



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 19, 2025 – 04:20 PM JST

PDB ID : 9W7F / pdb_00009w7f
Title : Crystal structure of African swine fever virus methyltransferase EP424R in complex with S-adenosylmethionine
Authors : Wang, Z.X.; Guo, F.L.; Liu, Y.; Peng, G.Q.
Deposited on : 2025-08-06
Resolution : 2.59 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

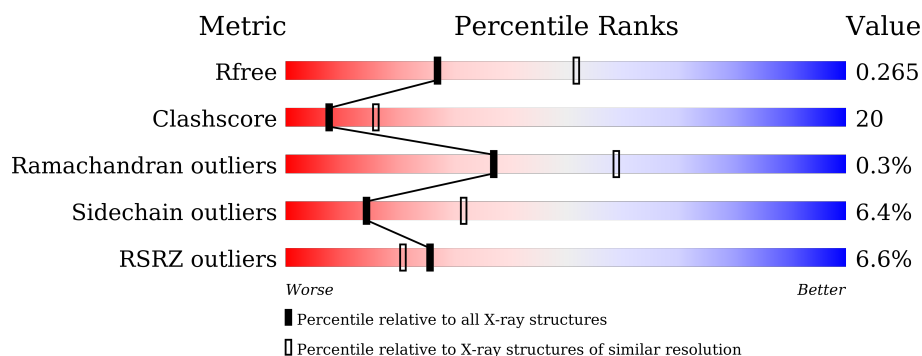
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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}	164625	3775 (2.60-2.60)
Clashscore	180529	4181 (2.60-2.60)
Ramachandran outliers	177936	4129 (2.60-2.60)
Sidechain outliers	177891	4129 (2.60-2.60)
RSRZ outliers	164620	3775 (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 $\leq 5\%$. 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	426	 5% 58% 31% 8%
1	B	426	 7% 51% 36% 5% 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6682 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.

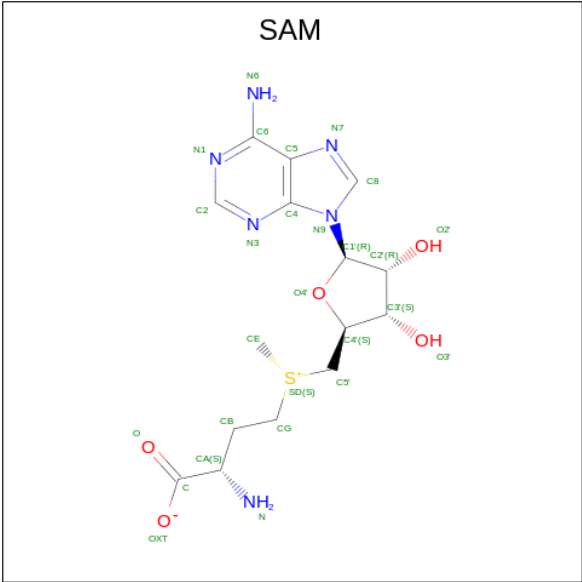
- Molecule 1 is a protein called Probable methyltransferase EP424R.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3236	2108	540	572	16			
1	B	392	Total	C	N	O	S	0	0	0
			3231	2102	538	575	16			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	419	HIS	-	expression tag	UNP A0A2X0RUW3
A	420	HIS	-	expression tag	UNP A0A2X0RUW3
A	421	HIS	-	expression tag	UNP A0A2X0RUW3
A	422	HIS	-	expression tag	UNP A0A2X0RUW3
A	423	HIS	-	expression tag	UNP A0A2X0RUW3
A	424	HIS	-	expression tag	UNP A0A2X0RUW3
A	425	HIS	-	expression tag	UNP A0A2X0RUW3
A	426	HIS	-	expression tag	UNP A0A2X0RUW3
B	419	HIS	-	expression tag	UNP A0A2X0RUW3
B	420	HIS	-	expression tag	UNP A0A2X0RUW3
B	421	HIS	-	expression tag	UNP A0A2X0RUW3
B	422	HIS	-	expression tag	UNP A0A2X0RUW3
B	423	HIS	-	expression tag	UNP A0A2X0RUW3
B	424	HIS	-	expression tag	UNP A0A2X0RUW3
B	425	HIS	-	expression tag	UNP A0A2X0RUW3
B	426	HIS	-	expression tag	UNP A0A2X0RUW3

- Molecule 2 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: C₁₅H₂₂N₆O₅S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	90	Total	O	0	0
			90	90		
3	B	71	Total	O	0	0
			71	71		

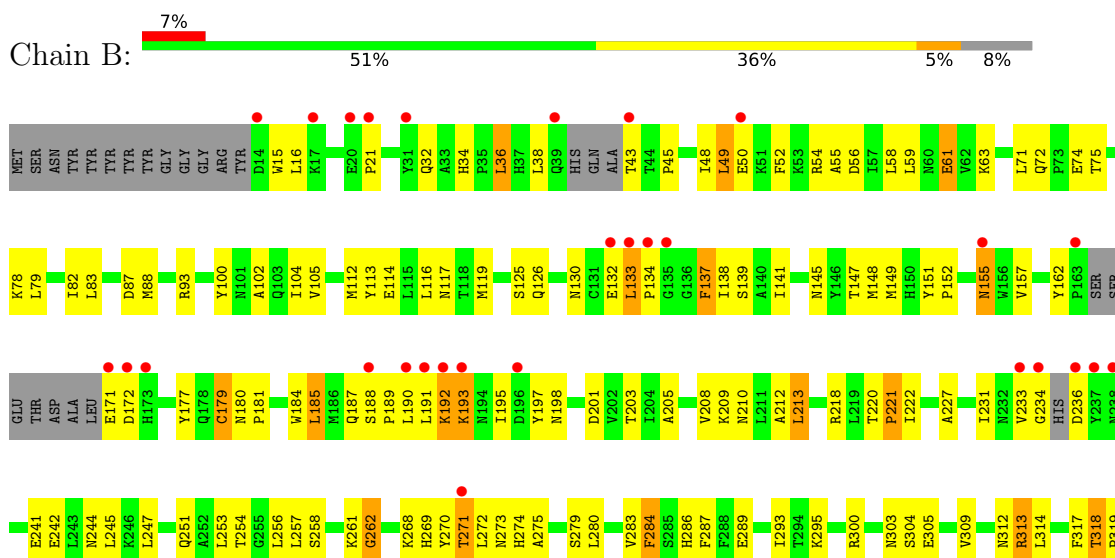
3 Residue-property plots [i](#)

