



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 07:28 AM UTC

PDB ID : 7WVS / pdb_00007wvs
Title : The structure of FinI complex with SAM
Authors : Lu, J.; Zhou, J.
Deposited on : 2022-02-11
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

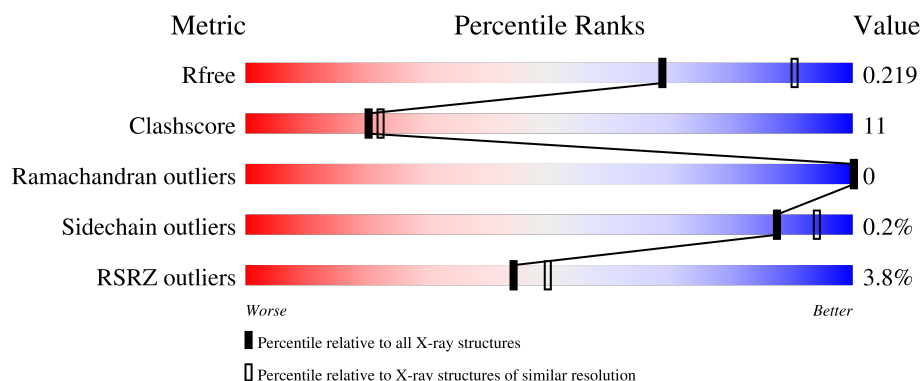
1 Overall quality at a glance

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	409	84% 11% .
1	B	409	7% 76% 20% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	A	514	-	-	X	-
3	EDO	A	523	-	-	X	-
3	EDO	A	528	-	-	X	-
3	EDO	B	503	-	-	X	-
3	EDO	B	509	-	-	X	-
4	GOL	A	512	-	-	X	-
4	GOL	B	508	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6624 atoms, of which 4 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.

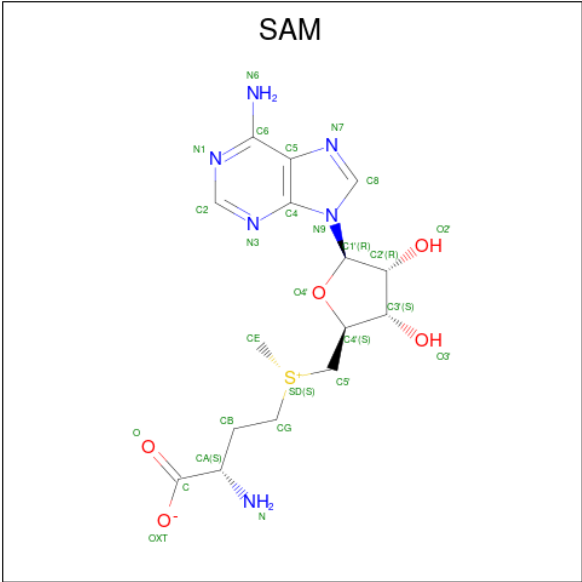
- Molecule 1 is a protein called Methyltransf_2 domain-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	392	Total	C	H	N	O	S	0	1	0
			3061	1952	2	523	565	19			
1	B	393	Total	C	H	N	O	S	0	0	0
			3063	1953	2	524	565	19			

There are 20 discrepancies between the modelled and reference sequences:

