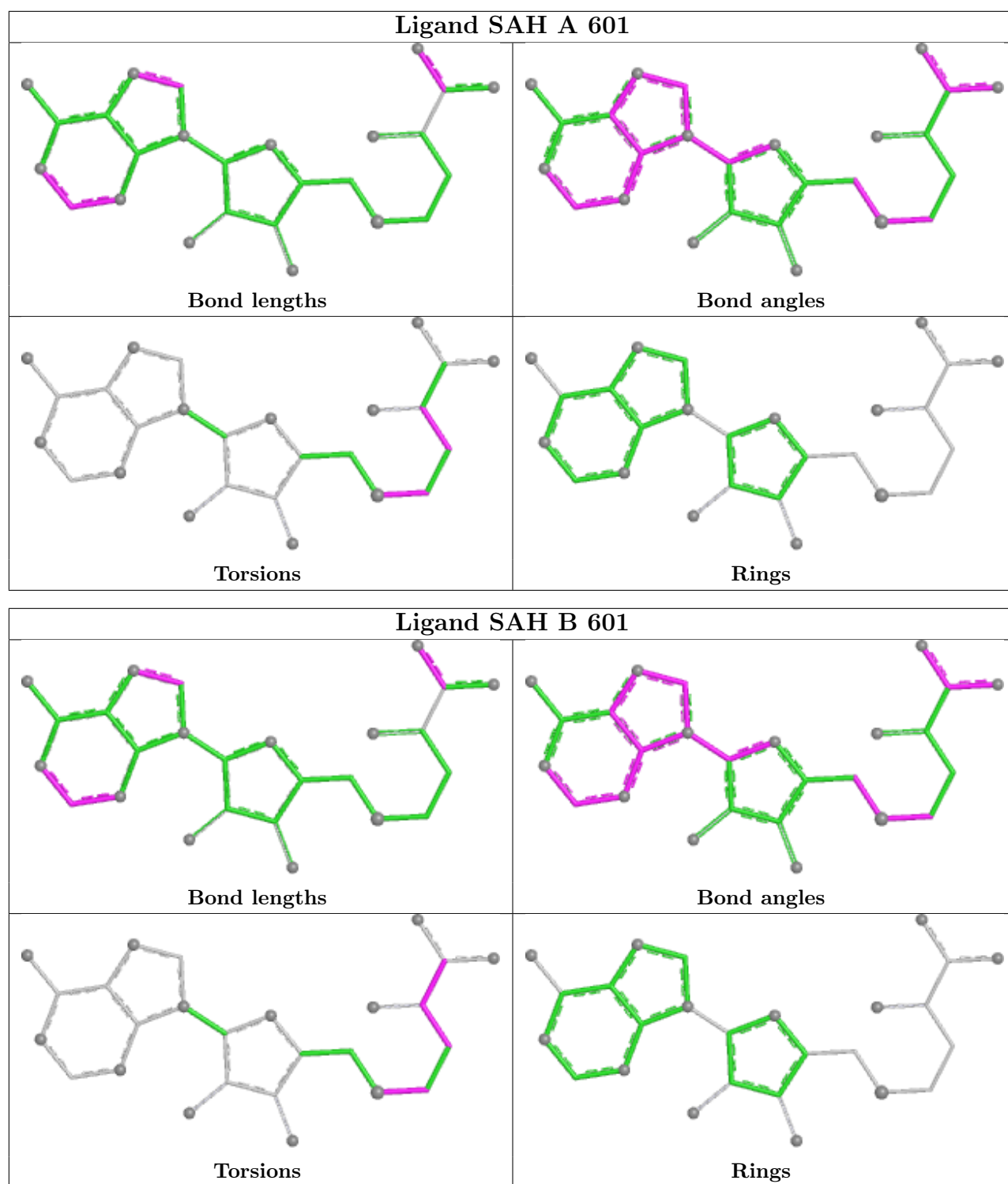
Mol	Chain	Res	Type	Atoms
2	A	601	SAH	N-CA-CB-CG
2	A	601	SAH	C-CA-CB-CG
2	B	601	SAH	N-CA-CB-CG
2	B	601	SAH	C-CA-CB-CG
2	B	601	SAH	O-C-CA-N
2	B	601	SAH	OXT-C-CA-N
2	B	601	SAH	CB-CG-SD-C5'
2	A	601	SAH	CB-CG-SD-C5'
2	B	601	SAH	OXT-C-CA-CB

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	SAH	2	0
2	B	601	SAH	2	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 than 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.