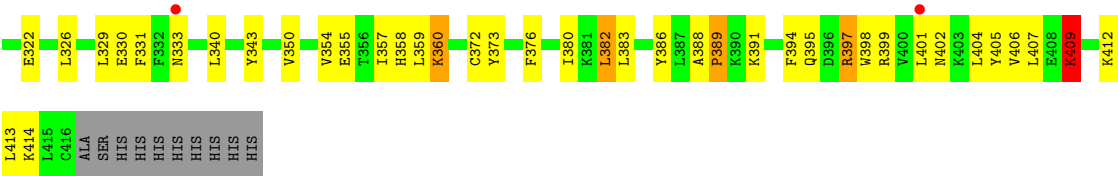
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Probable methyltransferase EP424R



• Molecule 1: Probable methyltransferase EP424R





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.60Å 57.72Å 101.43Å 90.00° 111.44° 90.00°	Depositor
Resolution (Å)	50.07 – 2.59 50.07 – 2.59	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.07-2.59) 98.7 (50.07-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.88 (at 2.58Å)	Xtriage
Refinement program	PHENIX v1.20.1	Depositor
R, R_{free}	0.203 , 0.276 0.211 , 0.265	Depositor DCC
R_{free} test set	1371 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	15.2	Xtriage
Anisotropy	0.792	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6682	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% 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: SAM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.50	0/3318	0.74	0/4489
1	B	0.77	0/3311	1.23	10/4479 (0.2%)
All	All	0.65	0/6629	1.01	10/8968 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	270	TYR	N-CA-C	6.28	124.17	110.80
1	B	284	PHE	CA-CB-CG	6.21	120.00	113.80
1	B	193	LYS	CB-CA-C	-5.65	100.72	111.06
1	B	262	GLY	N-CA-C	-5.61	107.92	115.21
1	B	155	ASN	CB-CA-C	5.49	118.81	109.80
1	B	389	PRO	N-CA-CB	-5.40	97.39	103.33
1	B	261	LYS	CB-CA-C	5.39	118.67	109.72
1	B	313	ARG	CB-CA-C	5.28	117.77	110.16
1	B	409	LYS	N-CA-CB	-5.12	102.33	110.22
1	B	137	PHE	CA-CB-CG	5.09	118.89	113.80

