



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:50 AM UTC

PDB ID : 6I5Z / pdb_00006i5z
Title : Papaver somniferum O-methyltransferase
Authors : Davies, G.J.; Cabry, M.P.; Offen, W.A.
Deposited on : 2018-11-15
Resolution : 3.00 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

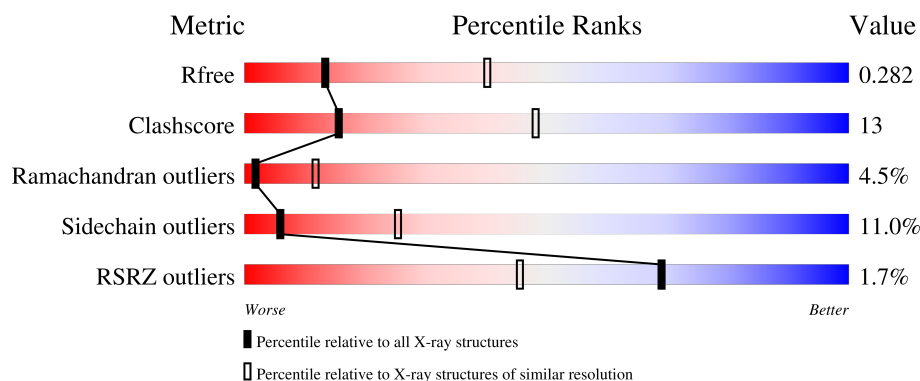
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	393	52% 31% • • 13%
1	B	393	62% 24% • 11%
1	C	393	63% 22% • 13%
1	D	393	3% 51% 31% 6% 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10191 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 O-methyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2560	1654	419	471	16			
1	B	349	Total	C	N	O	S	0	0	0
			2586	1659	430	481	16			
1	C	342	Total	C	N	O	S	0	0	0
			2463	1581	409	456	17			
1	D	347	Total	C	N	O	S	0	0	0
			2503	1604	411	472	16			

There are 12 discrepancies between the modelled and reference sequences:

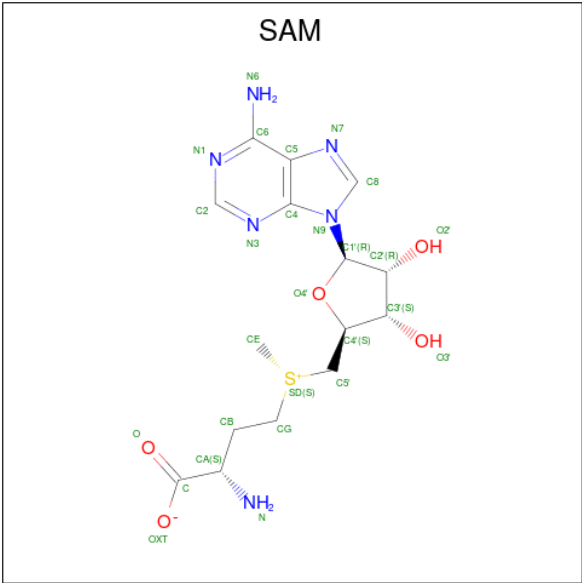
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP I3PLQ5
A	-1	PRO	-	expression tag	UNP I3PLQ5
A	0	ALA	-	expression tag	UNP I3PLQ5
B	-2	GLY	-	expression tag	UNP I3PLQ5
B	-1	PRO	-	expression tag	UNP I3PLQ5
B	0	ALA	-	expression tag	UNP I3PLQ5
C	-2	GLY	-	expression tag	UNP I3PLQ5
C	-1	PRO	-	expression tag	UNP I3PLQ5
C	0	ALA	-	expression tag	UNP I3PLQ5
D	-2	GLY	-	expression tag	UNP I3PLQ5
D	-1	PRO	-	expression tag	UNP I3PLQ5
D	0	ALA	-	expression tag	UNP I3PLQ5

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

- Molecule 3 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: C₁₅H₂₂N₆O₅S).

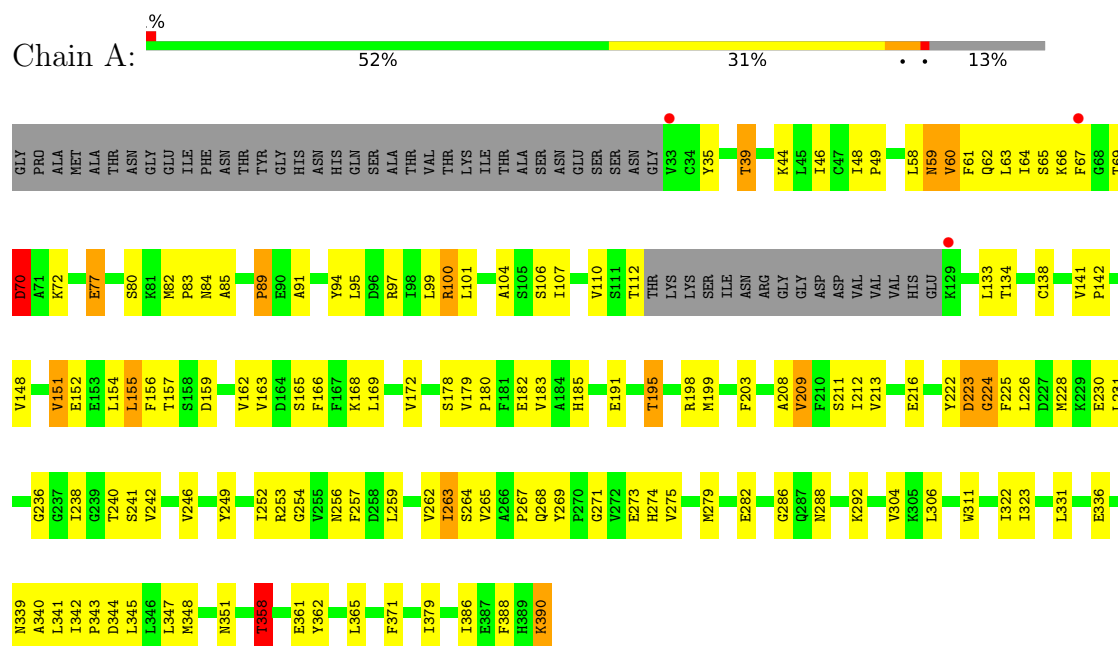


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

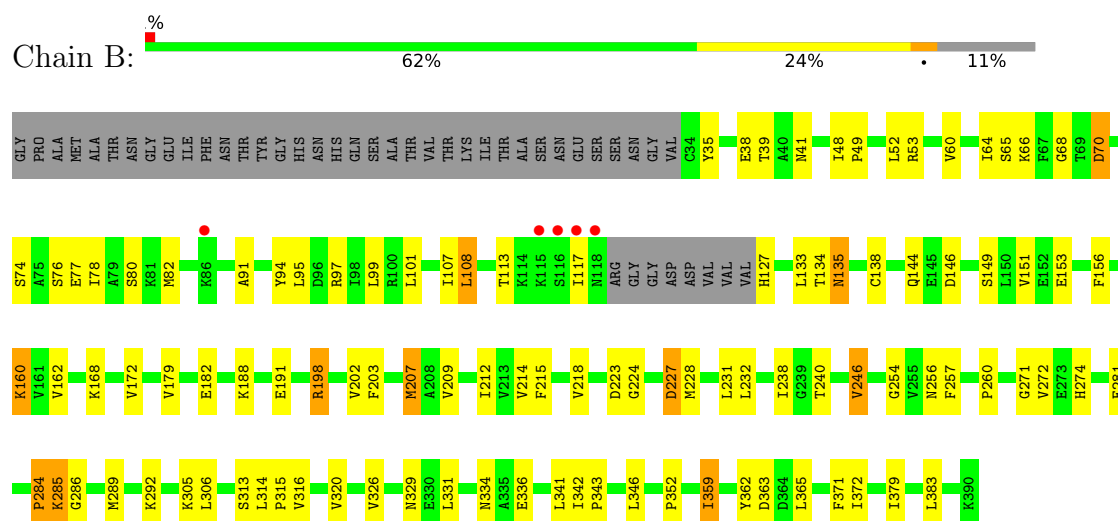
3 Residue-property plots [i](#)

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.