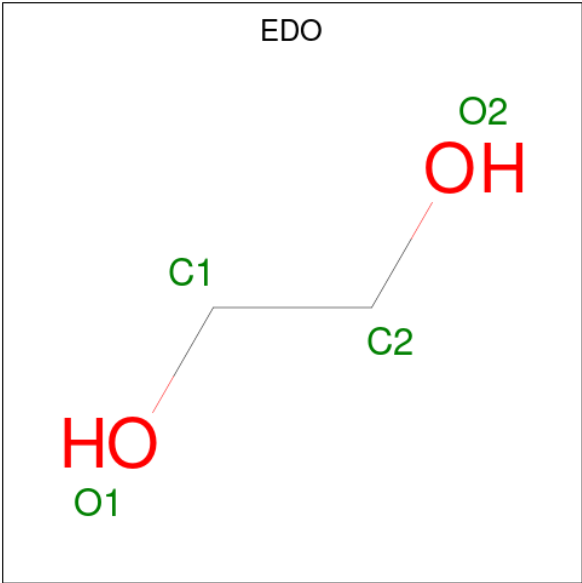
Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ILE	VAL	conflict	UNP A0A1R3S1W7
A	159	PRO	SER	conflict	UNP A0A1R3S1W7
A	227	PRO	ARG	conflict	UNP A0A1R3S1W7
A	403	GLU	-	expression tag	UNP A0A1R3S1W7
A	404	HIS	-	expression tag	UNP A0A1R3S1W7
A	405	HIS	-	expression tag	UNP A0A1R3S1W7
A	406	HIS	-	expression tag	UNP A0A1R3S1W7
A	407	HIS	-	expression tag	UNP A0A1R3S1W7
A	408	HIS	-	expression tag	UNP A0A1R3S1W7
A	409	HIS	-	expression tag	UNP A0A1R3S1W7
B	19	ILE	VAL	conflict	UNP A0A1R3S1W7
B	159	PRO	SER	conflict	UNP A0A1R3S1W7
B	227	PRO	ARG	conflict	UNP A0A1R3S1W7
B	403	GLU	-	expression tag	UNP A0A1R3S1W7
B	404	HIS	-	expression tag	UNP A0A1R3S1W7
B	405	HIS	-	expression tag	UNP A0A1R3S1W7
B	406	HIS	-	expression tag	UNP A0A1R3S1W7
B	407	HIS	-	expression tag	UNP A0A1R3S1W7
B	408	HIS	-	expression tag	UNP A0A1R3S1W7
B	409	HIS	-	expression tag	UNP A0A1R3S1W7

- 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 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		

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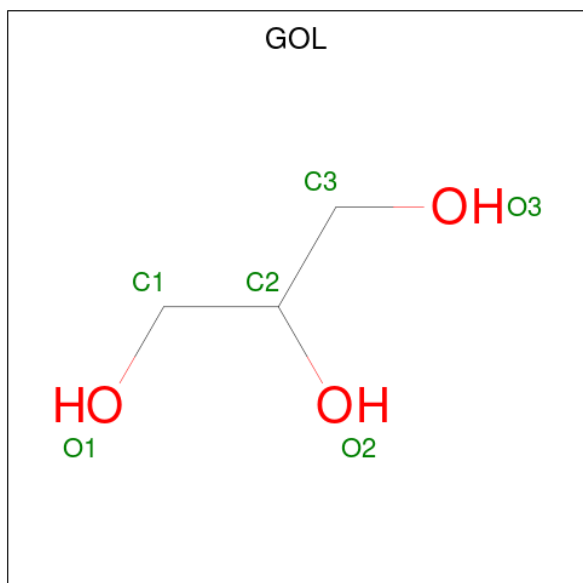
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



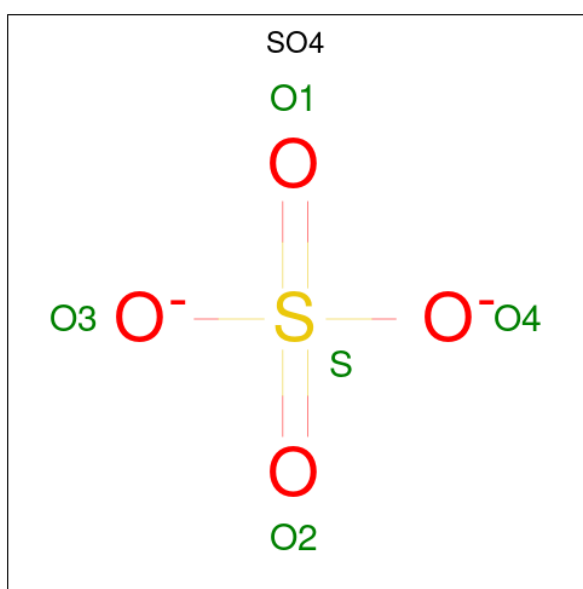
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