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	3236	0	3259	110	0
1	B	3231	0	3253	144	0
2	A	27	0	22	2	0
2	B	27	0	22	2	0
3	A	90	0	0	9	0
3	B	71	0	0	5	0
All	All	6682	0	6556	256	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 (256) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:LYS:H	1:A:94:LYS:HD2	1.22	1.04
1:A:129:CYS:HB3	1:A:132:GLU:HG2	1.40	1.00
1:B:59:LEU:CD2	1:B:63:LYS:HE3	1.93	0.98
1:A:65:GLU:HB2	1:A:370:MET:HE1	1.44	0.97
1:A:239:LYS:O	1:A:243:LEU:HG	1.69	0.92
1:B:59:LEU:HD22	1:B:63:LYS:HE3	1.49	0.90
1:A:227:ALA:HB1	1:A:251:GLN:HG2	1.57	0.87
1:A:228:ASP:OD1	1:A:268:LYS:HD3	1.75	0.86
1:B:253:LEU:HD13	1:B:326:LEU:HD23	1.58	0.85
1:B:185:LEU:HD12	1:B:218:ARG:NH1	1.89	0.85
1:A:94:LYS:HD2	1:A:94:LYS:N	1.95	0.80
1:B:256:LEU:HB3	1:B:317:PHE:CZ	2.18	0.79
1:A:233:VAL:HG21	1:A:243:LEU:HD12	1.66	0.76
1:A:209:LYS:NZ	1:A:322:GLU:OE2	2.20	0.75
1:A:268:LYS:HD2	1:A:305:GLU:OE2	1.87	0.74
1:B:242:GLU:HA	1:B:245:LEU:HD12	1.69	0.73
1:A:59:LEU:HD22	1:A:358:HIS:HB3	1.71	0.73
1:B:32:GLN:HG3	1:B:34:HIS:CE1	2.23	0.72
1:B:187:GLN:HB3	1:B:191:LEU:HD12	1.71	0.72
1:B:397:ARG:O	1:B:401:LEU:HG	1.89	0.72
1:B:289:GLU:HB2	1:B:314:LEU:HD21	1.72	0.72
1:A:39:GLN:NE2	1:A:336:PRO:O	2.23	0.71
1:A:237:TYR:N	3:A:604:HOH:O	2.26	0.69
1:A:90:LYS:O	1:A:94:LYS:NZ	2.24	0.69
1:B:355:GLU:HG2	1:B:360:LYS:HE3	1.75	0.68
1:B:130:ASN:ND2	1:B:254:THR:HG21	2.08	0.68
1:B:43:THR:N	3:B:603:HOH:O	2.25	0.68
1:A:65:GLU:CB	1:A:370:MET:HE1	2.21	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:GLN:NE2	1:B:197:TYR:HA	2.09	0.68
1:B:88:MET:HG3	1:B:394:PHE:CD2	2.28	0.67
1:B:187:GLN:HE22	1:B:197:TYR:HA	1.59	0.67
1:A:162:TYR:CD1	1:A:189:PRO:HD3	2.29	0.67
1:B:50:GLU:HG3	1:B:54:ARG:HH12	1.58	0.67
1:A:229:GLY:N	1:A:251:GLN:OE1	2.25	0.67
1:B:185:LEU:CD1	1:B:218:ARG:NH1	2.58	0.67
1:B:133:LEU:HB3	1:B:134:PRO:HD3	1.77	0.66
1:B:59:LEU:HD11	1:B:358:HIS:HB3	1.76	0.66
1:B:88:MET:HG3	1:B:394:PHE:HD2	1.59	0.66
1:A:23:ASN:ND2	3:A:607:HOH:O	2.29	0.66
1:B:179:CYS:SG	1:B:414:LYS:HG3	2.36	0.66
1:A:319:PRO:O	1:A:323:GLN:HG3	1.97	0.65
1:A:376:PHE:O	1:A:380:ILE:HD12	1.98	0.64
1:A:129:CYS:HB3	1:A:132:GLU:CG	2.23	0.64
1:B:388:ALA:HB3	1:B:389:PRO:HD3	1.79	0.63
1:A:65:GLU:HB2	1:A:370:MET:CE	2.25	0.63
1:B:192:LYS:O	1:B:193:LYS:HB2	1.99	0.62
1:A:162:TYR:CE1	1:A:189:PRO:HD3	2.34	0.62
1:A:272:LEU:HA	1:A:277:THR:HG21	1.82	0.62
1:B:401:LEU:HD12	1:B:402:ASN:ND2	2.15	0.62
1:B:32:GLN:HG3	1:B:34:HIS:HE1	1.65	0.61
1:B:192:LYS:HD2	1:B:193:LYS:HE2	1.83	0.60
1:B:179:CYS:C	1:B:181:PRO:HD3	2.27	0.60
1:B:205:ALA:HA	1:B:329:LEU:HD23	1.84	0.60
1:A:231:ILE:HD12	1:A:244:ASN:OD1	2.01	0.59
1:B:50:GLU:HG3	1:B:54:ARG:NH1	2.17	0.59
1:A:192:LYS:HA	1:A:197:TYR:CD2	2.38	0.59
1:A:45:PRO:HB2	1:A:49:LEU:HD12	1.84	0.58
1:B:88:MET:SD	1:B:391:LYS:HG2	2.43	0.58
1:B:177:TYR:HA	1:B:184:TRP:CD1	2.38	0.58
1:B:132:GLU:OE1	1:B:137:PHE:HB2	2.03	0.58
1:B:257:LEU:HD21	1:B:322:GLU:HG3	1.85	0.58
1:B:293:ILE:HD11	1:B:350:VAL:HG22	1.85	0.58
1:A:149:MET:HA	1:A:149:MET:HE2	1.84	0.58
1:A:77:LYS:O	1:A:81:GLN:HG3	2.04	0.57
1:B:407:LEU:HD23	1:B:412:LYS:HG2	1.86	0.57
1:B:380:ILE:HD12	1:B:380:ILE:H	1.68	0.57
1:B:300:ARG:HB2	1:B:303:ASN:ND2	2.20	0.57
1:A:59:LEU:HG	1:A:63:LYS:HE3	1.87	0.57
1:A:300:ARG:NH1	3:A:612:HOH:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:SER:HB2	1:B:189:PRO:HD2	1.87	0.56
1:B:382:LEU:HD22	1:B:386:TYR:CE2	2.39	0.56
1:B:148:MET:HE1	1:B:405:TYR:HD2	1.70	0.56
1:B:376:PHE:CD2	1:B:383:LEU:HD13	2.40	0.56
1:B:171:GLU:HG3	1:B:172:ASP:N	2.21	0.56
1:B:21:PRO:HG3	1:B:394:PHE:HE1	1.69	0.55
1:A:60:ASN:OD1	1:A:238:ASN:HA	2.05	0.55
1:B:79:LEU:HD11	1:B:83:LEU:HD11	1.88	0.55
1:B:100:TYR:HA	1:B:406:VAL:HG12	1.88	0.55
1:A:124:THR:HG23	1:A:151:TYR:HE2	1.71	0.55
1:A:104:ILE:HG23	1:A:174:TYR:CE1	2.42	0.55
1:B:330:GLU:HG2	1:B:331:PHE:CZ	2.42	0.55
1:B:36:LEU:HD11	1:B:38:LEU:HD23	1.87	0.55
1:B:55:ALA:HB1	1:B:359:LEU:HD21	1.89	0.55