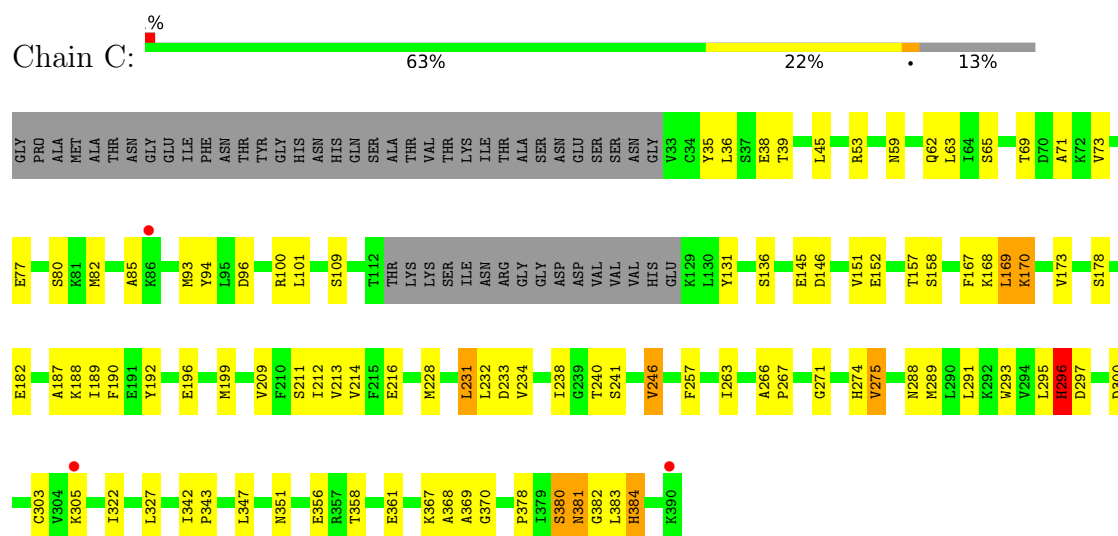
• Molecule 1: O-methyltransferase 1



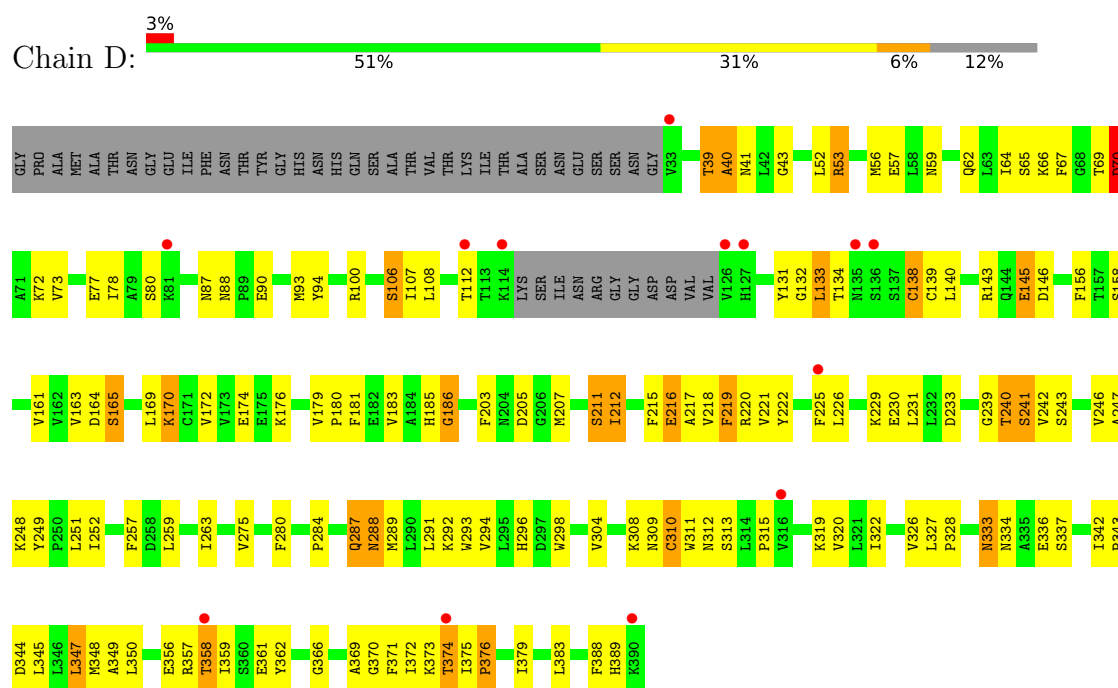
• Molecule 1: O-methyltransferase 1



• Molecule 1: O-methyltransferase 1



• Molecule 1: O-methyltransferase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	111.15Å 111.15Å 302.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	101.00 – 3.00 100.79 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (101.00-3.00) 100.0 (100.79-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.203 , 0.289 0.206 , 0.282	Depositor DCC
R_{free} test set	2123 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	94.8	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 85.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10191	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SAH, 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	1.13	1/2613 (0.0%)	1.58	9/3551 (0.3%)
1	B	1.17	0/2639	1.54	1/3581 (0.0%)
1	C	1.17	0/2511	1.60	5/3420 (0.1%)
1	D	1.20	1/2554 (0.0%)	1.55	6/3480 (0.2%)
All	All	1.17	2/10317 (0.0%)	1.57	21/14032 (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	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	376	PRO	C-O	-5.72	1.17	1.23
1	A	288	ASN	C-O	5.13	1.30	1.23

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	THR	CA-CB-OG1	-7.17	98.85	109.60
1	D	376	PRO	CB-CA-C	-6.96	103.04	111.46
1	A	379	ILE	CA-C-O	-6.11	115.51	120.70
1	C	169	LEU	N-CA-C	-6.03	103.67	111.02
1	C	178	SER	CA-C-N	5.98	126.67	122.60
1	C	178	SER	C-N-CA	5.98	126.67	122.60
1	A	358	THR	CB-CA-C	5.81	120.78	109.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	376	PRO	N-CA-C	5.76	119.50	110.80
1	A	142	PRO	CA-C-N	5.69	129.18	120.82
1	A	142	PRO	C-N-CA	5.69	129.18	120.82
1	C	267	PRO	N-CA-C	5.67	119.58	111.13
1	D	358	THR	CA-C-O	-5.65	115.40	121.56
1	D	333	ASN	N-CA-C	-5.46	106.12	112.89
1	B	223	ASP	CA-CB-CG	5.44	118.04	112.60
1	D	347	LEU	N-CA-C	-5.40	105.29	111.07
1	A	216	GLU	CB-CA-C	5.31	119.31	110.81
1	A	263	ILE	N-CA-C	-5.30	105.33	110.42
1	A	104	ALA	CA-C-N	5.21	127.52	120.38
1	A	104	ALA	C-N-CA	5.21	127.52	120.38
1	C	240	THR	CB-CA-C	5.08	119.32	110.68
1	D	356	GLU	CB-CA-C	5.02	118.10	109.51

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	384	HIS	Peptide

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	2560	0	2486	82	0
1	B	2586	0	2449	53	0
1	C	2463	0	2319	54	0
1	D	2503	0	2294	88	0
2	A	26	0	19	2	0
2	B	26	0	19	1	0
3	D	27	0	22	3	0
All	All	10191	0	9608	265	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 13.