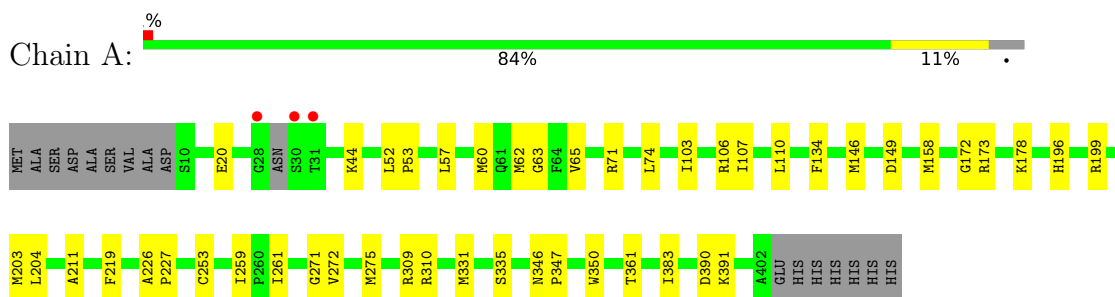
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	151	Total 151	O 151	0	0
6	B	103	Total 103	O 103	0	0

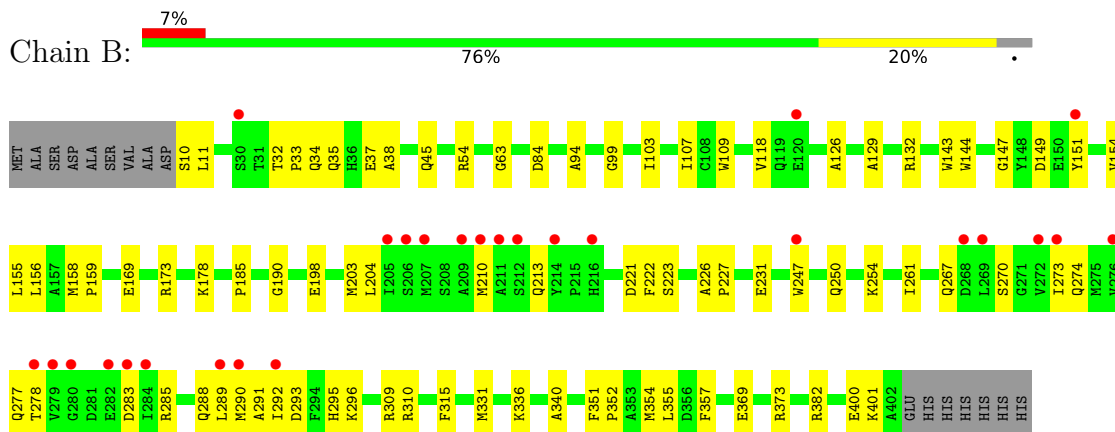
3 Residue-property plots

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: Methyltransf_2 domain-containing protein



- Molecule 1: Methyltransf_2 domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	73.56Å 108.76Å 124.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.60 – 2.35 28.60 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (28.60-2.35) 99.9 (28.60-2.35)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.36Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.170 , 0.218 0.172 , 0.219	Depositor DCC
R_{free} test set	2106 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	30.7	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 45.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6624	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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, SO4, GOL, EDO

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	0.30	0/3125	0.46	0/4242
1	B	0.29	0/3128	0.45	0/4248
All	All	0.29	0/6253	0.46	0/8490

There are no bond length outliers.

There are no bond angle outliers.