1:B:36:LEU:HB2	1:B:286:HIS:CD2	2.41	0.55
1:A:39:GLN:OE1	1:A:43:THR:HG22	2.07	0.54
1:B:59:LEU:HD21	1:B:63:LYS:HE3	1.85	0.54
1:B:59:LEU:CD1	1:B:358:HIS:HB3	2.38	0.54
1:A:129:CYS:CB	1:A:132:GLU:HG2	2.27	0.54
1:B:227:ALA:HB1	1:B:251:GLN:HB3	1.90	0.54
1:B:145:ASN:HA	1:B:149:MET:HB2	1.90	0.54
1:A:409:LYS:HA	1:A:412:LYS:HG3	1.90	0.54
1:A:16:LEU:O	1:A:19:VAL:HG13	2.08	0.53
1:A:45:PRO:CB	1:A:49:LEU:HD12	2.38	0.53
1:B:303:ASN:OD1	1:B:305:GLU:HB3	2.08	0.53
1:B:398:TRP:O	1:B:402:ASN:HB2	2.07	0.53
1:A:95:LYS:HE3	1:A:399:ARG:CZ	2.39	0.53
1:A:202:VAL:O	1:A:250:GLY:HA3	2.08	0.53
1:B:162:TYR:CE1	1:B:189:PRO:HD3	2.43	0.53
1:B:114:GLU:HG3	1:B:402:ASN:HD21	1.73	0.52
1:B:253:LEU:HD13	1:B:326:LEU:CD2	2.36	0.52
1:B:130:ASN:HD22	1:B:254:THR:HG21	1.72	0.52
1:B:241:GLU:HB2	1:B:271:THR:OG1	2.10	0.52
1:A:176:LEU:HD12	1:A:180:ASN:ND2	2.24	0.52
1:A:158:ALA:O	1:A:184:TRP:HA	2.10	0.52
1:B:269:HIS:HB3	1:B:272:LEU:HD21	1.91	0.52
1:A:231:ILE:HG22	1:A:232:ASN:N	2.25	0.52
1:B:126:GLN:HA	1:B:155:ASN:O	2.10	0.52
1:A:16:LEU:HD22	1:A:387:LEU:HD21	1.92	0.52
1:B:119:MET:HG3	1:B:309:VAL:HG11	1.91	0.52
1:B:227:ALA:CB	1:B:251:GLN:HB3	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:ARG:HG2	3:A:621:HOH:O	2.09	0.51
1:B:180:ASN:HD21	1:B:414:LYS:HB3	1.75	0.51
1:A:388:ALA:HB3	1:A:389:PRO:HD3	1.92	0.51
1:A:187:GLN:NE2	1:A:214:ARG:NH1	2.59	0.51
1:B:208:VAL:HG11	1:B:253:LEU:HB3	1.92	0.51
1:B:355:GLU:HG2	1:B:360:LYS:CE	2.39	0.51
1:A:274:HIS:CE1	1:A:334:ASP:HB2	2.45	0.51
1:B:147:THR:HB	1:B:405:TYR:HB2	1.91	0.51
1:B:280:LEU:HG	1:B:284:PHE:CZ	2.46	0.51
1:B:185:LEU:CD1	1:B:218:ARG:HH11	2.23	0.50
1:B:279:SER:O	1:B:283:VAL:HG23	2.11	0.50
1:B:395:GLN:O	1:B:399:ARG:HG3	2.11	0.50
1:B:180:ASN:N	1:B:181:PRO:HD3	2.25	0.50
1:B:78:LYS:NZ	3:B:610:HOH:O	2.43	0.50
1:B:274:HIS:HD2	1:B:275:ALA:N	2.09	0.50
1:B:355:GLU:HA	1:B:359:LEU:HB2	1.93	0.50
1:A:132:GLU:CD	1:A:137:PHE:HB2	2.36	0.50
1:B:93:ARG:HG2	1:B:105:VAL:HG12	1.93	0.50
1:B:82:ILE:HD12	1:B:373:TYR:HA	1.93	0.49
1:A:49:LEU:HD21	1:A:278:LEU:HD12	1.94	0.49
1:A:209:LYS:HD3	1:A:326:LEU:HD11	1.94	0.49
1:A:387:LEU:O	1:A:391:LYS:HG3	2.12	0.49
1:B:102:ALA:HB3	1:B:105:VAL:HG21	1.94	0.49
1:B:192:LYS:HG2	1:B:197:TYR:CE2	2.47	0.49
1:A:133:LEU:HD22	1:A:134:PRO:HA	1.94	0.49
1:A:333:ASN:OD1	1:A:335:THR:HB	2.12	0.49
1:A:172:ASP:CG	1:A:177:TYR:H	2.21	0.49
1:B:45:PRO:HB3	1:B:49:LEU:HD12	1.93	0.49
1:B:192:LYS:O	1:B:193:LYS:CB	2.61	0.49
1:B:407:LEU:CD2	1:B:412:LYS:HG2	2.43	0.48
1:A:150:HIS:HA	3:A:651:HOH:O	2.13	0.48
1:B:79:LEU:O	1:B:83:LEU:HG	2.13	0.48
1:A:241:GLU:HB2	1:A:271:THR:OG1	2.14	0.48
1:B:241:GLU:O	1:B:245:LEU:HG	2.13	0.48
1:A:74:GLU:HG3	1:A:75:THR:N	2.28	0.48
1:B:388:ALA:N	1:B:389:PRO:CD	2.76	0.48
1:A:130:ASN:O	1:A:131:CYS:C	2.56	0.47
1:B:382:LEU:HD22	1:B:386:TYR:CD2	2.49	0.47
1:A:138:ILE:HG21	1:A:176:LEU:HD21	1.95	0.47
1:B:56:ASP:OD1	3:B:601:HOH:O	2.20	0.47
1:A:21:PRO:HD3	1:A:394:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:TYR:CZ	1:B:404:LEU:HD23	2.50	0.47
1:A:133:LEU:HD13	1:A:171:GLU:C	2.40	0.47
1:B:275:ALA:HB3	3:B:622:HOH:O	2.14	0.47
1:B:132:GLU:HA	2:B:501:SAM:HB1	1.96	0.46
1:B:212:ALA:HA	1:B:258:SER:OG	2.15	0.46
1:B:247:LEU:HD23	1:B:247:LEU:O	2.15	0.46
1:A:132:GLU:OE1	1:A:137:PHE:HB2	2.15	0.46
1:B:273:ASN:HD21	1:B:354:VAL:HG11	1.80	0.46
1:A:175:GLY:HA3	1:A:416:CYS:HB2	1.98	0.46
1:B:192:LYS:HD2	1:B:193:LYS:H	1.81	0.46
1:B:177:TYR:HA	1:B:184:TRP:NE1	2.31	0.46
1:A:198:ASN:HD21	1:A:211:LEU:HG	1.79	0.46
1:A:30:PRO:HD2	1:A:346:LEU:HD12	1.97	0.46
1:B:409:LYS:HA	1:B:412:LYS:HD3	1.98	0.46
1:A:193:LYS:HZ3	1:A:197:TYR:N	2.13	0.46
1:B:247:LEU:HD23	1:B:247:LEU:C	2.40	0.46
1:A:193:LYS:O	1:A:193:LYS:HG3	2.15	0.45
1:B:247:LEU:O	1:B:251:GLN:HG3	2.16	0.45
1:B:355:GLU:O	1:B:360:LYS:HB2	2.15	0.45
1:B:233:VAL:O	1:B:234:GLY:C	2.58	0.45
1:A:130:ASN:ND2	1:A:159:SER:HB3	2.31	0.45
1:A:92:LEU:HD13	1:A:395:GLN:HB3	1.99	0.45