All (265) 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:378:PRO:HB3	1:C:384:HIS:NE2	1.92	0.83
1:D:292:LYS:NZ	3:D:401:SAM:OXT	2.11	0.82
1:A:199:MET:HE2	1:A:203:PHE:CZ	2.17	0.79
1:D:288:ASN:H	1:D:288:ASN:HD22	1.34	0.76
1:D:288:ASN:HD22	1:D:288:ASN:N	1.85	0.74
1:D:326:VAL:HG11	1:D:359:ILE:HG12	1.70	0.73
1:C:246:VAL:HG11	1:C:271:GLY:HA3	1.68	0.73
1:A:268:GLN:OE1	1:A:268:GLN:HA	1.91	0.71
1:A:100:ARG:NH2	1:D:327:LEU:HD21	2.07	0.70
1:D:374:THR:O	1:D:376:PRO:HD3	1.91	0.70
1:B:198:ARG:O	1:B:202:VAL:HG23	1.92	0.69
1:D:215:PHE:O	1:D:218:VAL:N	2.25	0.69
1:A:249:TYR:O	1:A:252:ILE:HG22	1.93	0.69
1:A:262:VAL:O	1:A:265:VAL:HG12	1.94	0.68
1:A:322:ILE:HB	1:A:386:ILE:HB	1.76	0.67
1:D:185:HIS:O	1:D:186:GLY:C	2.36	0.66
1:A:347:LEU:O	1:A:351:ASN:N	2.29	0.65
1:A:230:GLU:HG3	1:A:253:ARG:CG	2.26	0.65
1:A:62:GLN:HA	1:A:141:VAL:HG13	1.79	0.65
1:A:311:TRP:CE2	1:A:390:LYS:HD3	2.33	0.64
1:B:203:PHE:O	1:B:207:MET:HG3	1.98	0.64
1:B:285:LYS:HA	1:B:313:SER:O	1.98	0.64
1:A:199:MET:HE2	1:A:203:PHE:CE1	2.32	0.63
1:D:249:TYR:O	1:D:251:LEU:N	2.30	0.63
1:A:77:GLU:O	1:A:80:SER:CB	2.46	0.63
1:B:214:VAL:O	1:B:218:VAL:HG23	1.99	0.63
1:C:228:MET:HE3	1:C:288:ASN:HB2	1.81	0.63
1:C:367:LYS:O	1:C:369:ALA:N	2.32	0.63
1:D:288:ASN:H	1:D:288:ASN:ND2	1.96	0.63
1:A:223:ASP:O	1:A:225:PHE:N	2.31	0.62
1:D:293:TRP:O	3:D:401:SAM:HE3	2.00	0.61
1:D:242:VAL:O	1:D:243:SER:C	2.43	0.61
1:C:367:LYS:O	1:C:370:GLY:N	2.33	0.61
1:D:143:ARG:NH2	1:D:146:ASP:OD2	2.28	0.61
1:A:97:ARG:HA	1:A:100:ARG:HD3	1.81	0.61
1:D:64:ILE:CG2	1:D:133:LEU:HD12	2.31	0.60
1:A:64:ILE:CB	1:A:133:LEU:HD11	2.30	0.60
1:A:256:ASN:HB3	1:A:274:HIS:ND1	2.17	0.59
1:D:65:SER:C	1:D:67:PHE:H	2.09	0.59
1:C:234:VAL:HB	1:C:291:LEU:CD2	2.32	0.59
1:A:151:VAL:HG12	1:A:152:GLU:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:LYS:HA	1:D:131:TYR:O	2.03	0.59
1:C:228:MET:HE1	1:C:231:LEU:HD22	1.85	0.58
1:D:161:VAL:O	1:D:165:SER:OG	2.21	0.58
1:D:179:VAL:O	1:D:180:PRO:C	2.45	0.58
1:C:263:ILE:HG23	1:C:274:HIS:HB3	1.86	0.58
1:D:225:PHE:HB2	1:D:249:TYR:CE2	2.39	0.58
1:D:52:LEU:HG	1:D:56:MET:HE2	1.86	0.57
1:D:345:LEU:O	1:D:348:MET:N	2.36	0.57
1:C:342:ILE:HB	1:C:343:PRO:HD3	1.87	0.57
1:D:326:VAL:HG11	1:D:359:ILE:CG1	2.34	0.57
1:A:230:GLU:OE1	1:A:286:GLY:HA2	2.05	0.56
1:B:82:MET:HE1	1:B:95:LEU:CD1	2.35	0.56
1:D:53:ARG:NH1	1:D:158:SER:O	2.38	0.56
1:A:159:ASP:OD1	1:A:198:ARG:NH2	2.38	0.56
1:D:225:PHE:HB2	1:D:249:TYR:CZ	2.40	0.56
1:B:228:MET:HE1	1:B:231:LEU:HD22	1.87	0.56
1:D:311:TRP:C	1:D:313:SER:H	2.13	0.55
1:B:305:LYS:O	1:B:306:LEU:C	2.49	0.55
1:C:192:TYR:CZ	1:C:196:GLU:HG3	2.41	0.55
1:D:294:VAL:O	1:D:298:TRP:HD1	1.90	0.55
1:A:254:GLY:N	1:A:271:GLY:O	2.38	0.54
1:A:94:TYR:O	1:A:97:ARG:HB2	2.07	0.54
1:D:212:ILE:O	1:D:216:GLU:HG3	2.07	0.54
1:C:378:PRO:HB3	1:C:384:HIS:CD2	2.43	0.54
1:C:77:GLU:O	1:C:80:SER:HB3	2.08	0.54
1:B:156:PHE:HE1	1:B:203:PHE:CZ	2.26	0.53
1:A:228:MET:HE3	1:A:252:ILE:HD11	1.90	0.53
1:B:77:GLU:O	1:B:80:SER:CB	2.56	0.53
1:C:380:SER:O	1:C:381:ASN:C	2.52	0.53
1:C:96:ASP:O	1:C:100:ARG:HB2	2.10	0.52
1:B:227:ASP:OD1	1:B:227:ASP:N	2.38	0.52
1:D:90:GLU:HB3	1:D:94:TYR:CD2	2.44	0.52
1:D:229:LYS:O	1:D:252:ILE:HA	2.10	0.52
1:A:69:THR:O	1:A:70:ASP:C	2.53	0.52
1:A:159:ASP:O	1:A:162:VAL:HG12	2.10	0.52
1:A:246:VAL:HG22	1:A:252:ILE:HG23	1.92	0.52
1:A:342:ILE:HB	1:A:343:PRO:HD3	1.91	0.52
1:D:64:ILE:HG21	1:D:133:LEU:HD12	1.91	0.52
1:A:59:ASN:O	1:A:60:VAL:C	2.53	0.51
1:B:35:TYR:O	1:B:39:THR:HG23	2.10	0.51
1:C:59:ASN:O	1:C:63:LEU:HD13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:VAL:O	1:A:265:VAL:HG22	2.10	0.51
1:B:82:MET:HE1	1:B:95:LEU:HD11	1.92	0.51
1:A:311:TRP:CE2	1:A:390:LYS:CD	2.93	0.51
1:B:179:VAL:HG23	1:B:352:PRO:CD	2.40	0.51
1:C:212:ILE:O	1:C:216:GLU:HG3	2.09	0.51
1:D:358:THR:HG23	1:D:361:GLU:H	1.76	0.51
1:D:39:THR:O	1:D:41:ASN:N	2.44	0.51
1:A:345:LEU:HD12	1:A:348:MET:CE	2.41	0.51
1:A:163:VAL:O	1:A:166:PHE:HB2	2.11	0.50
1:A:279:MET:HE3	1:A:306:LEU:HD22	1.93	0.50
1:B:228:MET:HE1	1:B:231:LEU:HD13	1.93	0.50
1:D:77:GLU:O	1:D:80:SER:OG	2.15	0.50
1:D:342:ILE:HB	1:D:343:PRO:CD	2.42	0.50
1:B:78:ILE:HG22	1:B:82:MET:HE3	1.93	0.50
1:B:256:ASN:HD22	1:B:274:HIS:CE1	2.29	0.50
1:B:342:ILE:N	1:B:343:PRO:HD2	2.27	0.50
1:D:288:ASN:N	1:D:288:ASN:ND2	2.53	0.50
1:A:225:PHE:HB2	1:A:249:TYR:CE2	2.47	0.50
1:A:262:VAL:O	1:A:265:VAL:CG1	2.60	0.50
1:D:39:THR:C	1:D:41:ASN:H	2.20	0.50
1:D:373:LYS:CB	1:D:389:HIS:HB2	2.41	0.50
1:B:160:LYS:HA	1:C:167:PHE:CZ	2.47	0.49
1:D:280:PHE:O	1:D:309:ASN:ND2	2.45	0.49
1:C:59:ASN:ND2	1:C:62:GLN:HB3	2.27	0.49
1:D:145:GLU:CD	1:D:145:GLU:H	2.20	0.49
1:D:225:PHE:CB	1:D:249:TYR:CE2	2.95	0.49
1:D:289:MET:SD	1:D:310:CYS:SG	2.92	0.49
1:D:248:LYS:C	1:D:249:TYR:CD1	2.90	0.49
1:B:334:ASN:OD1	1:B:334:ASN:N	2.42	0.49
1:A:148:VAL:HG13	1:A:209:VAL:HG22	1.94	0.49
1:B:254:GLY:O	1:B:272:VAL:HA	2.13	0.49
1:D:169:LEU:O	1:D:170:LYS:C	2.55	0.49
1:C:182:GLU:HG2	1:C:187:ALA:O	2.12	0.48
1:C:234:VAL:HB	1:C:291:LEU:HD23	1.95	0.48
1:A:48:ILE:HB	1:A:49:PRO:HD3	1.95	0.48
1:A:263:ILE:O	1:A:265:VAL:N	2.46	0.48
1:B:94:TYR:O	1:B:97:ARG:N	2.44	0.48
1:A:44:LYS:O	1:A:48:ILE:HG12	2.13	0.48
1:A:64:ILE:CB	1:A:133:LEU:CD1	2.91	0.48
1:B:49:PRO:HG3	1:C:45:LEU:O	2.13	0.48
1:C:297:ASP:OD1	1:C:351:ASN:ND2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:ILE:HG22	1:D:133:LEU:HD12	1.94	0.48
1:A:236:GLY:HA3	1:A:256:ASN:ND2	2.28	0.48
1:B:188:LYS:HB2	1:B:191:GLU:HG3	1.94	0.48
1:D:311:TRP:O	1:D:313:SER:N	2.47	0.48
1:D:371:PHE:CD2	1:D:388:PHE:HB3	2.49	0.48
1:A:222:TYR:CE2	1:A:224:GLY:HA3	2.49	0.48
1:B:341:LEU:HB3	1:C:101:LEU:HD13	1.96	0.48
1:C:146:ASP:OD1	1:C:146:ASP:N	2.47	0.47
1:A:238:ILE:O	1:A:269:TYR:HE2	1.96	0.47
1:D:180:PRO:HG2	1:D:349:ALA:HA	1.94	0.47
1:C:214:VAL:HG13	1:C:383:LEU:HD21	1.95	0.47
1:B:65:SER:O	1:B:68:GLY:N	2.44	0.47
