



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:40 PM UTC

PDB ID : 7WDQ / pdb_00007wdq
Title : DsyB in complex with SAM
Authors : Li, C.Y.
Deposited on : 2021-12-22
Resolution : 2.35 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

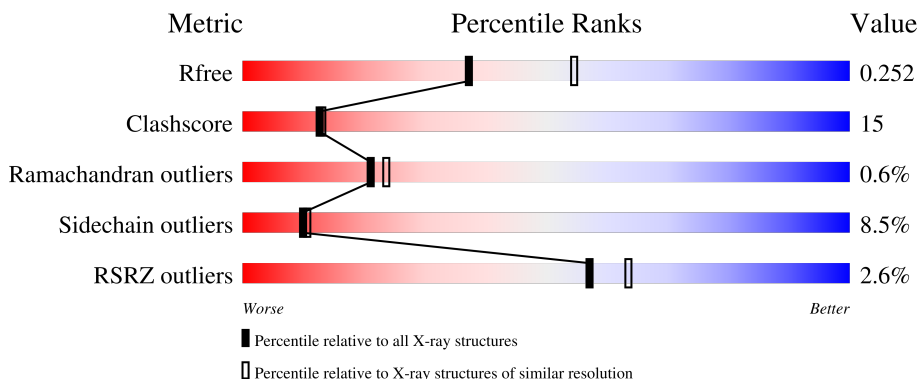
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	337	 81% 16% .
1	B	337	 77% 19% .
1	C	337	 9% 57% 34% 9% .
1	D	337	 % 69% 21% . 6%

2 Entry composition [i](#)

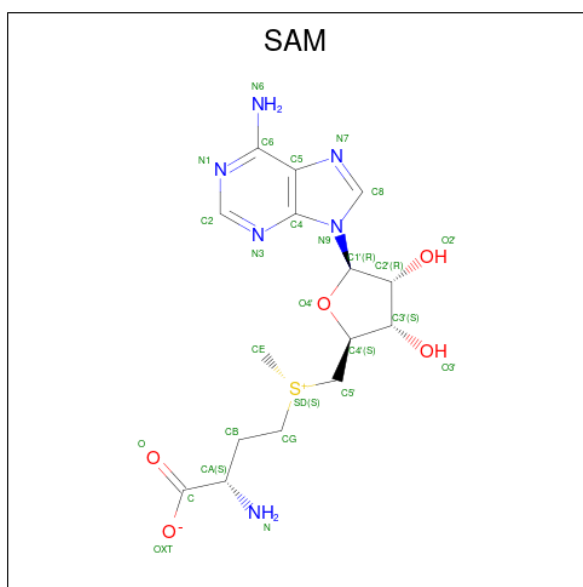
There are 3 unique types of molecules in this entry. The entry contains 10316 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 SAM-dependent MTHB methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	1	0
			2545	1618	427	491	9			
1	B	336	Total	C	N	O	S	0	0	0
			2539	1615	426	489	9			
1	C	335	Total	C	N	O	S	0	0	0
			2529	1610	425	485	9			
1	D	316	Total	C	N	O	S	0	0	0
			2375	1512	403	451	9			

- Molecule 2 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: $C_{15}H_{22}N_6O_5S$) (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		

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

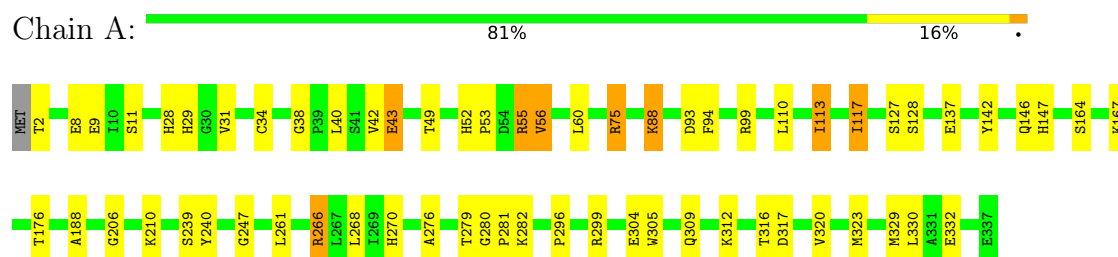
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	87	Total	O	0	0
			87	87		
3	B	88	Total	O	0	0
			88	88		
3	C	30	Total	O	0	0
			30	30		
3	D	42	Total	O	0	0
			42	42		

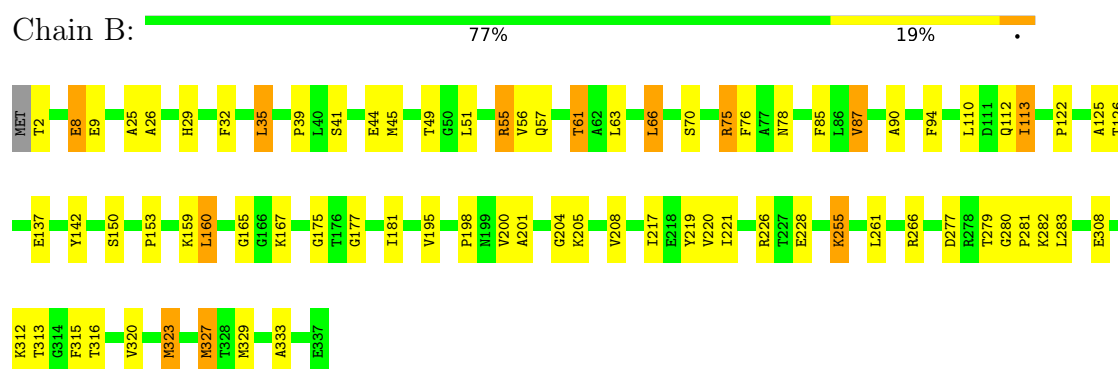
3 Residue-property plots

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.

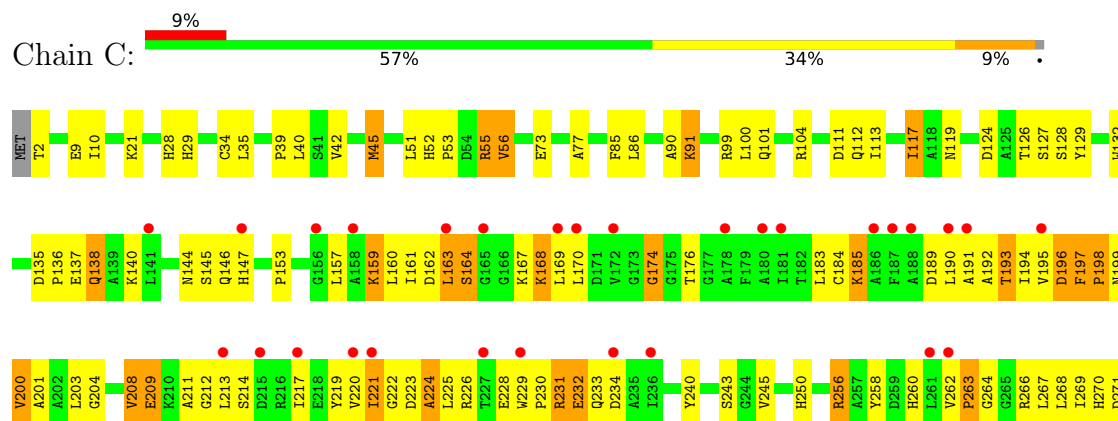
- Molecule 1: SAM-dependent MTHB methyltransferase