1:A:133:LEU:HD23	1:A:133:LEU:HA	1.80	0.45
1:B:274:HIS:CD2	1:B:275:ALA:N	2.84	0.45
1:B:401:LEU:CD1	1:B:402:ASN:ND2	2.79	0.45
1:B:48:ILE:O	1:B:48:ILE:HG12	2.16	0.45
1:B:231:ILE:HG12	1:B:244:ASN:OD1	2.16	0.45
1:B:257:LEU:HD21	1:B:322:GLU:CD	2.42	0.44
1:B:32:GLN:CG	1:B:34:HIS:CE1	2.98	0.44
1:B:192:LYS:HD2	1:B:193:LYS:N	2.32	0.44
1:A:192:LYS:HA	1:A:197:TYR:CG	2.53	0.44
1:B:220:THR:HA	1:B:221:PRO:HA	1.75	0.44
1:B:287:PHE:O	1:B:313:ARG:HA	2.17	0.43
1:B:382:LEU:CD2	1:B:386:TYR:CE2	3.01	0.43
1:B:133:LEU:HG	1:B:171:GLU:C	2.43	0.43
1:B:201:ASP:OD1	1:B:203:THR:HG23	2.18	0.43
1:A:149:MET:HE2	1:A:149:MET:CA	2.49	0.43
1:B:157:VAL:HB	1:B:185:LEU:HD21	1.99	0.43
1:B:398:TRP:HZ3	1:B:404:LEU:HD11	1.83	0.43
1:A:233:VAL:HG21	1:A:243:LEU:CD1	2.41	0.43
1:A:49:LEU:HD23	1:A:49:LEU:HA	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:CYS:HB3	2:A:501:SAM:H1'	2.01	0.43
1:A:209:LYS:CE	1:A:322:GLU:OE2	2.66	0.43
1:A:253:LEU:HD21	1:A:325:LEU:HB3	2.00	0.43
1:B:138:ILE:H	1:B:138:ILE:HG13	1.62	0.43
1:A:246:LYS:HE2	3:A:606:HOH:O	2.19	0.43
1:B:74:GLU:HG3	1:B:75:THR:N	2.32	0.43
1:A:260:SER:HB3	3:A:652:HOH:O	2.18	0.43
1:B:116:LEU:HD11	1:B:141:ILE:HG12	2.01	0.43
1:A:28:GLY:O	1:A:29:LEU:HD23	2.19	0.42
1:A:43:THR:HG21	1:A:339:ASP:HA	2.00	0.42
1:A:82:ILE:O	1:A:86:ILE:HG13	2.19	0.42
1:A:403:LYS:H	1:A:403:LYS:HG2	1.65	0.42
1:B:257:LEU:HD21	1:B:322:GLU:CG	2.49	0.42
1:A:69:LEU:HD12	1:A:79:LEU:HD13	2.01	0.42
1:A:103:GLN:O	1:A:104:ILE:C	2.63	0.42
1:A:137:PHE:CE2	1:A:228:ASP:HB2	2.54	0.42
1:A:392:LYS:HE3	1:A:396:ASP:OD2	2.19	0.42
1:B:87:ASP:OD1	1:B:87:ASP:C	2.63	0.42
1:B:88:MET:HA	1:B:391:LYS:HG2	2.02	0.42
1:B:192:LYS:CD	1:B:193:LYS:H	2.33	0.42
1:A:381:LYS:HD2	3:A:673:HOH:O	2.19	0.42
2:A:501:SAM:HG2	2:A:501:SAM:H4'	1.32	0.42
1:B:126:GLN:NE2	1:B:221:PRO:HD2	2.35	0.42
1:B:318:THR:O	1:B:319:PRO:C	2.63	0.42
1:A:16:LEU:HD11	1:A:376:PHE:CE2	2.55	0.41
1:A:95:LYS:HD2	1:A:99:THR:OG1	2.20	0.41
1:A:127:ALA:HA	1:A:224:LEU:O	2.20	0.41
1:A:160:SER:O	1:A:186:MET:HG3	2.20	0.41
1:B:376:PHE:CE2	1:B:383:LEU:HD13	2.55	0.41
1:B:58:LEU:O	1:B:61:GLU:HB2	2.21	0.41
1:B:125:SER:C	1:B:126:GLN:HG3	2.45	0.41
1:B:213:LEU:HD23	1:B:213:LEU:HA	1.93	0.41
1:A:92:LEU:HB2	1:A:395:GLN:HG2	2.00	0.41
1:B:16:LEU:HD11	1:B:383:LEU:HD11	2.01	0.41
1:B:198:ASN:HD22	1:B:210:ASN:HB3	1.86	0.41
1:A:112:MET:HE3	1:A:137:PHE:CD2	2.55	0.41
1:A:190:LEU:H	1:A:190:LEU:HG	1.69	0.41
1:A:253:LEU:HD23	1:A:253:LEU:HA	1.88	0.41
1:B:262:GLY:HA2	1:B:312:ASN:OD1	2.20	0.41
1:A:35:PRO:HA	3:A:617:HOH:O	2.20	0.41
1:B:71:LEU:HA	1:B:71:LEU:HD23	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:ASP:O	3:B:602:HOH:O	2.21	0.41
1:A:231:ILE:HD12	1:A:231:ILE:H	1.86	0.41
1:B:104:ILE:HG22	1:B:104:ILE:O	2.20	0.41
1:B:295:LYS:HD2	1:B:357:ILE:HG23	2.02	0.41
1:A:256:LEU:HD23	1:A:256:LEU:HA	1.92	0.41
1:B:32:GLN:HG2	1:B:343:TYR:CD2	2.55	0.41
1:B:52:PHE:HD1	1:B:273:ASN:HD22	1.68	0.41
1:B:151:TYR:HA	1:B:152:PRO:HD3	1.92	0.41
1:B:195:ILE:N	1:B:195:ILE:HD13	2.36	0.41
1:A:260:SER:O	1:A:261:LYS:C	2.62	0.41
1:B:15:TRP:HZ3	1:B:372:CYS:SG	2.43	0.41
1:B:133:LEU:CB	1:B:134:PRO:HD3	2.49	0.41
2:B:501:SAM:H4'	2:B:501:SAM:HG2	1.75	0.40
1:A:25:LEU:O	1:A:294:THR:HA	2.20	0.40
1:A:128:PHE:CD1	1:A:157:VAL:HG23	2.56	0.40
1:A:198:ASN:OD1	1:A:198:ASN:C	2.64	0.40
1:A:394:PHE:N	1:A:394:PHE:CD1	2.89	0.40
1:A:269:HIS:ND1	1:A:308:ILE:HD12	2.36	0.40
1:B:139:SER:HA	1:B:413:LEU:HD11	2.03	0.40
1:A:372:CYS:O	1:A:373:TYR:C	2.65	0.40
1:A:25:LEU:HD23	1:A:25:LEU:HA	1.95	0.40
1:A:191:LEU:HD13	1:A:191:LEU:HA	1.91	0.40
1:B:112:MET:HB2	1:B:137:PHE:CD1	2.57	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	384/426 (90%)	364 (95%)	18 (5%)	2 (0%)	25	47
1	B	384/426 (90%)	368 (96%)	16 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	768/852 (90%)	732 (95%)	34 (4%)	2 (0%)	37	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	GLY
1	A	134	PRO