1:B:134:THR:O	1:B:135:ASN:C	2.56	0.47
1:B:246:VAL:HG11	1:B:271:GLY:HA3	1.96	0.47
1:D:211:SER:O	1:D:212:ILE:C	2.57	0.47
1:C:59:ASN:HD21	1:C:62:GLN:CB	2.28	0.47
1:D:371:PHE:HD2	1:D:388:PHE:C	2.22	0.47
1:A:168:LYS:HE3	1:A:183:VAL:HG12	1.96	0.47
1:A:257:PHE:HA	1:A:275:VAL:O	2.15	0.47
1:B:331:LEU:HD22	1:B:341:LEU:HD11	1.95	0.47
1:D:138:CYS:C	1:D:140:LEU:H	2.23	0.47
1:D:239:GLY:O	1:D:241:SER:N	2.48	0.47
1:A:340:ALA:C	1:A:343:PRO:HD2	2.40	0.47
1:B:149:SER:O	1:B:209:VAL:HG11	2.15	0.47
1:D:215:PHE:O	1:D:217:ALA:N	2.48	0.47
1:A:267:PRO:HG2	1:A:269:TYR:CZ	2.50	0.46
1:B:215:PHE:O	1:B:218:VAL:N	2.48	0.46
1:D:231:LEU:HA	1:D:288:ASN:O	2.15	0.46
1:A:65:SER:C	1:A:67:PHE:H	2.23	0.46
1:A:253:ARG:NH2	1:A:273:GLU:OE1	2.49	0.46
1:A:159:ASP:O	1:A:162:VAL:CG1	2.64	0.46
1:D:156:PHE:HE1	1:D:203:PHE:CZ	2.33	0.46
1:B:326:VAL:HG11	1:B:359:ILE:HG13	1.96	0.46
1:C:188:LYS:O	1:C:189:ILE:C	2.59	0.46
1:D:308:LYS:CE	1:D:369:ALA:HA	2.46	0.46
1:A:259:LEU:HD21	2:A:401:SAH:C6	2.46	0.46
1:B:331:LEU:HD13	1:C:100:ARG:HG2	1.96	0.46
1:A:154:LEU:C	1:A:156:PHE:N	2.72	0.46
1:A:222:TYR:CZ	1:A:224:GLY:HA3	2.51	0.46
1:C:380:SER:O	1:C:382:GLY:N	2.49	0.46
1:C:257:PHE:HA	1:C:275:VAL:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:PHE:HD1	1:A:275:VAL:O	1.99	0.45
1:A:263:ILE:C	1:A:265:VAL:H	2.24	0.45
1:C:93:MET:HG3	1:C:94:TYR:N	2.30	0.45
1:C:358:THR:HG23	1:C:361:GLU:H	1.80	0.45
1:A:97:ARG:NH2	1:D:344:ASP:OD1	2.49	0.45
1:B:95:LEU:O	1:B:99:LEU:HG	2.17	0.45
1:B:292:LYS:O	2:B:401:SAH:N	2.49	0.45
1:A:35:TYR:O	1:A:39:THR:HB	2.16	0.45
1:D:240:THR:O	1:D:241:SER:C	2.60	0.45
1:A:151:VAL:O	1:A:152:GLU:C	2.59	0.45
1:C:295:LEU:C	1:C:297:ASP:H	2.25	0.45
1:A:292:LYS:HB3	2:A:401:SAH:HN2	1.82	0.45
1:A:362:TYR:HA	1:A:365:LEU:HD12	1.99	0.45
1:B:232:LEU:HD23	1:B:289:MET:HG2	1.98	0.45
1:C:53:ARG:NH1	1:C:158:SER:OG	2.49	0.45
1:D:56:MET:O	1:D:59:ASN:N	2.36	0.44
1:D:181:PHE:CD1	1:D:181:PHE:C	2.95	0.44
1:B:362:TYR:O	1:B:365:LEU:HB2	2.16	0.44
1:A:84:ASN:CB	1:D:174:GLU:OE2	2.66	0.44
1:A:182:GLU:O	1:A:185:HIS:O	2.35	0.44
1:D:145:GLU:CD	1:D:145:GLU:N	2.76	0.44
1:B:38:GLU:CD	1:B:41:ASN:HD22	2.26	0.44
1:C:228:MET:HE3	1:C:288:ASN:CB	2.47	0.44
1:A:279:MET:HG3	1:A:306:LEU:HD13	1.99	0.44
1:B:232:LEU:O	1:B:289:MET:HA	2.18	0.44
1:D:53:ARG:HA	1:D:56:MET:HE3	1.99	0.43
1:D:108:LEU:HD23	1:D:132:GLY:O	2.17	0.43
1:D:163:VAL:O	1:D:164:ASP:C	2.61	0.43
1:D:257:PHE:HA	1:D:275:VAL:O	2.18	0.43
1:D:233:ASP:HB2	1:D:242:VAL:CG1	2.47	0.43
1:B:286:GLY:O	1:B:315:PRO:HD3	2.19	0.43
1:D:259:LEU:HD21	3:D:401:SAM:C6	2.48	0.43
1:B:48:ILE:HG22	1:C:45:LEU:HD13	2.00	0.43
1:A:344:ASP:OD2	1:D:100:ARG:NH2	2.51	0.43
1:C:238:ILE:HA	1:C:266:ALA:HB2	2.01	0.43
1:D:366:GLY:HA2	1:D:388:PHE:CD2	2.54	0.43
1:D:219:PHE:O	1:D:220:ARG:C	2.62	0.43
1:A:99:LEU:O	1:A:100:ARG:C	2.62	0.43
1:A:159:ASP:CG	1:A:198:ARG:HH22	2.27	0.43
1:A:331:LEU:HD22	1:A:341:LEU:HD11	2.01	0.43
1:C:169:LEU:O	1:C:170:LYS:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:MET:O	1:D:57:GLU:C	2.62	0.43
1:D:65:SER:O	1:D:67:PHE:N	2.48	0.43
1:B:38:GLU:CD	1:C:136:SER:HA	2.44	0.43
1:B:285:LYS:HE3	1:B:285:LYS:HB3	1.81	0.43
1:C:295:LEU:O	1:C:297:ASP:N	2.51	0.43
1:B:108:LEU:HD12	1:B:108:LEU:HA	1.86	0.42
1:C:73:VAL:CG1	1:C:77:GLU:CB	2.96	0.42
1:C:295:LEU:HD12	1:C:322:ILE:CG2	2.48	0.42
1:B:343:PRO:O	1:B:346:LEU:HB2	2.19	0.42
1:C:233:ASP:OD2	1:C:241:SER:OG	2.35	0.42
1:C:296:HIS:ND1	1:C:356:GLU:OE2	2.52	0.42
1:A:339:ASN:CG	1:D:40:ALA:HB2	2.44	0.42
1:B:153:GLU:O	1:B:156:PHE:HB3	2.19	0.42
1:B:179:VAL:HG13	1:B:182:GLU:HB2	2.00	0.42
1:D:106:SER:C	1:D:108:LEU:H	2.27	0.42
1:D:211:SER:OG	1:D:292:LYS:NZ	2.27	0.42
1:A:179:VAL:O	1:A:180:PRO:C	2.62	0.42
1:A:154:LEU:C	1:A:156:PHE:H	2.28	0.42
1:A:230:GLU:OE2	1:A:253:ARG:NH1	2.50	0.42
1:D:328:PRO:HG2	1:D:336:GLU:HG3	2.02	0.42
1:C:232:LEU:HD23	1:C:289:MET:HE2	2.02	0.42
1:C:300:ASP:HA	1:C:303:CYS:HB2	2.02	0.42
1:A:292:LYS:HG3	1:A:323:ILE:HB	2.01	0.42
1:D:319:LYS:HD3	1:D:389:HIS:CE1	2.55	0.42
1:B:257:PHE:CE2	1:B:284:PRO:HD2	2.55	0.41
1:D:343:PRO:O	1:D:347:LEU:HG	2.20	0.41
1:A:48:ILE:HB	1:A:49:PRO:CD	2.50	0.41
1:A:59:ASN:O	1:A:61:PHE:N	2.53	0.41
1:A:358:THR:HG22	1:A:361:GLU:HG3	2.01	0.41
1:A:58:LEU:HB3	1:A:82:MET:HE2	2.02	0.41
1:B:66:LYS:C	1:B:68:GLY:H	2.27	0.41
1:C:35:TYR:O	1:C:39:THR:HG23	2.21	0.41
1:D:69:THR:O	1:D:70:ASP:C	2.64	0.41
1:D:287:GLN:HA	1:D:315:PRO:CG	2.51	0.41
1:D:357:ARG:HD2	1:D:362:TYR:CE1	2.55	0.41
1:A:230:GLU:HG3	1:A:253:ARG:HG3	2.00	0.41
1:B:286:GLY:O	1:B:314:LEU:HD12	2.20	0.41
1:D:106:SER:C	1:D:108:LEU:N	2.79	0.41
1:A:83:PRO:C	1:A:85:ALA:H	2.28	0.41
1:A:211:SER:O	1:A:212:ILE:C	2.63	0.41
1:C:109:SER:O	1:C:131:TYR:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:VAL:O	1:C:152:GLU:C	2.63	0.41
1:A:97:ARG:HE	1:D:344:ASP:CG	2.29	0.41
1:A:347:LEU:O	1:A:351:ASN:C	2.64	0.41
1:A:371:PHE:CG	1:A:388:PHE:HB3	2.56	0.41
1:B:379:ILE:N	1:B:383:LEU:O	2.50	0.41
1:C:347:LEU:O	1:C:351:ASN:C	2.64	0.41
1:D:156:PHE:HE1	1:D:203:PHE:CE1	2.39	0.41
1:D:379:ILE:HB	1:D:383:LEU:O	2.21	0.41
1:D:88:ASN:OD1	1:D:88:ASN:C	2.64	0.41
1:B:209:VAL:O	1:B:212:ILE:HB	2.20	0.40
1:C:82:MET:HB2	1:C:85:ALA:HB3	2.04	0.40
1:C:168:LYS:O	1:C:169:LEU:C	2.63	0.40
1:D:230:GLU:O	1:D:288:ASN:ND2	2.54	0.40
1:B:365:LEU:HD23	1:B:365:LEU:HA	1.92	0.40
1:A:231:LEU:HB2	1:A:252:ILE:HD11	2.03	0.40
1:C:274:HIS:C	1:C:275:VAL:HG23	2.47	0.40
1:B:179:VAL:HG23	1:B:352:PRO:HD3	2.03	0.40
1:C:69:THR:C	1:C:71:ALA:N	2.77	0.40
1:D:39:THR:O	1:D:43:GLY:N	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	338/393 (86%)	288 (85%)	35 (10%)	15 (4%)	2	12
1	B	345/393 (88%)	299 (87%)	39 (11%)	7 (2%)	6	28
1	C	338/393 (86%)	286 (85%)	44 (13%)	8 (2%)	4	24
1	D	343/393 (87%)	248 (72%)	63 (18%)	32 (9%)	0	2
All	All	1364/1572 (87%)	1121 (82%)	181 (13%)	62 (4%)	2	12