5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	520/535 (97%)	-0.22	2 (0%) 88 79	33, 68, 101, 126	1 (0%)
1	B	512/535 (95%)	-0.07	8 (1%) 70 51	32, 77, 105, 121	1 (0%)
All	All	1032/1070 (96%)	-0.15	10 (0%) 79 63	32, 72, 104, 126	2 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	147	PHE	4.5
1	B	447	THR	3.6
1	A	499	ASP	3.2
1	B	448	ASN	3.1
1	B	177	HIS	2.9
1	A	15	TYR	2.3
1	B	509	LYS	2.3
1	B	22	TYR	2.1
1	B	514	PHE	2.1
1	B	144	GLY	2.1

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](#)

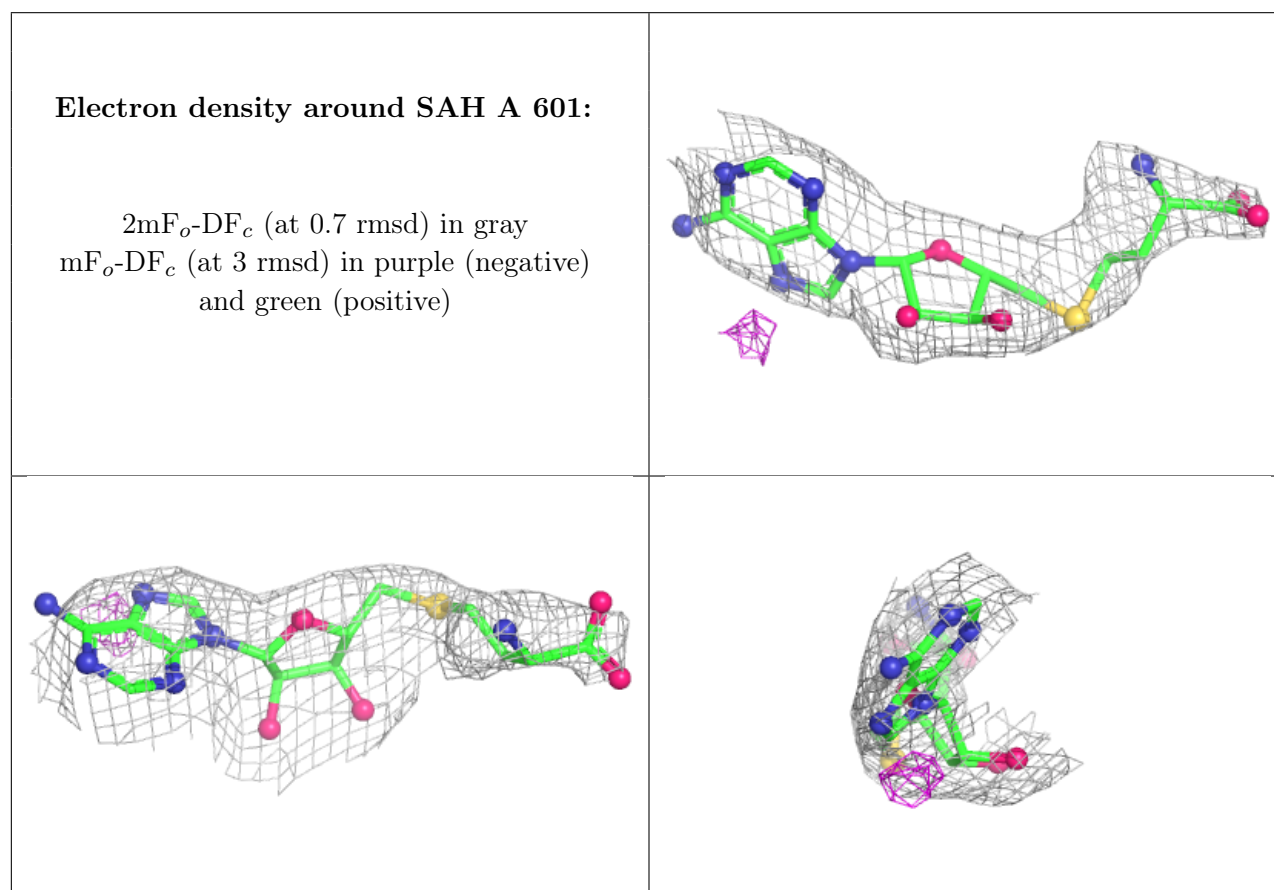
There are no oligosaccharides in this entry.