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	360/389 (92%)	339 (94%)	21 (6%)	17	36
1	B	361/389 (93%)	336 (93%)	25 (7%)	13	28
All	All	721/778 (93%)	675 (94%)	46 (6%)	14	32

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	HIS
1	A	43	THR
1	A	47	SER
1	A	97	GLU
1	A	124	THR
1	A	132	GLU
1	A	138	ILE
1	A	139	SER
1	A	153	THR
1	A	160	SER
1	A	161	LEU
1	A	171	GLU
1	A	190	LEU
1	A	191	LEU
1	A	193	LYS
1	A	219	LEU

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Mol	Chain	Res	Type
1	A	220	THR
1	A	233	VAL
1	A	251	GLN
1	A	271	THR
1	A	338	VAL
1	B	36	LEU
1	B	49	LEU
1	B	61	GLU
1	B	72	GLN
1	B	117	ASN
1	B	133	LEU
1	B	179	CYS
1	B	185	LEU
1	B	190	LEU
1	B	192	LYS
1	B	209	LYS
1	B	213	LEU
1	B	221	PRO
1	B	222	ILE
1	B	236	ASP
1	B	268	LYS
1	B	271	THR
1	B	304	SER
1	B	318	THR
1	B	333	ASN
1	B	340	LEU
1	B	360	LYS
1	B	382	LEU
1	B	397	ARG
1	B	409	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	101	ASN
1	A	126	GLN
1	A	150	HIS
1	A	248	HIS
1	A	323	GLN
1	B	34	HIS
1	B	126	GLN

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Mol	Chain	Res	Type
1	B	173	HIS
1	B	180	ASN
1	B	238	ASN
1	B	273	ASN
1	B	274	HIS
1	B	362	GLN
1	B	402	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	SAM	B	501	-	24,29,29	0.86	1 (4%)	23,42,42	0.94	2 (8%)
2	SAM	A	501	-	24,29,29	0.68	0	23,42,42	0.94	1 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAM	B	501	-	-	7/12/33/33	0/3/3/3
2	SAM	A	501	-	-	5/12/33/33	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	SAM	OXT-C	-3.02	1.20	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	SAM	C5-C6-N6	2.60	124.30	120.35
2	A	501	SAM	C5-C6-N6	2.35	123.92	120.35
2	B	501	SAM	CG-SD-C5'	-2.27	97.62	103.40

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	SAM	CB-CG-SD-CE
2	A	501	SAM	C4'-C5'-SD-CG
2	B	501	SAM	O-C-CA-N
2	B	501	SAM	CB-CG-SD-CE
2	B	501	SAM	CB-CG-SD-C5'
2	B	501	SAM	OXT-C-CA-N
2	A	501	SAM	CB-CG-SD-C5'
2	A	501	SAM	O4'-C4'-C5'-SD
2	B	501	SAM	CA-CB-CG-SD
2	B	501	SAM	O-C-CA-CB
2	B	501	SAM	OXT-C-CA-CB
2	A	501	SAM	OXT-C-CA-N