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	VAL
1	A	110	VAL
1	A	224	GLY
1	B	91	ALA
1	C	170	LYS
1	C	190	PHE
1	C	368	ALA
1	D	170	LYS
1	D	176	LYS
1	D	219	PHE
1	D	221	VAL
1	D	240	THR
1	D	312	ASN
1	A	70	ASP
1	A	155	LEU
1	B	60	VAL
1	B	284	PRO
1	C	381	ASN
1	D	66	LYS
1	D	139	CYS
1	D	186	GLY
1	D	207	MET
1	D	216	GLU
1	D	241	SER
1	D	247	ALA
1	D	287	GLN
1	D	334	ASN
1	D	372	ILE
1	D	374	THR
1	A	59	ASN
1	A	91	ALA
1	A	106	SER
1	A	208	ALA
1	A	264	SER
1	B	70	ASP
1	B	135	ASN
1	C	145	GLU
1	D	40	ALA
1	D	222	TYR
1	D	284	PRO
1	A	66	LYS
1	A	72	LYS

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Mol	Chain	Res	Type
1	B	371	PHE
1	C	293	TRP
1	C	296	HIS
1	D	70	ASP
1	D	87	ASN
1	D	370	GLY
1	D	39	THR
1	D	107	ILE
1	D	375	ILE
1	A	89	PRO
1	A	100	ARG
1	A	151	VAL
1	B	224	GLY
1	D	106	SER
1	D	205	ASP
1	D	212	ILE
1	C	275	VAL
1	D	304	VAL
1	D	246	VAL
1	D	320	VAL

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	261/333 (78%)	229 (88%)	32 (12%)	4	21
1	B	255/333 (77%)	218 (86%)	37 (14%)	3	15
1	C	238/333 (72%)	223 (94%)	15 (6%)	16	48
1	D	237/333 (71%)	212 (90%)	25 (10%)	6	27
All	All	991/1332 (74%)	882 (89%)	109 (11%)	6	25