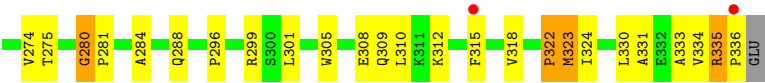


- Molecule 1: SAM-dependent MTHB methyltransferase

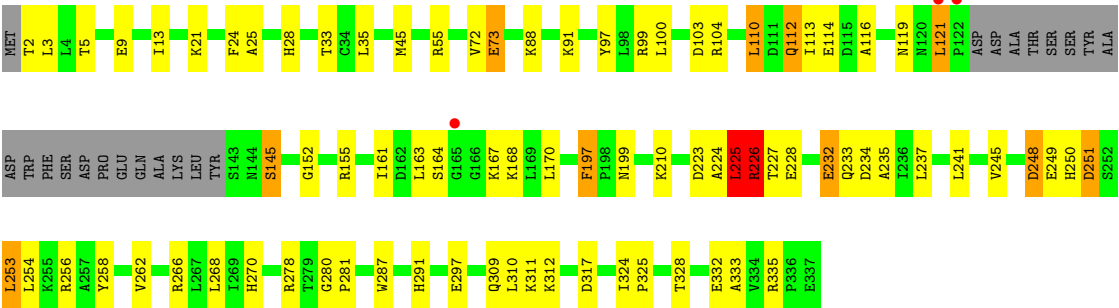


- Molecule 1: SAM-dependent MTHB methyltransferase





● Molecule 1: SAM-dependent MTHB methyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.49Å 115.93Å 153.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.94 – 2.35 31.94 – 2.35	Depositor EDS
% Data completeness (in resolution range)	93.4 (31.94-2.35) 97.4 (31.94-2.35)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.6.4 _486	Depositor
R, R_{free}	0.192 , 0.253 0.196 , 0.252	Depositor DCC
R_{free} test set	2841 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 31.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10316	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.91% 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: 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	0.56	1/2598 (0.0%)	0.89	5/3526 (0.1%)
1	B	0.58	1/2592 (0.0%)	0.89	3/3518 (0.1%)
1	C	0.53	3/2582 (0.1%)	0.89	4/3506 (0.1%)
1	D	0.54	1/2421 (0.0%)	0.90	7/3283 (0.2%)
All	All	0.55	6/10193 (0.1%)	0.89	19/13833 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	281	PRO	N-CD	5.48	1.55	1.47
1	C	322	PRO	N-CD	5.41	1.55	1.47
1	C	198	PRO	N-CD	5.40	1.55	1.47
1	B	281	PRO	N-CD	5.33	1.55	1.47
1	A	281	PRO	N-CD	5.26	1.55	1.47
1	C	281	PRO	N-CD	5.06	1.54	1.47

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	280	GLY	C-N-CD	8.19	138.62	120.60
1	A	280	GLY	C-N-CD	8.09	138.40	120.60
1	B	280	GLY	C-N-CD	8.08	138.37	120.60
1	D	280	GLY	C-N-CD	7.97	138.12	120.60
1	C	174	GLY	N-CA-C	7.40	123.12	114.16
1	D	253	LEU	N-CA-C	-6.88	104.76	113.43
1	D	225	LEU	N-CA-C	6.64	121.73	111.56
1	B	165	GLY	N-CA-C	-6.15	103.71	112.81
1	A	38	GLY	CA-C-N	5.70	125.63	119.76
1	A	38	GLY	C-N-CA	5.70	125.63	119.76
1	A	31	VAL	N-CA-C	5.44	116.07	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	197	PHE	CA-C-N	-5.43	113.13	119.32
1	C	197	PHE	C-N-CA	-5.43	113.13	119.32
1	A	188	ALA	N-CA-C	5.24	116.99	111.28
1	B	313	THR	N-CA-C	-5.16	106.98	113.28
1	D	225	LEU	CA-C-N	5.16	130.99	121.70
1	D	225	LEU	C-N-CA	5.16	130.99	121.70
1	D	197	PHE	CA-C-N	5.04	126.14	119.84
1	D	197	PHE	C-N-CA	5.04	126.14	119.84

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	2545	0	2506	52	0
1	B	2539	0	2502	54	0
1	C	2529	0	2496	139	0
1	D	2375	0	2366	82	0
2	A	27	0	22	5	0
2	B	27	0	22	2	0
2	C	27	0	22	6	0
3	A	87	0	0	0	0
3	B	88	0	0	0	0
3	C	30	0	0	0	0
3	D	42	0	0	2	0
All	All	10316	0	9936	304	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 15.