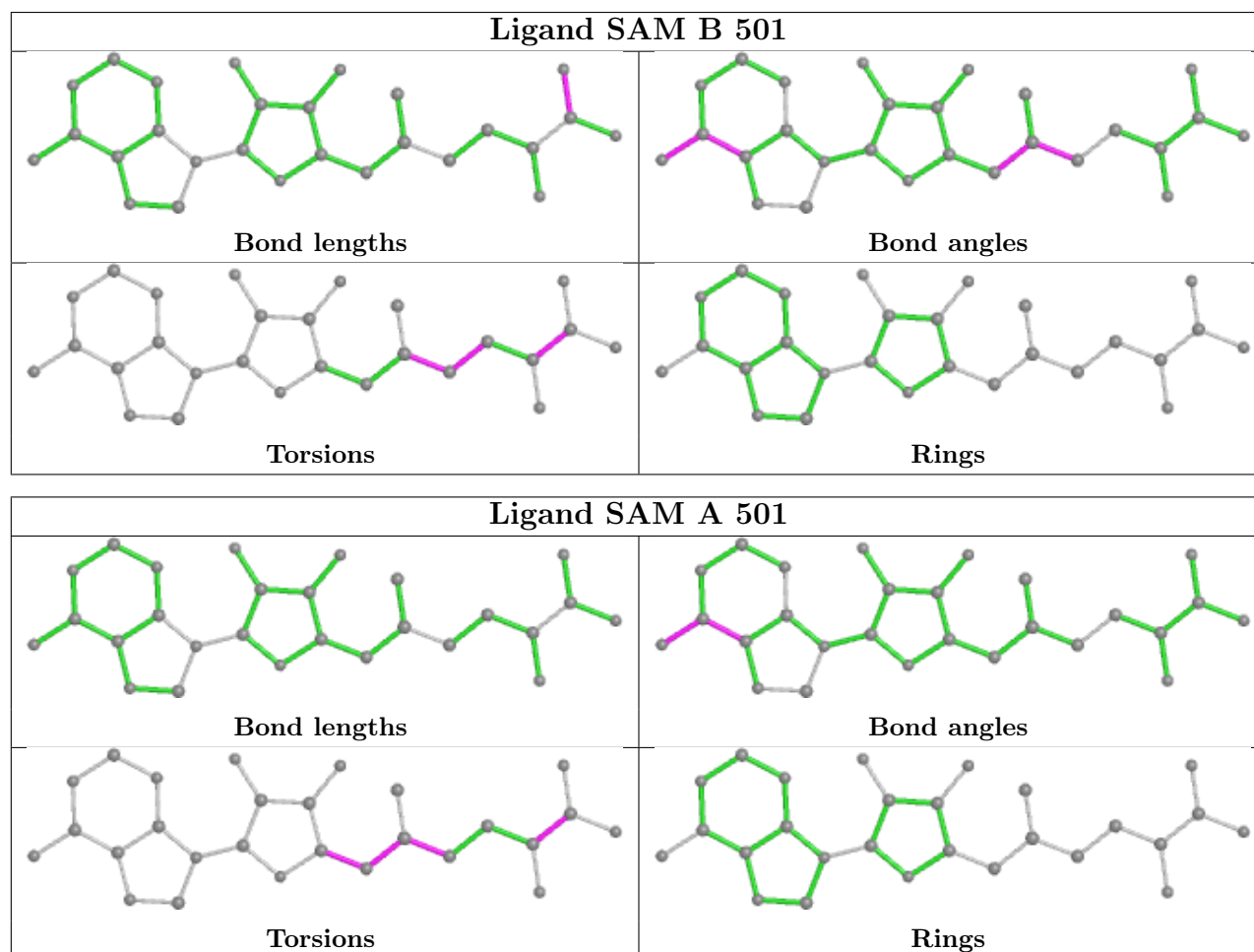
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	SAM	2	0
2	A	501	SAM	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 ⓘ

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, 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	392/426 (92%)	0.11	21 (5%) 32 27	5, 14, 34, 58	0
1	B	392/426 (92%)	0.46	31 (7%) 20 16	5, 16, 40, 66	0
All	All	784/852 (92%)	0.29	52 (6%) 26 21	5, 15, 38, 66	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	133	LEU	6.6
1	B	234	GLY	6.5
1	B	237	TYR	5.9
1	B	132	GLU	5.2
1	B	163	PRO	4.6
1	A	232	ASN	4.5
1	B	14	ASP	4.1
1	B	190	LEU	3.9
1	A	13	TYR	3.9
1	B	193	LYS	3.7
1	A	134	PRO	3.6
1	A	217	GLN	3.5
1	A	218	ARG	3.4
1	B	21	PRO	3.3
1	B	192	LYS	3.1
1	B	50	GLU	3.0
1	B	238	ASN	2.9
1	A	163	PRO	2.8
1	A	171	GLU	2.8
1	A	14	ASP	2.8
1	A	231	ILE	2.8
1	A	40	HIS	2.8
1	A	193	LYS	2.6
1	A	191	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	134	PRO	2.6
1	B	39	GLN	2.5
1	B	401	LEU	2.4
1	B	271	THR	2.4
1	A	378	ASN	2.4
1	B	333	ASN	2.4
1	A	238	ASN	2.4
1	B	171	GLU	2.4
1	B	155	ASN	2.3
1	B	233	VAL	2.3
1	B	196	ASP	2.3
1	B	31	TYR	2.3
1	B	135	GLY	2.2
1	B	43	THR	2.2
1	B	172	ASP	2.2
1	A	233	VAL	2.2
1	A	98	PHE	2.2
1	A	237	TYR	2.2
1	B	17	LYS	2.2
1	A	230	GLY	2.2
1	B	236	ASP	2.2
1	A	190	LEU	2.1
1	A	220	THR	2.1
1	A	334	ASP	2.1
1	B	188	SER	2.1
1	B	173	HIS	2.0
1	B	191	LEU	2.0
1	B	20	GLU	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 oligosaccharides in this entry.