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	THR

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Mol	Chain	Res	Type
1	A	46	ILE
1	A	63	LEU
1	A	70	ASP
1	A	77	GLU
1	A	89	PRO
1	A	95	LEU
1	A	101	LEU
1	A	107	ILE
1	A	112	THR
1	A	134	THR
1	A	138	CYS
1	A	155	LEU
1	A	157	THR
1	A	165	SER
1	A	169	LEU
1	A	172	VAL
1	A	178	SER
1	A	191	GLU
1	A	195	THR
1	A	209	VAL
1	A	213	VAL
1	A	223	ASP
1	A	226	LEU
1	A	240	THR
1	A	241	SER
1	A	242	VAL
1	A	282	GLU
1	A	304	VAL
1	A	336	GLU
1	A	358	THR
1	A	390	LYS
1	B	52	LEU
1	B	53	ARG
1	B	64	ILE
1	B	70	ASP
1	B	74	SER
1	B	76	SER
1	B	101	LEU
1	B	107	ILE
1	B	108	LEU
1	B	113	THR
1	B	117	ILE

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Mol	Chain	Res	Type
1	B	127	HIS
1	B	133	LEU
1	B	138	CYS
1	B	144	GLN
1	B	146	ASP
1	B	151	VAL
1	B	160	LYS
1	B	162	VAL
1	B	168	LYS
1	B	172	VAL
1	B	198	ARG
1	B	207	MET
1	B	227	ASP
1	B	238	ILE
1	B	240	THR
1	B	246	VAL
1	B	260	PRO
1	B	281	GLU
1	B	285	LYS
1	B	316	VAL
1	B	320	VAL
1	B	329	ASN
1	B	336	GLU
1	B	359	ILE
1	B	363	ASP
1	B	372	ILE
1	C	36	LEU
1	C	38	GLU
1	C	65	SER
1	C	157	THR
1	C	173	VAL
1	C	199	MET
1	C	209	VAL
1	C	211	SER
1	C	213	VAL
1	C	231	LEU
1	C	246	VAL
1	C	296	HIS
1	C	305	LYS
1	C	327	LEU
1	C	380	SER
1	D	53	ARG

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Mol	Chain	Res	Type
1	D	62	GLN
1	D	70	ASP
1	D	73	VAL
1	D	78	ILE
1	D	93	MET
1	D	112	THR
1	D	133	LEU
1	D	134	THR
1	D	138	CYS
1	D	145	GLU
1	D	165	SER
1	D	172	VAL
1	D	183	VAL
1	D	211	SER
1	D	226	LEU
1	D	263	ILE
1	D	288	ASN
1	D	291	LEU
1	D	296	HIS
1	D	310	CYS
1	D	322	ILE
1	D	333	ASN
1	D	337	SER
1	D	350	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	381	ASN
1	B	41	ASN
1	B	201	GLN
1	B	256	ASN
1	C	333	ASN
1	D	84	ASN
1	D	256	ASN
1	D	268	GLN
1	D	288	ASN

5.3.3 RNA ⓘ

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](#)

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	B	401	-	27,28,28	1.85	8 (29%)	36,40,40	1.89	15 (41%)
2	SAH	A	401	-	27,28,28	2.01	7 (25%)	36,40,40	2.43	14 (38%)
3	SAM	D	401	-	27,29,29	0.54	1 (3%)	34,42,42	0.71	1 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAH	B	401	-	-	5/15/31/31	0/3/3/3
2	SAH	A	401	-	-	5/15/31/31	0/3/3/3
3	SAM	D	401	-	-	0/17/33/33	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	SAH	C5-N7	-4.95	1.30	1.39
2	A	401	SAH	C5-C4	4.33	1.46	1.39
2	B	401	SAH	C5-C4	4.20	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	SAH	O-C	4.11	1.34	1.22
2	B	401	SAH	C4-N9	-3.90	1.29	1.37
2	B	401	SAH	O-C	3.85	1.33	1.22
2	B	401	SAH	C5-N7	-3.42	1.32	1.39
2	A	401	SAH	C8-N9	-3.29	1.31	1.37
2	B	401	SAH	OXT-C	-2.89	1.21	1.30
2	A	401	SAH	OXT-C	-2.78	1.21	1.30
2	A	401	SAH	C4-N9	-2.47	1.32	1.37
2	B	401	SAH	C8-N7	2.37	1.36	1.31
2	A	401	SAH	C8-N7	2.17	1.35	1.31
2	B	401	SAH	C8-N9	-2.10	1.34	1.37
2	B	401	SAH	C5-C6	2.04	1.46	1.41
3	D	401	SAM	OXT-C	-2.03	1.24	1.30

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	SAH	C5'-SD-CG	6.47	121.46	102.26
2	A	401	SAH	C5-C4-N3	-4.74	120.19	126.72
2	A	401	SAH	OXT-C-O	-4.45	113.97	124.08
2	A	401	SAH	CB-CA-C	4.26	121.72	110.45
2	A	401	SAH	C4-C5-N7	-4.06	105.94	110.58
2	B	401	SAH	C4-N9-C8	3.54	109.45	105.74
2	A	401	SAH	N3-C4-N9	3.53	133.17	127.17
2	A	401	SAH	O4'-C1'-N9	3.48	114.78	108.09
2	B	401	SAH	C5-C4-N3	-3.41	122.02	126.72
2	A	401	SAH	C5-N7-C8	3.24	108.54	103.45
2	B	401	SAH	C5'-SD-CG	3.14	111.57	102.26
2	B	401	SAH	C4-N9-C1'	-3.02	119.56	126.63
2	B	401	SAH	C4-C5-N7	-2.87	107.30	110.58
2	A	401	SAH	O4'-C4'-C5'	-2.85	101.50	108.83
2	B	401	SAH	N3-C2-N1	-2.79	124.35	128.58
2	B	401	SAH	N3-C4-N9	2.72	131.79	127.17
2	A	401	SAH	N3-C2-N1	-2.71	124.47	128.58
2	A	401	SAH	C2-N1-C6	2.67	123.11	118.73
2	B	401	SAH	CB-CG-SD	-2.62	107.60	113.45
2	B	401	SAH	C2-N3-C4	2.35	117.57	111.83
2	B	401	SAH	O4'-C4'-C5'	-2.34	102.80	108.83
2	B	401	SAH	OXT-C-O	-2.32	118.82	124.08
2	A	401	SAH	C2-N3-C4	2.32	117.50	111.83
2	B	401	SAH	N9-C8-N7	-2.32	110.65	113.94
2	B	401	SAH	C2-N1-C6	2.30	122.50	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	SAH	CB-CA-N	2.29	116.09	110.12
3	D	401	SAM	O4'-C1'-C2'	-2.18	101.96	106.62
2	A	401	SAH	N9-C8-N7	-2.15	110.88	113.94
2	A	401	SAH	C4-N9-C8	2.12	107.97	105.74
2	B	401	SAH	C6-C5-N7	2.08	136.10	132.09

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	SAH	C-CA-CB-CG
2	A	401	SAH	C4'-C5'-SD-CG
2	A	401	SAH	O4'-C4'-C5'-SD
2	A	401	SAH	C3'-C4'-C5'-SD
2	B	401	SAH	N-CA-CB-CG
2	B	401	SAH	C-CA-CB-CG
2	A	401	SAH	CA-CB-CG-SD
2	B	401	SAH	O-C-CA-CB
2	B	401	SAH	OXT-C-CA-CB
2	B	401	SAH	CB-CG-SD-C5'