All (304) 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:168:LYS:H	1:C:168:LYS:HE2	0.97	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:PRO:HA	1:C:335:ARG:HD2	1.41	1.01
1:D:225:LEU:H	1:D:226:ARG:HB2	1.26	0.99
1:D:225:LEU:N	1:D:226:ARG:HB2	1.78	0.99
1:A:75:ARG:HG3	1:A:75:ARG:HH11	1.25	0.96
1:C:193:THR:HG21	1:C:230:PRO:HG3	1.47	0.95
1:C:168:LYS:HE2	1:C:168:LYS:N	1.82	0.93
1:C:231:ARG:HB2	1:C:231:ARG:CZ	2.00	0.90
1:B:75:ARG:HG3	1:B:75:ARG:HH11	1.35	0.89
1:C:168:LYS:HA	1:C:191:ALA:HB3	1.55	0.89
1:A:9:GLU:OE2	1:D:2:THR:HG23	1.73	0.87
1:C:266:ARG:HG2	1:C:334:VAL:HG22	1.56	0.85
1:D:225:LEU:CA	1:D:226:ARG:HB2	2.07	0.85
1:C:274:VAL:HG23	1:C:280:GLY:O	1.77	0.84
1:C:168:LYS:H	1:C:168:LYS:CE	1.90	0.80
1:C:174:GLY:HA3	1:C:194:ILE:HG23	1.65	0.79
1:C:140:LYS:HA	1:C:203:LEU:HD21	1.66	0.78
1:A:320:VAL:HG12	1:A:329:MET:HE2	1.65	0.78
1:C:231:ARG:HB2	1:C:231:ARG:NH1	1.99	0.78
2:C:401:SAM:HB1	2:C:401:SAM:H4'	1.66	0.78
1:B:110:LEU:O	1:B:113:ILE:HG13	1.86	0.76
1:C:192:ALA:HB3	1:C:217:ILE:HA	1.66	0.75
1:B:113:ILE:HD11	1:D:21:LYS:HE3	1.68	0.75
1:A:113:ILE:O	1:A:117:ILE:HG13	1.87	0.74
1:B:320:VAL:HG12	1:B:329:MET:HE2	1.69	0.74
1:D:72:VAL:HG22	1:D:73:GLU:HG2	1.71	0.73
1:B:61:THR:HG21	1:D:278:ARG:HD2	1.71	0.72
1:C:267:LEU:HD12	1:C:268:LEU:N	2.05	0.72
1:C:229:TRP:CZ3	1:C:256:ARG:HB3	2.24	0.72
1:A:113:ILE:HD11	1:C:21:LYS:HD2	1.71	0.72
1:D:28:HIS:CE1	1:D:99:ARG:HG2	2.26	0.71
1:C:168:LYS:HE3	1:C:234:ASP:HB2	1.71	0.71
1:C:198:PRO:HG3	1:C:221:ILE:CG2	2.20	0.70
1:C:315:PHE:HB3	1:C:333:ALA:HB1	1.73	0.70
1:A:305:TRP:CZ2	1:A:309:GLN:HG3	2.26	0.70
1:C:28:HIS:CE1	1:C:99:ARG:HG2	2.26	0.70
1:A:2:THR:HG23	1:D:9:GLU:OE2	1.92	0.69
1:C:185:LYS:HE3	1:C:185:LYS:HA	1.74	0.69
1:D:225:LEU:HB2	1:D:226:ARG:CG	2.22	0.68
1:C:223:ASP:O	1:C:225:LEU:N	2.27	0.68
1:D:251:ASP:HA	1:D:254:LEU:HD12	1.76	0.68
1:C:229:TRP:HZ3	1:C:256:ARG:HB3	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:ASP:OD1	2:C:401:SAM:H1'	1.95	0.67
1:A:316:THR:CG2	1:A:317:ASP:N	2.57	0.67
1:C:284:ALA:O	1:C:288:GLN:HG3	1.94	0.67
1:D:155:ARG:HG3	1:D:155:ARG:HH11	1.59	0.67
1:D:258:TYR:CZ	1:D:335:ARG:HG3	2.30	0.66
1:C:28:HIS:HA	1:C:99:ARG:HD2	1.76	0.66
1:B:75:ARG:HH11	1:B:75:ARG:CG	2.09	0.65
1:C:101:GLN:HB2	1:C:145:SER:OG	1.95	0.65
2:B:401:SAM:HB1	2:B:401:SAM:H4'	1.79	0.64
1:C:204:GLY:O	1:C:208:VAL:HG13	1.96	0.64
2:A:401:SAM:H4'	2:A:401:SAM:HB1	1.80	0.63
1:C:132:TRP:CD1	1:C:138:GLN:HG2	2.33	0.63
1:A:323:MET:CE	1:A:330:LEU:HD22	2.29	0.63
1:B:25:ALA:HB2	1:D:113:ILE:HD13	1.80	0.63
1:A:42:VAL:HG13	1:A:56:VAL:CG2	2.28	0.63
1:C:42:VAL:HG13	1:C:56:VAL:HG22	1.80	0.63
1:C:168:LYS:HE3	1:C:234:ASP:CB	2.28	0.62
1:D:72:VAL:HG22	1:D:73:GLU:CG	2.29	0.62
1:D:104:ARG:HG3	1:D:104:ARG:HH11	1.64	0.62
1:A:316:THR:HG22	1:A:317:ASP:N	2.14	0.61
1:B:181:ILE:HD11	1:B:208:VAL:HG22	1.81	0.61
1:D:310:LEU:HD13	1:D:333:ALA:HB2	1.80	0.61
1:A:29:HIS:CE1	1:C:117:ILE:CD1	2.83	0.61
1:B:9:GLU:OE2	1:C:2:THR:HB	2.00	0.61
1:D:249:GLU:O	1:D:253:LEU:HB2	2.01	0.61
1:A:312:LYS:O	1:A:312:LYS:HD3	2.00	0.61
1:C:163:LEU:HD12	1:C:167:LYS:HD3	1.82	0.61
1:C:157:LEU:HD23	1:C:157:LEU:O	2.00	0.61
1:B:75:ARG:HG3	1:B:75:ARG:NH1	2.14	0.60
1:C:28:HIS:ND1	1:C:99:ARG:HG2	2.17	0.60
1:D:270:HIS:HE1	1:D:328:THR:OG1	1.84	0.60
1:B:201:ALA:O	1:B:205:LYS:HG3	2.03	0.59
1:A:75:ARG:HG3	1:A:75:ARG:NH1	2.05	0.59
1:C:195:VAL:O	1:C:196:ASP:HB2	2.01	0.59
1:C:193:THR:CG2	1:C:230:PRO:HG3	2.28	0.58
1:A:164:SER:O	1:A:167:LYS:HD2	2.04	0.58
1:B:2:THR:HG23	1:C:9:GLU:OE2	2.04	0.58
1:C:308:GLU:OE1	1:C:312:LYS:HD2	2.04	0.58
1:C:267:LEU:HD12	1:C:268:LEU:H	1.68	0.58
1:C:163:LEU:HD23	1:C:183:LEU:HD13	1.85	0.58
1:B:61:THR:HG21	1:D:278:ARG:HH21	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:ASP:O	1:C:222:GLY:O	2.22	0.57
1:C:198:PRO:HG3	1:C:221:ILE:HG23	1.85	0.57
1:C:243:SER:HB2	1:C:271:ASP:OD1	2.04	0.57
1:C:100:LEU:O	1:C:104:ARG:HB2	2.05	0.57
1:A:75:ARG:HH11	1:A:75:ARG:CG	2.05	0.57
1:A:276:ALA:HB2	1:A:304:GLU:HG2	1.86	0.56
1:A:117:ILE:CD1	1:C:29:HIS:CE1	2.88	0.56
1:D:233:GLN:NE2	3:D:401:HOH:O	2.38	0.56
1:A:117:ILE:HD11	1:C:29:HIS:CE1	2.40	0.56
1:D:223:ASP:CG	1:D:226:ARG:HG3	2.31	0.56
1:C:263:PRO:HA	1:C:335:ARG:CD	2.28	0.56
1:B:66:LEU:HG	1:D:13:ILE:HD13	1.88	0.56
1:C:195:VAL:HG22	1:C:220:VAL:HB	1.87	0.56
1:A:29:HIS:CE1	1:C:117:ILE:HD13	2.41	0.56
1:C:161:ILE:HD13	1:C:163:LEU:HD22	1.87	0.55
1:C:192:ALA:HB1	1:C:217:ILE:HG23	1.87	0.55
1:D:225:LEU:CB	1:D:226:ARG:HB2	2.35	0.55
1:C:163:LEU:C	1:C:167:LYS:HD2	2.32	0.55