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	3059	2	3075	57	0
1	B	3061	2	3078	93	0
2	A	27	0	22	1	0
2	B	27	0	22	1	0
3	A	76	0	114	32	0
3	B	56	0	84	16	0
4	A	24	0	32	8	0
4	B	6	0	8	5	0
5	A	20	0	0	1	0
5	B	10	0	0	1	0
6	A	151	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	103	0	0	3	0
All	All	6620	4	6435	144	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 11.

All (144) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:LYS:HA	1:B:254:LYS:HE3	1.18	1.16
1:B:132:ARG:HH12	4:B:508:GOL:H31	1.13	1.08
3:A:511:EDO:H12	1:B:63:GLY:HA3	1.38	1.04
1:A:253:CYS:HB3	3:A:514:EDO:H22	1.46	0.98
1:B:221:ASP:HA	3:B:509:EDO:H12	1.46	0.97
1:B:185:PRO:HG3	3:B:512:EDO:H22	1.43	0.96
1:B:254:LYS:HA	1:B:254:LYS:CE	2.00	0.85
1:A:62:MET:CG	1:B:354:MET:HE1	2.07	0.85
1:A:390:ASP:OD1	1:A:391:LYS:HE2	1.75	0.84
3:A:518:EDO:H12	6:A:648:HOH:O	1.79	0.82
1:A:146:MET:HE1	1:A:203:MET:HG2	1.61	0.81
1:B:132:ARG:NH1	4:B:508:GOL:H31	1.92	0.81
1:B:254:LYS:HE3	1:B:254:LYS:CA	2.09	0.80
1:B:32:THR:HG23	1:B:35:GLN:H	1.46	0.79
1:B:32:THR:HG22	1:B:35:GLN:HB2	1.65	0.78
1:B:10:SER:HA	3:B:503:EDO:H22	1.65	0.78
1:A:275:MET:HE2	4:A:512:GOL:H11	1.66	0.76
3:A:523:EDO:H21	1:B:156:LEU:HA	1.67	0.74
1:A:62:MET:HG2	1:B:354:MET:HE1	1.68	0.74
1:A:253:CYS:HB3	3:A:514:EDO:C2	2.16	0.73
1:A:259:ILE:O	3:A:514:EDO:H21	1.88	0.73
1:A:71:ARG:HG2	3:A:523:EDO:H11	1.69	0.73
1:A:62:MET:HG3	1:B:354:MET:HE1	1.71	0.72
1:B:147:GLY:O	1:B:151:TYR:HB3	1.91	0.71
1:B:32:THR:CG2	1:B:35:GLN:HB2	2.21	0.70
1:A:178:LYS:NZ	3:A:502:EDO:H12	2.07	0.70
3:A:523:EDO:H21	1:B:156:LEU:O	1.92	0.69
1:A:158:MET:HE3	1:A:361:THR:CG2	2.23	0.68
1:B:285:ARG:HH21	1:B:289:LEU:HD12	1.57	0.68
1:B:11:LEU:H	3:B:503:EDO:C2	2.06	0.68
1:B:267:GLN:HB3	1:B:292:ILE:HG12	1.75	0.66
1:A:178:LYS:HZ2	3:A:502:EDO:H12	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:ARG:HG3	1:B:340:ALA:HB3	1.77	0.65
1:B:273:ILE:O	1:B:277:GLN:HG3	1.97	0.64
1:B:149:ASP:OD1	3:B:506:EDO:H21	1.96	0.64
1:A:383:ILE:H	3:A:508:EDO:H12	1.62	0.64
1:B:129:ALA:H	4:B:508:GOL:H12	1.62	0.64
1:B:190:GLY:H	3:B:516:EDO:H22	1.62	0.64
1:B:227:PRO:O	1:B:231:GLU:HG3	1.98	0.64
1:B:222:PHE:H	3:B:509:EDO:H11	1.63	0.63
1:A:149:ASP:OD2	4:A:522:GOL:H12	1.99	0.62
1:B:118:VAL:HG23	1:B:126:ALA:HB3	1.81	0.61
1:A:60:MET:HE2	1:B:144:TRP:NE1	2.16	0.60
1:A:204:LEU:HD21	1:A:272:VAL:HG13	1.84	0.60
1:A:44:LYS:NZ	3:A:506:EDO:H11	2.17	0.60