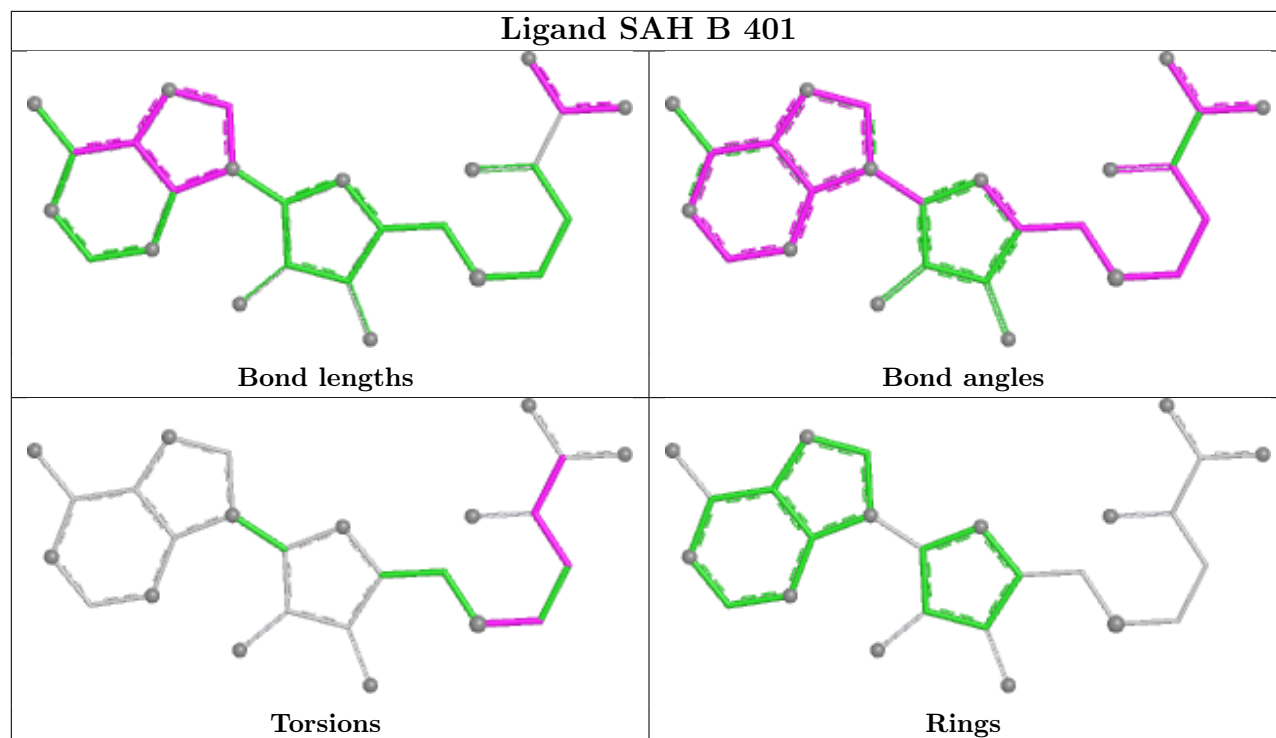
There are no ring outliers.

3 monomers are involved in 6 short contacts:

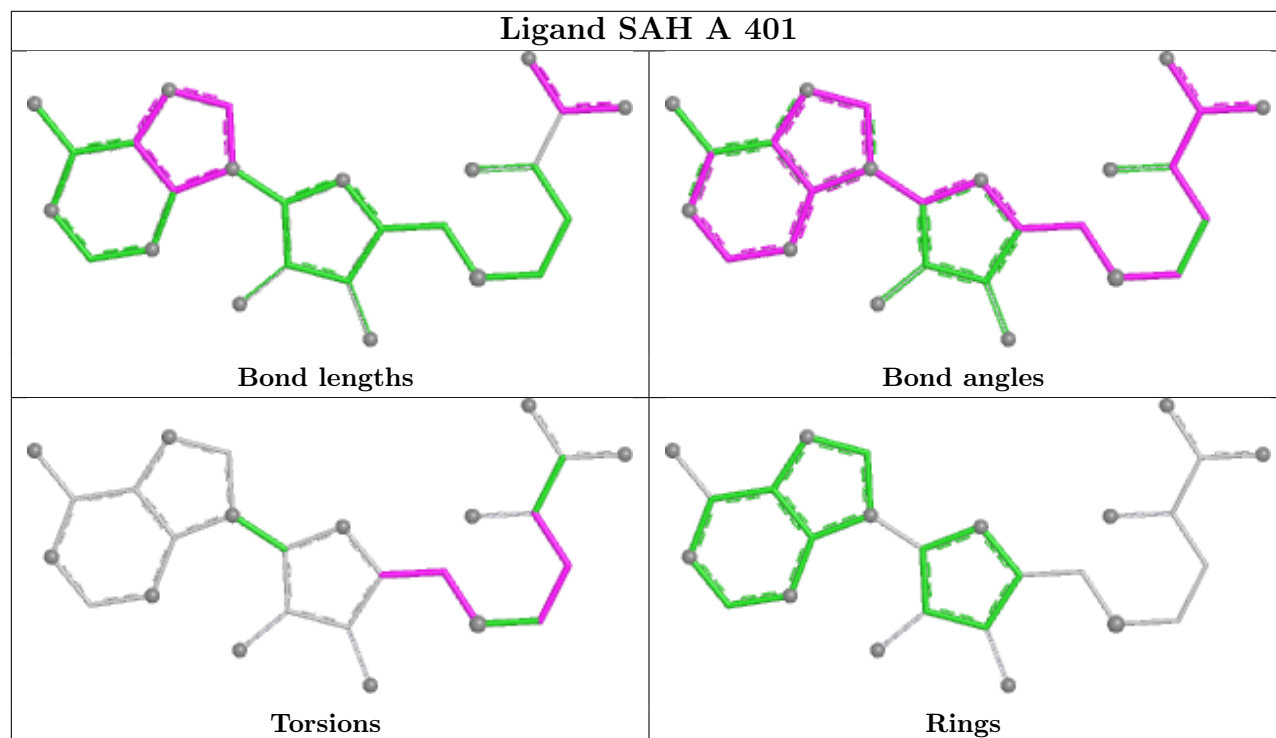
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	SAH	1	0
2	A	401	SAH	2	0
3	D	401	SAM	3	0

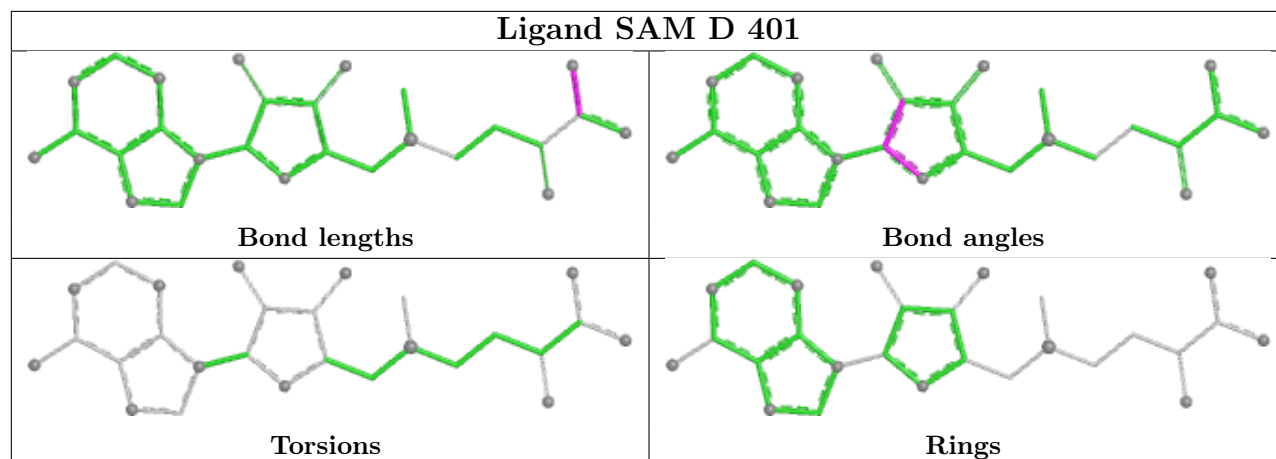
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