1:D:155:ARG:HG3	1:D:155:ARG:NH1	2.22	0.55
1:D:225:LEU:CB	1:D:226:ARG:HG2	2.37	0.55
1:D:227:THR:HG22	1:D:228:GLU:N	2.21	0.55
1:C:250:HIS:CE1	1:C:301:LEU:HD11	2.42	0.55
1:C:34:CYS:HB2	1:C:45:MET:HE1	1.89	0.55
1:C:223:ASP:O	1:C:224:ALA:C	2.48	0.54
1:C:223:ASP:OD1	1:C:225:LEU:HB2	2.07	0.54
1:D:225:LEU:CB	1:D:226:ARG:CG	2.86	0.54
1:C:231:ARG:HG3	1:C:260:HIS:HA	1.89	0.54
1:A:53:PRO:O	1:A:56:VAL:HG22	2.06	0.54
1:A:55:ARG:HD3	1:C:119:ASN:OD1	2.07	0.54
1:D:110:LEU:C	1:D:112:GLN:H	2.15	0.54
1:D:168:LYS:HB3	1:D:233:GLN:NE2	2.22	0.54
1:A:28:HIS:CE1	1:A:99:ARG:HB2	2.43	0.53
1:D:28:HIS:HA	1:D:99:ARG:HD2	1.90	0.53
1:C:159:LYS:HG3	1:C:159:LYS:O	2.09	0.53
1:D:113:ILE:HD12	1:D:114:GLU:N	2.23	0.53
1:C:213:LEU:HD12	1:C:213:LEU:N	2.24	0.53
1:D:223:ASP:OD1	1:D:226:ARG:HG3	2.09	0.53
1:C:140:LYS:HA	1:C:203:LEU:CD2	2.37	0.53
1:D:225:LEU:CA	1:D:226:ARG:CB	2.85	0.53
1:C:52:HIS:CG	1:C:53:PRO:HD2	2.44	0.52
1:C:112:GLN:HE22	1:C:126:THR:H	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:HIS:HB2	1:C:176:THR:OG1	2.09	0.52
1:A:2:THR:N	1:D:5:THR:HG1	2.07	0.52
1:B:177:GLY:O	1:B:181:ILE:HG12	2.10	0.52
1:A:266:ARG:HH12	1:A:332:GLU:HG2	1.74	0.52
1:B:61:THR:HB	1:D:278:ARG:HB3	1.92	0.52
1:D:254:LEU:CD2	1:D:310:LEU:HD23	2.40	0.52
1:D:100:LEU:O	1:D:104:ARG:HB2	2.09	0.52
1:B:85:PHE:HB3	1:B:94:PHE:CE2	2.45	0.51
1:C:135:ASP:OD1	1:C:137:GLU:HB2	2.09	0.51
1:A:88:LYS:HE2	1:A:88:LYS:N	2.26	0.51
1:C:119:ASN:ND2	1:C:296:PRO:O	2.44	0.51
1:A:110:LEU:O	1:A:113:ILE:HG13	2.10	0.51
1:B:75:ARG:CG	1:B:75:ARG:NH1	2.72	0.51
1:D:225:LEU:HB2	1:D:226:ARG:HB2	1.93	0.51
1:C:195:VAL:HG21	1:C:229:TRP:HD1	1.75	0.50
1:D:161:ILE:HD12	1:D:163:LEU:HD21	1.92	0.50
1:C:240:TYR:HB3	2:C:401:SAM:HE3	1.93	0.50
1:C:225:LEU:O	1:C:226:ARG:NH1	2.45	0.50
1:B:198:PRO:HG3	1:B:221:ILE:CG2	2.42	0.50
1:C:113:ILE:O	1:C:117:ILE:HG13	2.12	0.50
1:C:231:ARG:CZ	1:C:231:ARG:CB	2.83	0.50
1:C:168:LYS:HE3	1:C:234:ASP:CG	2.37	0.49
1:A:88:LYS:NZ	1:A:93:ASP:OD1	2.46	0.49
1:B:142:TYR:OH	2:B:401:SAM:HE1	2.12	0.49
1:D:116:ALA:HA	1:D:121:LEU:HG	1.93	0.49
1:B:113:ILE:HD13	1:D:25:ALA:HB2	1.95	0.49
1:D:104:ARG:HG3	1:D:104:ARG:NH1	2.26	0.49
1:A:43:GLU:CD	1:A:43:GLU:H	2.19	0.49
1:B:29:HIS:CD2	1:B:51:LEU:HD21	2.47	0.49
1:B:51:LEU:HB2	1:B:56:VAL:HG23	1.95	0.48
1:B:255:LYS:HE2	1:B:255:LYS:O	2.14	0.48
1:A:147:HIS:HD2	1:A:176:THR:OG1	1.97	0.48
1:C:129:TYR:OH	2:C:401:SAM:HE1	2.14	0.48
1:D:225:LEU:HB3	1:D:226:ARG:HG2	1.95	0.48
1:C:162:ASP:OD1	1:C:164:SER:HB2	2.13	0.48
1:C:268:LEU:N	1:C:268:LEU:HD12	2.29	0.48
1:B:315:PHE:HB3	1:B:333:ALA:HB1	1.96	0.48
1:D:232:GLU:HG3	1:D:262:VAL:HG12	1.96	0.48
1:B:39:PRO:HA	1:B:76:PHE:O	2.14	0.48
1:C:199:ASN:O	1:C:203:LEU:CD1	2.62	0.48
1:C:258:TYR:HD2	1:C:315:PHE:CE1	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ARG:NH1	1:A:75:ARG:CG	2.70	0.47
1:B:8:GLU:CD	1:B:8:GLU:H	2.22	0.47
1:A:240:TYR:CB	2:A:401:SAM:HE3	2.44	0.47
1:C:140:LYS:HG2	1:C:203:LEU:HD21	1.97	0.47
1:D:97:TYR:HB2	1:D:145:SER:HB3	1.97	0.47
1:A:127:SER:O	1:A:128:SER:HB3	2.15	0.47
1:A:34:CYS:SG	1:A:49:THR:HG22	2.54	0.46
1:B:41:SER:OG	1:B:44:GLU:HG3	2.15	0.46
1:B:181:ILE:HD13	1:B:217:ILE:HD12	1.97	0.46
1:B:308:GLU:HG3	1:B:312:LYS:HE3	1.96	0.46
1:C:223:ASP:C	1:C:225:LEU:N	2.73	0.46
1:C:262:VAL:O	1:C:263:PRO:C	2.58	0.46
1:D:110:LEU:C	1:D:112:GLN:N	2.73	0.46
1:C:240:TYR:CB	2:C:401:SAM:HE3	2.46	0.46
1:D:270:HIS:CE1	1:D:328:THR:OG1	2.65	0.46
1:B:57:GLN:O	1:B:61:THR:HG22	2.15	0.46
1:B:198:PRO:HG3	1:B:221:ILE:HG22	1.96	0.46
1:D:223:ASP:OD1	1:D:225:LEU:HB2	2.16	0.46
1:B:57:GLN:O	1:B:61:THR:CG2	2.64	0.45
1:D:24:PHE:CD2	1:D:103:ASP:HB2	2.51	0.45
1:B:70:SER:HB3	1:D:3:LEU:HD21	1.97	0.45
1:B:327:MET:HE2	1:B:327:MET:HB2	1.71	0.45
1:C:135:ASP:HB3	1:C:138:GLN:HB2	1.97	0.45
1:B:175:GLY:HA2	1:B:200:VAL:HG11	1.98	0.45
1:D:225:LEU:HB2	1:D:226:ARG:CB	2.46	0.45
1:A:142:TYR:OH	2:A:401:SAM:CE	2.65	0.45
1:C:229:TRP:CH2	1:C:256:ARG:HB3	2.50	0.45
1:D:287:TRP:CH2	1:D:291:HIS:CD2	3.05	0.45
1:A:29:HIS:HE1	1:C:117:ILE:CD1	2.30	0.45
1:B:277:ASP:OD1	1:B:279:THR:HG22	2.16	0.45
1:C:157:LEU:HD23	1:C:161:ILE:HG13	1.98	0.45
1:A:239:SER:HB3	2:A:401:SAM:HN1	1.82	0.45
1:D:33:THR:OG1	1:D:88:LYS:HE3	2.17	0.45
1:C:140:LYS:O	1:C:144:ASN:HB2	2.16	0.45
1:C:231:ARG:HG2	1:C:232:GLU:CD	2.41	0.45
1:D:170:LEU:HB2	1:D:233:GLN:HG2	1.98	0.45
1:C:264:GLY:N	1:C:335:ARG:O	2.50	0.45
1:D:225:LEU:CB	1:D:226:ARG:CB	2.94	0.45
1:C:163:LEU:HD12	1:C:163:LEU:HA	1.88	0.45
1:B:110:LEU:HG	1:D:21:LYS:HG3	2.00	0.44
1:C:135:ASP:O	1:C:138:GLN:N	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:GLU:CD	1:C:260:HIS:HE2	2.24	0.44