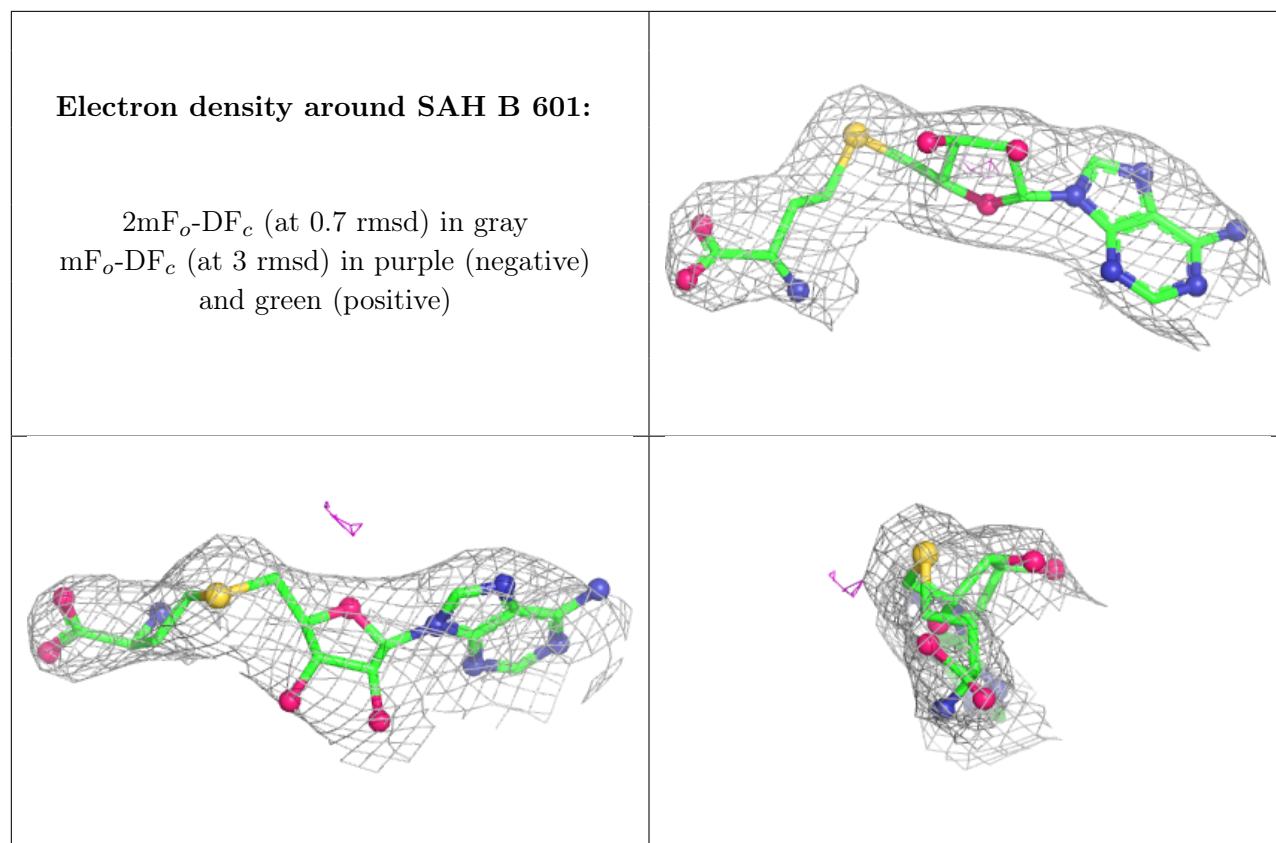
6.4 Ligands ⓘ

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	A	601	26/26	0.87	0.09	66,76,87,113	0
2	SAH	B	601	26/26	0.91	0.08	53,67,78,85	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.





6.5 Other polymers ⓘ

There are no such residues in this entry.