Ligand SAH B 401



Ligand SAH A 401





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	342/393 (87%)	-0.32	3 (0%)	81 61	40, 73, 104, 126	26 (7%)
1	B	349/393 (88%)	-0.19	5 (1%)	73 51	46, 85, 121, 148	27 (7%)
1	C	342/393 (87%)	-0.20	3 (0%)	81 61	52, 86, 116, 157	25 (7%)
1	D	347/393 (88%)	0.05	13 (3%)	45 25	41, 86, 122, 139	43 (12%)
All	All	1380/1572 (87%)	-0.16	24 (1%)	69 45	40, 83, 118, 157	121 (8%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	126	VAL	8.2
1	D	33	VAL	6.5
1	A	33	VAL	5.4
1	D	112	THR	5.4
1	D	114	LYS	5.1
1	B	86	LYS	4.8
1	B	118	ASN	4.4
1	C	86	LYS	4.3
1	D	136	SER	3.3
1	D	127	HIS	3.0
1	D	225	PHE	2.9
1	A	129	LYS	2.7
1	C	305	LYS	2.5
1	D	316	VAL	2.5
1	B	117	ILE	2.4
1	A	67	PHE	2.4
1	D	358	THR	2.3
1	B	115	LYS	2.2
1	D	135	ASN	2.2
1	D	81	LYS	2.1
1	D	390	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	374	THR	2.1
1	C	390	LYS	2.0
1	B	116	SER	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](#)

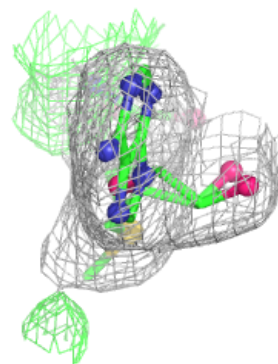
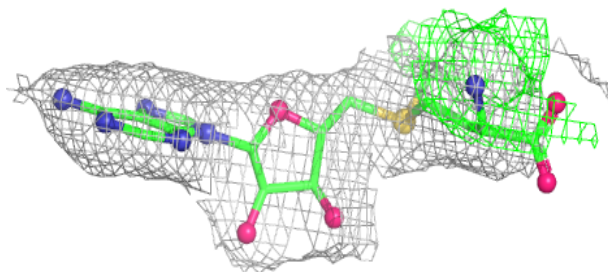
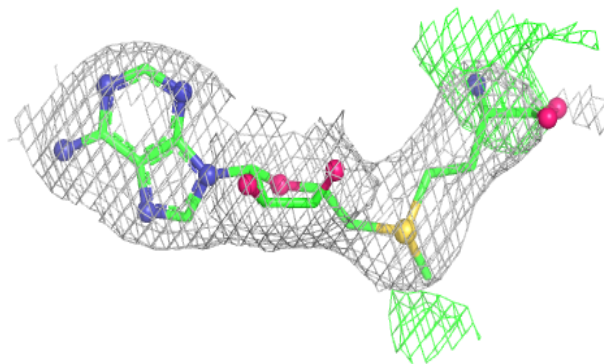
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SAM	D	401	27/27	0.90	0.14	53,62,90,93	5
2	SAH	B	401	26/26	0.94	0.08	70,81,89,92	0
2	SAH	A	401	26/26	0.94	0.08	58,64,82,106	0

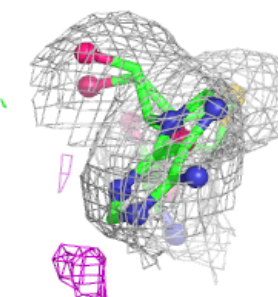
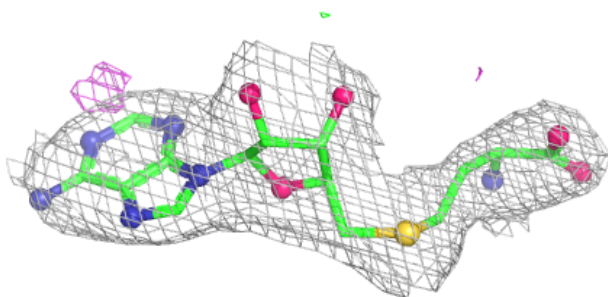
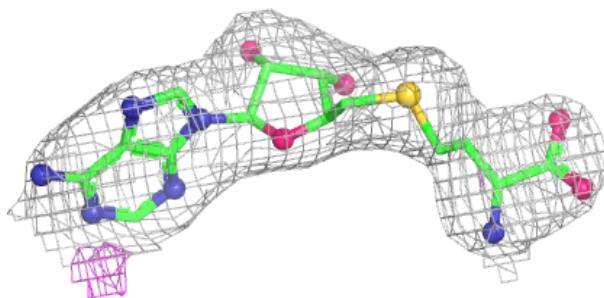
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

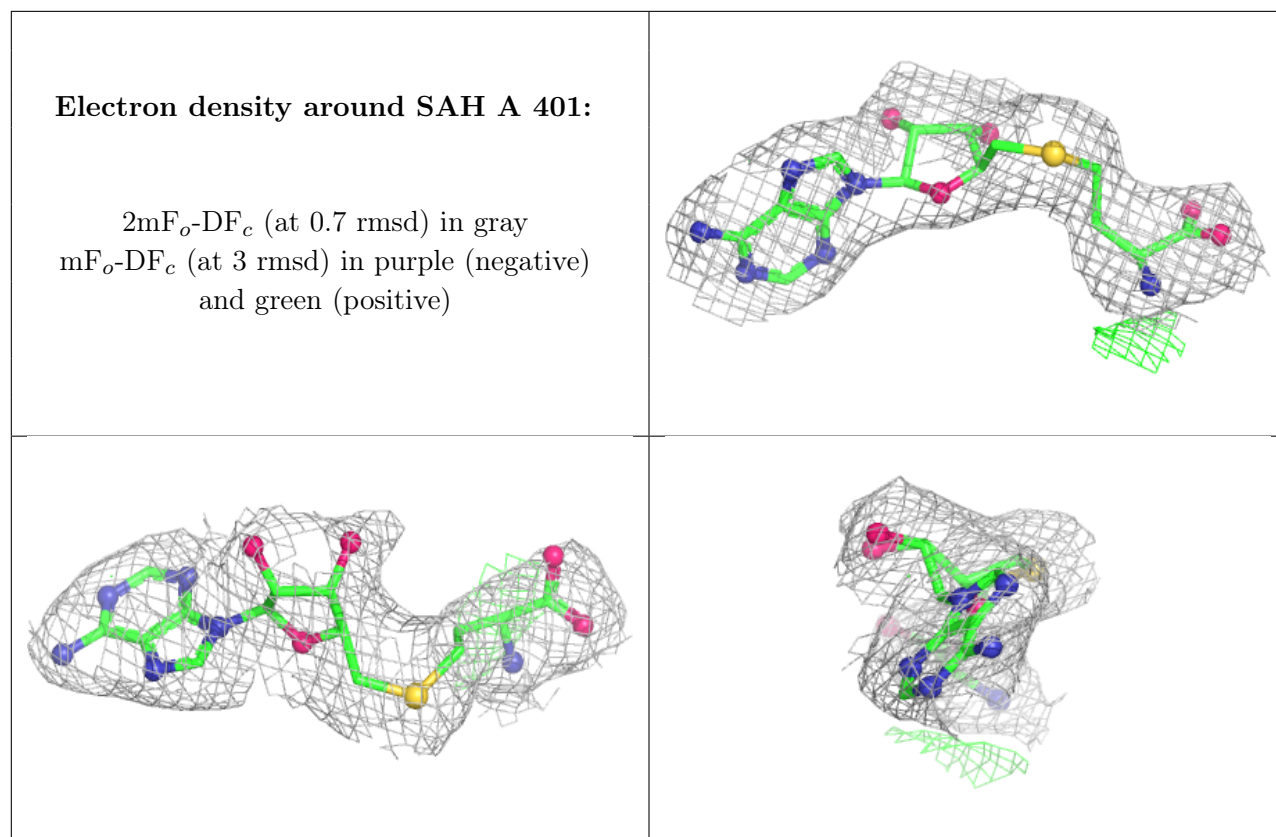
Electron density around SAM D 401:

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

**Electron density around SAH B 401:**

$2mF_o-DF_c$ (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.