1:A:146:GLN:HG2	2:A:401:SAM:HG1	1.98	0.44
1:D:167:LYS:HD2	1:D:234:ASP:OD2	2.17	0.44
1:C:299:ARG:HH22	1:C:305:TRP:CG	2.35	0.44
1:D:210:LYS:HE3	3:D:410:HOH:O	2.18	0.44
1:C:194:ILE:O	1:C:219:TYR:CD1	2.71	0.44
1:A:206:GLY:O	1:A:210:LYS:HG3	2.17	0.44
1:A:323:MET:HE2	1:A:330:LEU:HB2	2.00	0.44
1:B:159:LYS:HB2	1:B:159:LYS:NZ	2.33	0.44
1:C:35:LEU:HD23	1:C:40:LEU:HD12	2.00	0.44
1:C:270:HIS:CD2	1:C:323:MET:HG2	2.53	0.44
1:B:160:LEU:CD2	1:B:323:MET:HE3	2.47	0.44
1:C:305:TRP:CE2	1:C:309:GLN:HG3	2.53	0.44
1:D:324:ILE:HA	1:D:325:PRO:HD3	1.84	0.44
1:A:316:THR:CG2	1:A:317:ASP:H	2.30	0.44
1:C:274:VAL:HG22	1:C:275:THR:O	2.17	0.44
1:D:113:ILE:HA	1:D:116:ALA:HB3	2.00	0.44
1:D:223:ASP:C	1:D:225:LEU:H	2.26	0.44
1:C:258:TYR:OH	1:C:336:PRO:HD2	2.18	0.43
1:C:190:LEU:HD12	1:C:191:ALA:H	1.83	0.43
1:C:194:ILE:O	1:C:219:TYR:HD1	2.01	0.43
1:C:308:GLU:C	1:C:308:GLU:CD	2.84	0.43
1:C:192:ALA:C	1:C:193:THR:OG1	2.61	0.43
1:C:211:ALA:HB3	1:C:213:LEU:HD13	1.99	0.43
1:C:229:TRP:CH2	1:C:256:ARG:CZ	3.02	0.43
1:D:72:VAL:CG2	1:D:73:GLU:HG2	2.44	0.43
1:B:87:VAL:HG22	1:B:90:ALA:HB2	2.01	0.43
1:C:228:GLU:OE2	1:C:260:HIS:NE2	2.50	0.43
1:D:24:PHE:CG	1:D:103:ASP:HB2	2.53	0.43
1:A:270:HIS:CD2	1:A:323:MET:HG2	2.54	0.43
1:C:194:ILE:HB	1:C:219:TYR:CE1	2.54	0.43
1:A:316:THR:HG23	1:A:317:ASP:H	1.84	0.43
1:C:266:ARG:CG	1:C:334:VAL:HG22	2.39	0.43
1:A:29:HIS:HE1	1:C:117:ILE:HD11	1.84	0.42
1:A:247:GLY:HA2	1:A:299:ARG:HG2	2.01	0.42
1:B:195:VAL:HA	1:B:220:VAL:O	2.18	0.42
1:C:192:ALA:CB	1:C:217:ILE:HG23	2.49	0.42
1:C:169:LEU:HD12	1:C:170:LEU:H	1.84	0.42
1:D:227:THR:CG2	1:D:228:GLU:N	2.82	0.42
1:B:45:MET:HE3	1:B:49:THR:HG23	2.00	0.42
1:C:127:SER:O	1:C:128:SER:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:LEU:HD23	1:C:310:LEU:HA	1.78	0.42
1:D:311:LYS:O	1:D:312:LYS:C	2.61	0.42
1:C:39:PRO:HB3	1:C:77:ALA:HB2	2.01	0.42
1:C:161:ILE:HD12	1:C:161:ILE:O	2.20	0.42
1:C:184:CYS:N	1:C:190:LEU:HD23	2.35	0.42
1:C:200:VAL:O	1:C:201:ALA:C	2.62	0.42
1:D:152:GLY:O	1:D:155:ARG:HB2	2.19	0.42
1:C:135:ASP:HA	1:C:136:PRO:HD2	1.87	0.42
1:B:61:THR:CG2	1:D:278:ARG:HD2	2.46	0.42
1:D:28:HIS:ND1	1:D:99:ARG:HG2	2.34	0.42
1:B:150:SER:C	1:B:153:PRO:HD2	2.45	0.42
1:D:197:PHE:CE1	1:D:223:ASP:HB2	2.54	0.42
1:D:225:LEU:O	1:D:256:ARG:NH1	2.53	0.42
1:A:52:HIS:O	1:A:56:VAL:HG13	2.20	0.41
1:A:88:LYS:HD3	1:A:88:LYS:HA	1.79	0.41
1:D:28:HIS:CE1	1:D:99:ARG:CG	3.02	0.41
1:D:287:TRP:CH2	1:D:291:HIS:CG	3.08	0.41
1:A:29:HIS:CE1	1:C:117:ILE:HD11	2.54	0.41
1:A:296:PRO:O	1:C:55:ARG:HD3	2.20	0.41
1:C:73:GLU:HA	1:C:73:GLU:OE2	2.20	0.41
1:C:161:ILE:HD12	1:C:161:ILE:C	2.45	0.41
1:A:117:ILE:O	1:C:51:LEU:HD22	2.21	0.41
1:B:35:LEU:HD13	1:B:45:MET:SD	2.61	0.41
1:B:122:PRO:HD2	1:B:125:ALA:HB2	2.03	0.41
1:C:194:ILE:O	1:C:219:TYR:HA	2.20	0.41
1:C:228:GLU:CD	1:C:229:TRP:N	2.79	0.41
1:D:45:MET:HB3	1:D:45:MET:HE3	1.72	0.41
1:B:55:ARG:HD3	1:B:55:ARG:HA	1.83	0.41
1:C:85:PHE:O	1:C:86:LEU:HD23	2.21	0.41
1:C:250:HIS:HE1	1:C:301:LEU:HD11	1.84	0.41
1:B:113:ILE:HG13	1:B:113:ILE:H	1.77	0.41
1:B:26:ALA:HB2	1:B:63:LEU:HD11	2.03	0.41
1:B:283:LEU:HD13	1:B:327:MET:HE2	2.03	0.41
1:C:330:LEU:HG	1:C:331:ALA:O	2.21	0.41
1:D:223:ASP:HB3	1:D:226:ARG:HB3	2.02	0.41
1:D:250:HIS:O	1:D:254:LEU:HD12	2.20	0.41
1:B:32:PHE:HA	1:B:78:ASN:HD21	1.85	0.41
1:B:112:GLN:HE22	1:B:126:THR:H	1.69	0.41
1:C:200:VAL:HA	1:C:203:LEU:HD13	2.02	0.41
1:C:212:GLY:C	1:C:213:LEU:HD12	2.46	0.41
1:D:225:LEU:HB2	1:D:226:ARG:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:ILE:HB	1:C:331:ALA:HB3	2.02	0.40
1:B:204:GLY:HA3	1:B:219:TYR:OH	2.20	0.40
1:C:153:PRO:HB3	1:C:324:ILE:HD11	2.03	0.40
1:D:235:ALA:HA	1:D:266:ARG:O	2.21	0.40
1:C:197:PHE:HB2	1:C:200:VAL:CG2	2.51	0.40
1:C:90:ALA:O	1:C:91:LYS:C	2.65	0.40
1:C:136:PRO:O	1:C:140:LYS:HG3	2.20	0.40
1:C:209:GLU:HA	1:C:214:SER:OG	2.22	0.40
1:D:248:ASP:OD1	1:D:248:ASP:N	2.38	0.40
1:D:268:LEU:HD23	1:D:332:GLU:HB3	2.02	0.40
1:A:56:VAL:O	1:A:60:LEU:HD23	2.21	0.40
1:A:316:THR:O	1:A:317:ASP:C	2.65	0.40
1:C:129:TYR:CD2	2:C:401:SAM:H8	2.57	0.40
1:C:208:VAL:HG23	1:C:214:SER:HA	2.04	0.40
1:D:223:ASP:O	1:D:225:LEU:N	2.54	0.40
1:D:278:ARG:HA	1:D:278:ARG:HD3	1.70	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	335/337 (99%)	325 (97%)	10 (3%)	0	100	100
1	B	334/337 (99%)	325 (97%)	9 (3%)	0	100	100
1	C	333/337 (99%)	290 (87%)	37 (11%)	6 (2%)	6	5
1	D	312/337 (93%)	298 (96%)	12 (4%)	2 (1%)	21	24
All	All	1314/1348 (98%)	1238 (94%)	68 (5%)	8 (1%)	21	24