1:A:60:MET:HE2	1:B:144:TRP:CE2	2.39	0.58
1:A:196:HIS:HB3	3:A:528:EDO:C2	2.33	0.58
3:A:523:EDO:H21	1:B:156:LEU:CA	2.33	0.58
1:A:110:LEU:HD21	1:B:354:MET:HG3	1.86	0.58
1:A:44:LYS:HZ2	3:A:506:EDO:H11	1.68	0.58
1:B:293:ASP:OD2	1:B:296:LYS:HD3	2.04	0.57
1:B:382:ARG:NH2	1:B:400:GLU:OE1	2.38	0.57
3:A:523:EDO:H12	1:B:159:PRO:CD	2.34	0.56
3:A:523:EDO:H12	1:B:159:PRO:CG	2.36	0.56
1:B:10:SER:CA	3:B:503:EDO:H22	2.33	0.56
1:B:222:PHE:N	3:B:509:EDO:H11	2.19	0.56
3:B:507:EDO:H11	6:B:693:HOH:O	2.05	0.56
1:B:103:ILE:O	1:B:107:ILE:HG12	2.06	0.56
1:B:154:VAL:HG21	1:B:178:LYS:HD3	1.87	0.56
1:A:60:MET:HG3	5:A:527:SO4:O4	2.06	0.56
1:A:196:HIS:HB3	3:A:528:EDO:O2	2.05	0.55
1:A:309:ARG:HG2	1:A:310:ARG:HG3	1.89	0.55
1:B:247:TRP:HA	1:B:250:GLN:OE1	2.07	0.55
1:B:277:GLN:O	1:B:285:ARG:HD2	2.07	0.55
1:B:173:ARG:HD3	1:B:315:PHE:HE1	1.72	0.54
1:A:178:LYS:HZ2	3:A:502:EDO:C1	2.21	0.54
1:B:351:PHE:HB3	1:B:352:PRO:HD3	1.89	0.54
1:B:222:PHE:H	3:B:509:EDO:C1	2.22	0.53
1:B:288:GLN:OE1	1:B:290:MET:HE3	2.09	0.53
1:A:331:MET:HB3	1:A:335:SER:HB2	1.91	0.52
1:A:57:LEU:HD21	1:B:143:TRP:CD1	2.44	0.52
1:B:203:MET:CE	1:B:204:LEU:HD23	2.40	0.52
1:A:275:MET:HE2	4:A:512:GOL:C1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:504:EDO:H12	6:A:746:HOH:O	2.09	0.52
1:B:54:ARG:NE	6:B:602:HOH:O	2.28	0.52
1:B:129:ALA:N	4:B:508:GOL:H12	2.23	0.52
1:A:172:GLY:HA2	3:A:509:EDO:H22	1.92	0.51
1:A:219:PHE:HA	3:A:519:EDO:H22	1.91	0.51
1:B:37:GLU:HG3	1:B:38:ALA:N	2.25	0.51
1:B:203:MET:HE2	1:B:204:LEU:HD23	1.93	0.50
1:A:275:MET:CE	4:A:512:GOL:H11	2.39	0.50
1:B:129:ALA:H	4:B:508:GOL:C1	2.24	0.50
1:B:261:ILE:HG21	1:B:283:ASP:HB2	1.93	0.50
1:A:173:ARG:HG2	3:A:509:EDO:H11	1.92	0.50
4:A:521:GOL:H32	1:B:54:ARG:HD3	1.93	0.49
1:A:63:GLY:HA3	3:A:511:EDO:C1	2.43	0.49
1:B:277:GLN:HA	1:B:285:ARG:HD2	1.94	0.49
1:B:94:ALA:HB1	1:B:99:GLY:O	2.14	0.48
1:B:285:ARG:NH2	1:B:289:LEU:HD12	2.27	0.48
1:A:71:ARG:CG	3:A:523:EDO:H11	2.41	0.48
1:A:196:HIS:HB3	3:A:528:EDO:H11	1.96	0.48
1:B:295:HIS:HD2	6:B:607:HOH:O	1.97	0.48
1:B:10:SER:N	1:B:45:GLN:HE22	2.12	0.48
1:B:309:ARG:HG2	1:B:310:ARG:HG3	1.96	0.47
1:B:274:GLN:O	1:B:278:THR:HG23	2.14	0.47
1:B:369:GLU:O	1:B:373:ARG:HG3	2.14	0.47
1:A:346:ASN:OD1	1:B:109:TRP:CH2	2.68	0.47
1:B:11:LEU:H	3:B:503:EDO:H22	1.79	0.47
3:A:523:EDO:H21	1:B:156:LEU:C	2.39	0.47
1:B:285:ARG:HH21	1:B:289:LEU:CD1	2.25	0.47