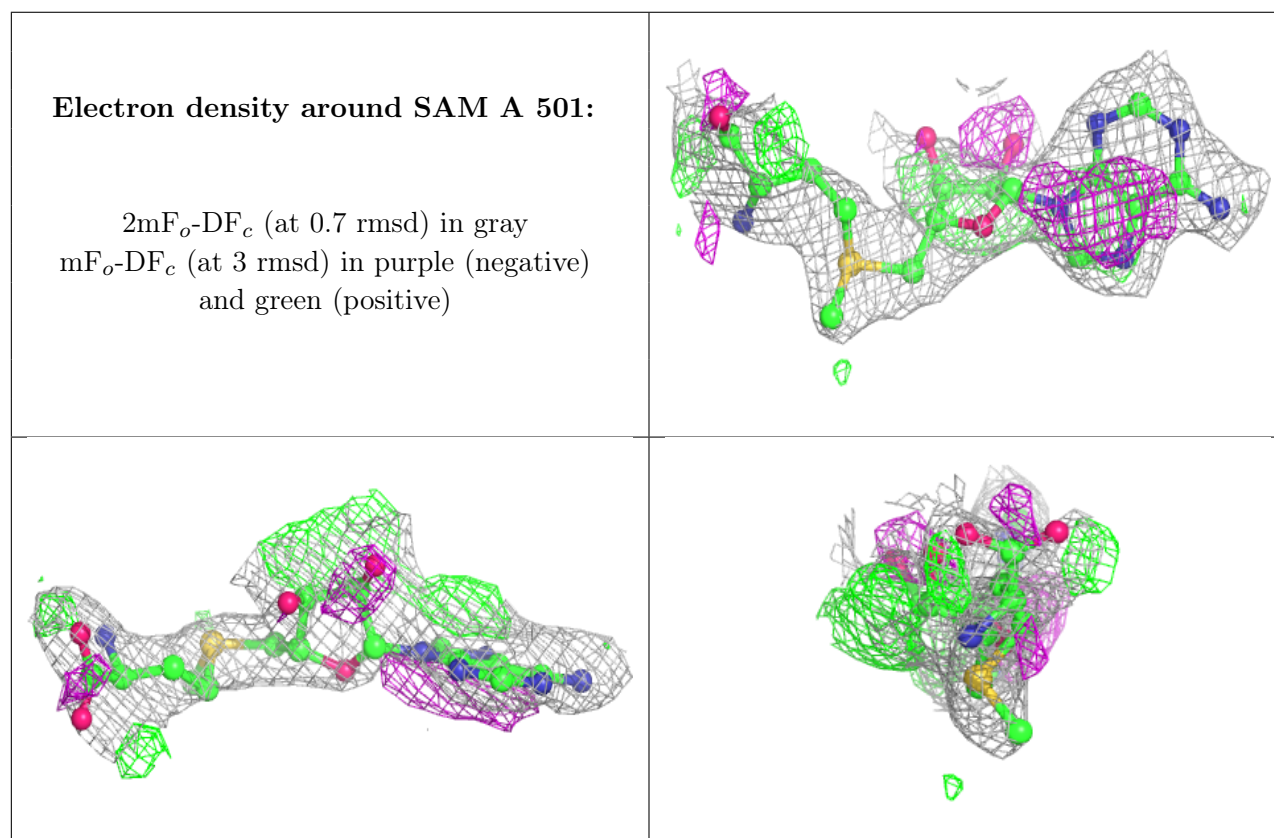
6.4 Ligands [i](#)

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.

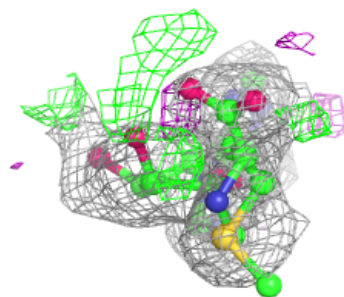
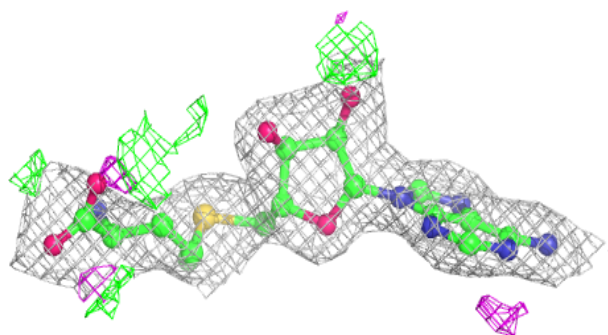
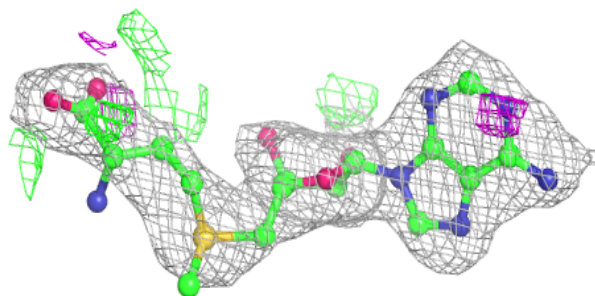
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SAM	A	501	27/27	0.67	0.23	21,28,39,48	0
2	SAM	B	501	27/27	0.88	0.14	14,25,39,47	0

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



Electron density around SAM B 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.