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	221	ILE
1	D	226	ARG
1	C	196	ASP
1	C	224	ALA
1	C	323	MET
1	D	224	ALA
1	C	322	PRO
1	C	263	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	261/261 (100%)	244 (94%)	17 (6%)	15	18
1	B	260/261 (100%)	240 (92%)	20 (8%)	12	13
1	C	259/261 (99%)	231 (89%)	28 (11%)	6	5
1	D	243/261 (93%)	221 (91%)	22 (9%)	9	9
All	All	1023/1044 (98%)	936 (92%)	87 (8%)	10	11

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	11	SER
1	A	40	LEU
1	A	43	GLU
1	A	55	ARG
1	A	56	VAL
1	A	75	ARG
1	A	88	LYS
1	A	94	PHE
1	A	113	ILE
1	A	117	ILE
1	A	137	GLU
1	A	261	LEU
1	A	266	ARG

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Mol	Chain	Res	Type
1	A	268	LEU
1	A	279	THR
1	A	282	LYS
1	B	8	GLU
1	B	35	LEU
1	B	55	ARG
1	B	61	THR
1	B	66	LEU
1	B	75	ARG
1	B	87	VAL
1	B	113	ILE
1	B	137	GLU
1	B	160	LEU
1	B	167	LYS
1	B	226	ARG
1	B	228	GLU
1	B	255	LYS
1	B	261	LEU
1	B	266	ARG
1	B	282	LYS
1	B	316	THR
1	B	323	MET
1	B	327	MET
1	C	10	ILE
1	C	45	MET
1	C	55	ARG
1	C	56	VAL
1	C	91	LYS
1	C	111	ASP
1	C	117	ILE
1	C	124	ASP
1	C	138	GLN
1	C	146	GLN
1	C	159	LYS
1	C	160	LEU
1	C	163	LEU
1	C	164	SER
1	C	168	LYS
1	C	185	LYS
1	C	189	ASP
1	C	193	THR
1	C	200	VAL

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Mol	Chain	Res	Type
1	C	208	VAL
1	C	209	GLU
1	C	231	ARG
1	C	232	GLU
1	C	233	GLN
1	C	245	VAL
1	C	256	ARG
1	C	318	VAL
1	C	335	ARG
1	D	35	LEU
1	D	55	ARG
1	D	73	GLU
1	D	91	LYS
1	D	110	LEU
1	D	112	GLN
1	D	119	ASN
1	D	121	LEU
1	D	145	SER
1	D	164	SER
1	D	199	ASN
1	D	225	LEU
1	D	226	ARG
1	D	232	GLU
1	D	237	LEU
1	D	241	LEU
1	D	245	VAL
1	D	248	ASP
1	D	251	ASP
1	D	297	GLU
1	D	309	GLN
1	D	317	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	HIS
1	A	144	ASN
1	A	147	HIS
1	A	233	GLN
1	B	6	ASN
1	B	78	ASN
1	B	112	GLN

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Mol	Chain	Res	Type
1	B	309	GLN
1	C	29	HIS
1	C	57	GLN
1	C	101	GLN
1	C	112	GLN
1	C	250	HIS
1	C	288	GLN
1	C	291	HIS
1	C	309	GLN
1	D	29	HIS
1	D	119	ASN
1	D	146	GLN
1	D	233	GLN
1	D	270	HIS

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](#)

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	SAM	C	401	-	27,29,29	1.53	5 (18%)	34,42,42	2.34	11 (32%)
2	SAM	A	401	-	27,29,29	1.52	5 (18%)	34,42,42	2.27	11 (32%)
2	SAM	B	401	-	27,29,29	1.43	4 (14%)	34,42,42	2.24	10 (29%)

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	C	401	-	-	3/17/33/33	0/3/3/3
2	SAM	A	401	-	-	5/17/33/33	0/3/3/3
2	SAM	B	401	-	-	1/17/33/33	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	SAM	C5'-C4'	-3.53	1.43	1.53
2	B	401	SAM	C5'-C4'	-3.44	1.43	1.53
2	A	401	SAM	C5'-C4'	-3.39	1.43	1.53
2	B	401	SAM	C6-N6	3.21	1.42	1.34
2	C	401	SAM	C6-N6	3.10	1.42	1.34
2	A	401	SAM	C6-N6	2.98	1.41	1.34
2	C	401	SAM	C3'-C4'	-2.49	1.46	1.53
2	A	401	SAM	C3'-C4'	-2.42	1.46	1.53
2	A	401	SAM	C2'-C3'	-2.24	1.47	1.53
2	C	401	SAM	C2'-C3'	-2.13	1.47	1.53
2	B	401	SAM	C5-N7	-2.12	1.35	1.39
2	C	401	SAM	O2'-C2'	-2.07	1.37	1.43
2	A	401	SAM	O-C	2.04	1.28	1.22
2	B	401	SAM	O-C	2.04	1.28	1.22