1:A:103:ILE:O	1:A:107:ILE:HG12	2.15	0.47
3:A:511:EDO:H11	6:A:717:HOH:O	2.13	0.47
1:B:198:GLU:HG2	5:B:517:SO4:O2	2.15	0.47
1:A:275:MET:HB2	4:A:512:GOL:H12	1.95	0.47
1:B:32:THR:OG1	1:B:33:PRO:HD2	2.16	0.46
1:B:277:GLN:HA	1:B:285:ARG:CD	2.45	0.46
1:A:158:MET:HE3	1:A:361:THR:HG22	1.95	0.46
1:A:390:ASP:OD1	1:A:391:LYS:HG3	2.16	0.46
1:A:226:ALA:HB3	1:A:227:PRO:HD3	1.97	0.46
1:A:211:ALA:H	4:A:521:GOL:H11	1.80	0.46
1:B:173:ARG:HD3	1:B:315:PHE:CE1	2.51	0.46
1:A:350:TRP:HB2	3:A:510:EDO:H12	1.98	0.46
1:B:155:LEU:HD23	1:B:158:MET:HE3	1.98	0.46
1:B:283:ASP:N	1:B:283:ASP:OD1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:501:SAM:HG2	2:B:501:SAM:O	2.16	0.45
1:B:295:HIS:CB	1:B:296:LYS:HD2	2.46	0.45
1:B:331:MET:HB2	1:B:401:LYS:CE	2.47	0.45
1:B:34:GLN:HA	1:B:37:GLU:HG2	1.98	0.45
1:A:196:HIS:HB2	1:A:199:ARG:HD3	1.99	0.44
1:B:277:GLN:HA	1:B:285:ARG:NE	2.32	0.44
1:A:74:LEU:HD11	1:A:134:PHE:HD1	1.83	0.44
1:A:310:ARG:O	2:A:501:SAM:HE3	2.17	0.43
1:A:65:VAL:HG13	1:B:357:PHE:CD2	2.53	0.43
1:B:210:MET:HA	1:B:213:GLN:OE1	2.18	0.43
1:A:196:HIS:HB3	3:A:528:EDO:C1	2.48	0.43
1:A:146:MET:HE1	1:A:203:MET:CG	2.41	0.43
3:A:523:EDO:H12	1:B:159:PRO:HG2	2.01	0.43
1:B:223:SER:HB3	3:B:509:EDO:H22	2.00	0.43
1:B:293:ASP:CG	1:B:296:LYS:HD3	2.43	0.43
1:B:351:PHE:CE2	1:B:355:LEU:HD11	2.54	0.43
1:B:190:GLY:N	3:B:516:EDO:H22	2.31	0.42
1:A:52:LEU:HB3	1:A:53:PRO:HD2	2.00	0.42
1:A:271:GLY:O	4:A:512:GOL:H12	2.19	0.42
1:B:84:ASP:OD2	3:B:511:EDO:H22	2.20	0.42
1:A:106:ARG:NH1	1:B:169:GLU:OE2	2.50	0.42
1:B:11:LEU:HG	3:B:503:EDO:H21	2.02	0.42
1:A:71:ARG:HD2	1:A:71:ARG:HA	1.89	0.41
1:B:270:SER:HA	1:B:291:ALA:HB2	2.01	0.41
1:B:336:LYS:CD	1:B:400:GLU:HG2	2.50	0.41
1:A:261:ILE:HB	3:A:514:EDO:H11	2.02	0.41
1:A:346:ASN:HA	1:A:347:PRO:C	2.45	0.41
1:B:309:ARG:HG3	1:B:340:ALA:CB	2.45	0.40
1:B:226:ALA:HB3	1:B:227:PRO:HD3	2.03	0.40
1:A:57:LEU:HD21	1:B:143:TRP:HD1	1.87	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	389/409 (95%)	380 (98%)	9 (2%)	0	100	100
1	B	391/409 (96%)	380 (97%)	11 (3%)	0	100	100
All	All	780/818 (95%)	760 (97%)	20 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	325/338 (96%)	324 (100%)	1 (0%)	86	92
1	B	325/338 (96%)	325 (100%)	0	100	100
All	All	650/676 (96%)	649 (100%)	1 (0%)	87	94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	346	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](#)