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	SAM	C5-C4-N3	-6.06	118.37	126.72
2	C	401	SAM	C5-C4-N3	-5.39	119.30	126.72
2	A	401	SAM	C5-C4-N3	-5.34	119.36	126.72
2	C	401	SAM	N3-C2-N1	-4.92	121.13	128.58
2	C	401	SAM	N3-C4-N9	4.65	135.07	127.17
2	B	401	SAM	N3-C4-N9	4.60	134.98	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	SAM	N9-C8-N7	-4.55	107.48	113.94
2	A	401	SAM	N3-C2-N1	-4.52	121.75	128.58
2	A	401	SAM	N3-C4-N9	4.39	134.64	127.17
2	C	401	SAM	C4-N9-C8	4.21	110.16	105.74
2	A	401	SAM	N9-C8-N7	-4.15	108.05	113.94
2	B	401	SAM	N9-C8-N7	-4.15	108.05	113.94
2	B	401	SAM	N3-C2-N1	-4.01	122.51	128.58
2	B	401	SAM	C5-N7-C8	3.90	109.58	103.45
2	A	401	SAM	C4-N9-C8	3.77	109.69	105.74
2	C	401	SAM	C2-N3-C4	3.62	120.66	111.83
2	C	401	SAM	C5-N7-C8	3.57	109.06	103.45
2	A	401	SAM	CG-SD-C5'	3.52	112.03	103.43
2	B	401	SAM	C2-N3-C4	3.45	120.27	111.83
2	A	401	SAM	C5-N7-C8	3.43	108.84	103.45
2	B	401	SAM	C4-C5-N7	-3.39	106.71	110.58
2	A	401	SAM	C2-N3-C4	3.35	120.01	111.83
2	B	401	SAM	C4-N9-C8	3.12	109.01	105.74
2	C	401	SAM	CG-SD-C5'	2.89	110.49	103.43
2	A	401	SAM	C4-C5-N7	-2.77	107.41	110.58
2	A	401	SAM	OXT-C-O	-2.74	117.87	124.08
2	B	401	SAM	CG-SD-C5'	2.73	110.10	103.43
2	C	401	SAM	C4-C5-N7	-2.56	107.66	110.58
2	C	401	SAM	OXT-C-O	-2.53	118.33	124.08
2	C	401	SAM	C3'-C2'-C1'	2.36	105.92	101.46
2	B	401	SAM	C6-C5-C4	2.17	120.14	117.18
2	A	401	SAM	C3'-C2'-C1'	2.11	105.45	101.46

There are no chirality outliers.

All (9) torsion outliers are listed below:

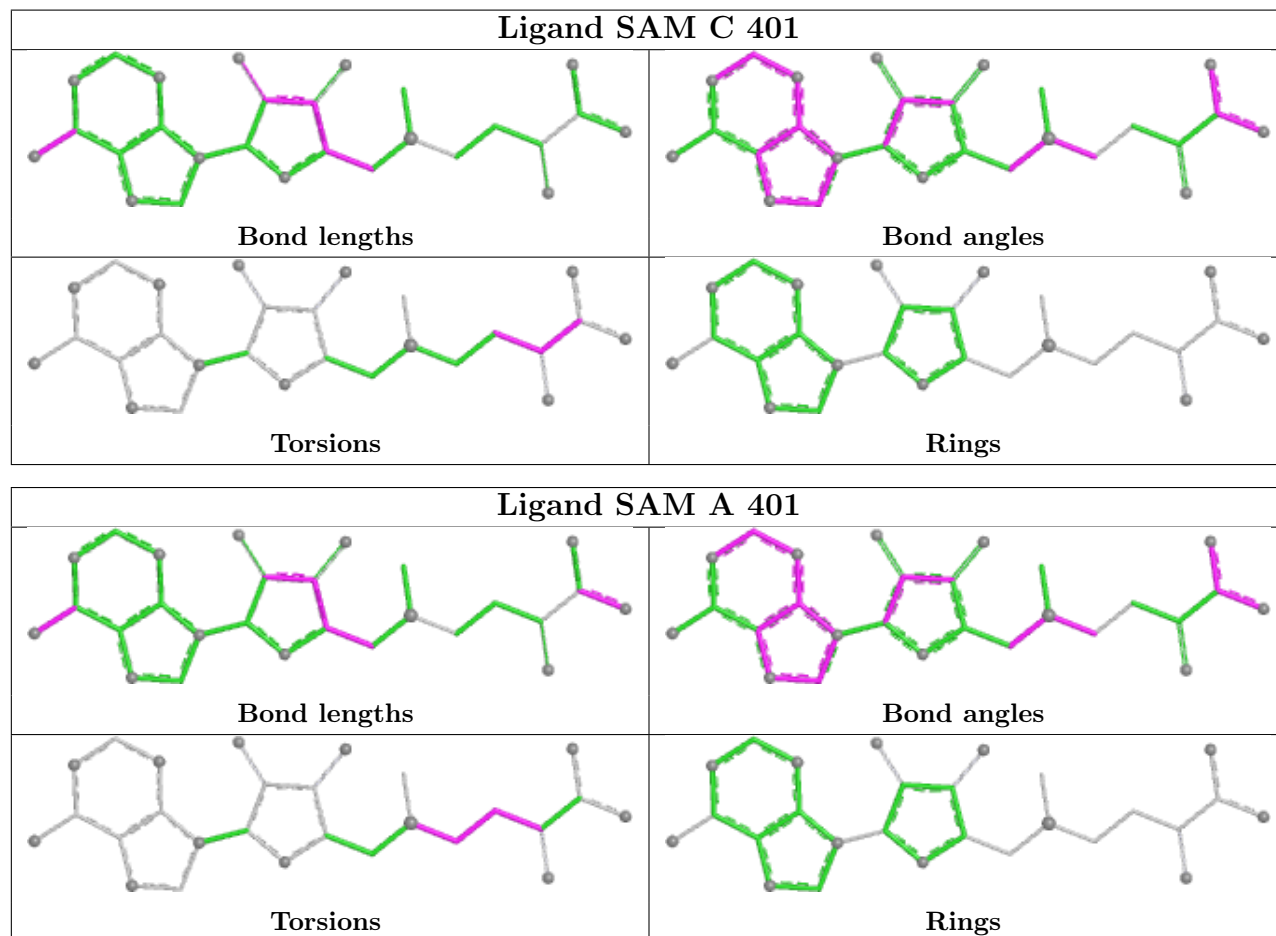
Mol	Chain	Res	Type	Atoms
2	A	401	SAM	C-CA-CB-CG
2	A	401	SAM	CA-CB-CG-SD
2	B	401	SAM	C-CA-CB-CG
2	C	401	SAM	C-CA-CB-CG
2	A	401	SAM	N-CA-CB-CG
2	C	401	SAM	O-C-CA-CB
2	C	401	SAM	OXT-C-CA-CB
2	A	401	SAM	CB-CG-SD-CE
2	A	401	SAM	CB-CG-SD-C5'

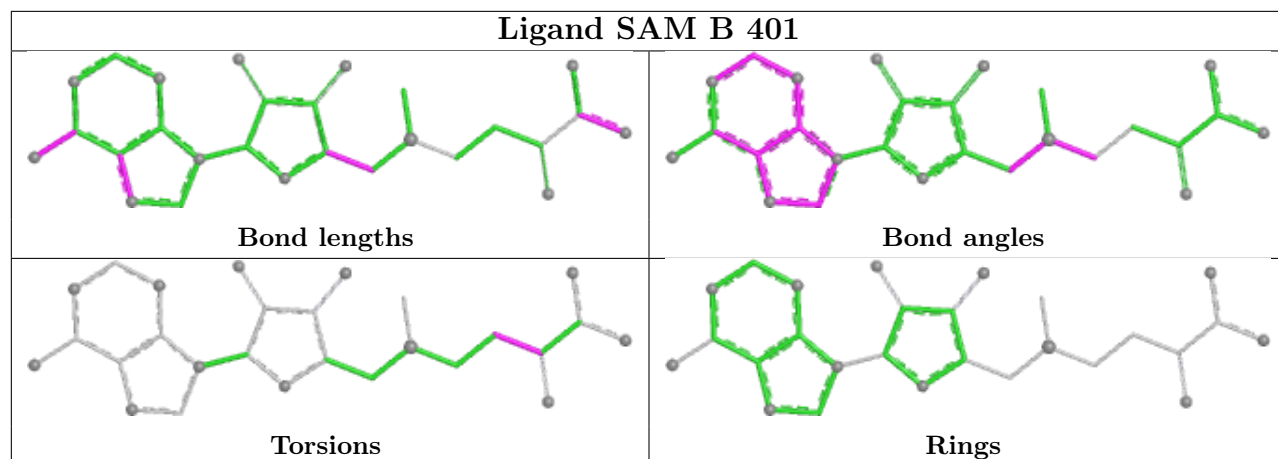
There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	SAM	6	0
2	A	401	SAM	5	0
2	B	401	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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	336/337 (99%)	-0.35	0 100 100	16, 37, 54, 67	1 (0%)
1	B	336/337 (99%)	-0.41	0 100 100	24, 35, 51, 65	0
1	C	335/337 (99%)	0.53	31 (9%) 14 17	27, 57, 97, 109	0
1	D	316/337 (93%)	0.11	3 (0%) 81 84	23, 49, 73, 110	0
All	All	1323/1348 (98%)	-0.03	34 (2%) 57 63	16, 41, 86, 110	1 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	122	PRO	3.7
1	C	181	ILE	3.3
1	C	262	VAL	3.1
1	C	220	VAL	3.1
1	C	141	LEU	3.1
1	C	217	ILE	2.9
1	C	236	ILE	2.9
1	D	121	LEU	2.7
1	C	190	LEU	2.7
1	C	191	ALA	2.7
1	C	180	ALA	2.7
1	C	172	VAL	2.5
1	C	163	LEU	2.5
1	D	165	GLY	2.5
1	C	169	LEU	2.5
1	C	261	LEU	2.4
1	C	156	GLY	2.3
1	C	213	LEU	2.3
1	C	221	ILE	2.3
1	C	234	ASP	2.2
1	C	165	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	229	TRP	2.2
1	C	158	ALA	2.2
1	C	195	VAL	2.1
1	C	188	ALA	2.1
1	C	336	PRO	2.1
1	C	170	LEU	2.1
1	C	215	ASP	2.1
1	C	315	PHE	2.1
1	C	227	THR	2.1
1	C	186	ALA	2.1
1	C	178	ALA	2.0
1	C	147	HIS	2.0
1	C	187	PHE	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](#)

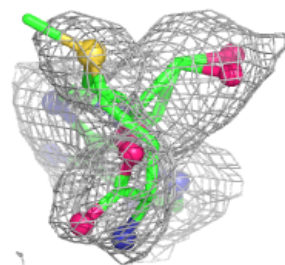
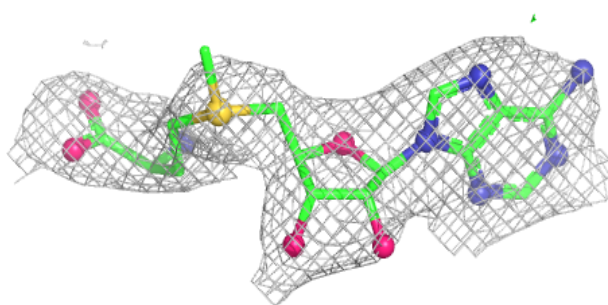
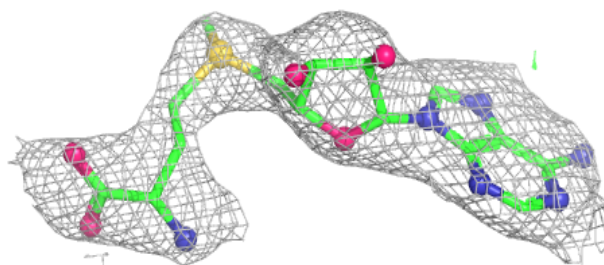
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SAM	C	401	27/27	0.90	0.11	54,65,70,73	0
2	SAM	A	401	27/27	0.93	0.08	30,35,44,51	0
2	SAM	B	401	27/27	0.95	0.07	29,34,38,41	0

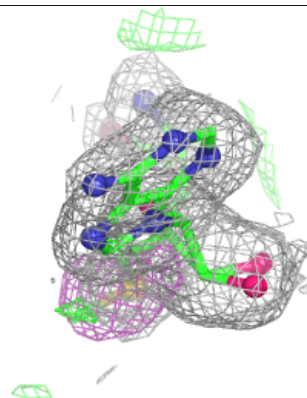
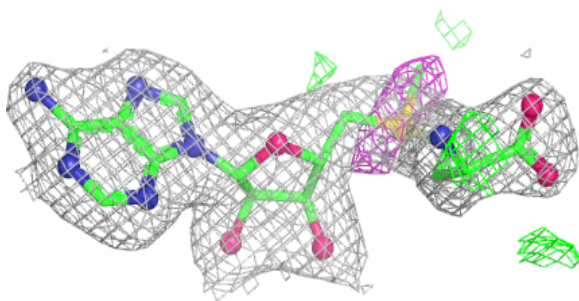
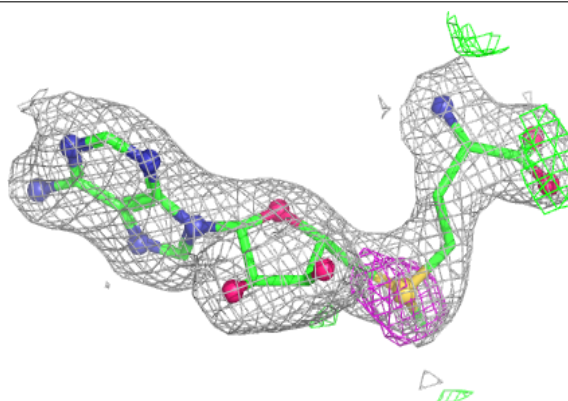
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAM C 401:

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

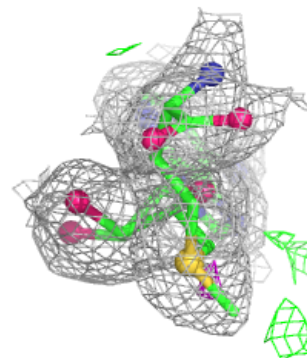
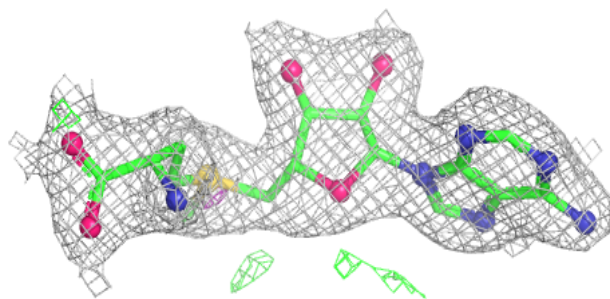
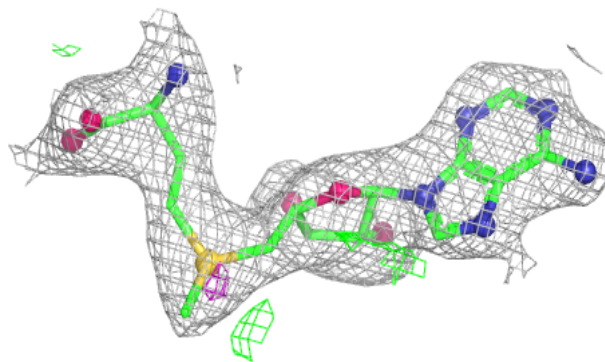
**Electron density around SAM A 401:**

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



Electron density around SAM 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.