46 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	$\# Z > 2$
3	EDO	A	502	-	3,3,3	0.32	0	2,2,2	0.84	0
3	EDO	A	511	-	3,3,3	0.38	0	2,2,2	0.53	0
3	EDO	B	504	-	3,3,3	0.46	0	2,2,2	0.46	0
3	EDO	A	520	-	3,3,3	0.48	0	2,2,2	0.32	0
5	SO4	B	518	-	4,4,4	0.32	0	6,6,6	0.23	0
3	EDO	A	514	-	3,3,3	0.42	0	2,2,2	0.36	0
4	GOL	B	508	-	5,5,5	1.00	0	5,5,5	1.05	0
3	EDO	A	517	-	3,3,3	0.49	0	2,2,2	0.33	0
3	EDO	B	509	-	3,3,3	0.46	0	2,2,2	0.25	0
3	EDO	A	523	-	3,3,3	0.41	0	2,2,2	0.39	0
5	SO4	A	525	-	4,4,4	0.27	0	6,6,6	0.20	0
3	EDO	B	512	-	3,3,3	0.42	0	2,2,2	0.40	0
4	GOL	A	512	-	5,5,5	0.93	0	5,5,5	1.11	0
5	SO4	A	526	-	4,4,4	0.26	0	6,6,6	0.09	0
3	EDO	A	509	-	3,3,3	0.56	0	2,2,2	0.17	0
3	EDO	A	515	-	3,3,3	0.51	0	2,2,2	0.27	0
3	EDO	B	515	-	3,3,3	0.60	0	2,2,2	0.27	0
3	EDO	B	503	-	3,3,3	0.45	0	2,2,2	0.34	0
4	GOL	A	521	-	5,5,5	0.88	0	5,5,5	1.31	1 (20%)
5	SO4	A	527	-	4,4,4	0.24	0	6,6,6	0.33	0
3	EDO	B	507	-	3,3,3	0.49	0	2,2,2	0.45	0
4	GOL	A	503	-	5,5,5	0.86	0	5,5,5	1.30	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SAM	B	501	-	27,29,29	1.13	4 (14%)	34,42,42	2.01	9 (26%)
3	EDO	A	510	-	3,3,3	0.55	0	2,2,2	0.30	0
3	EDO	A	528	-	3,3,3	0.34	0	2,2,2	0.84	0
3	EDO	B	506	-	3,3,3	0.51	0	2,2,2	0.35	0
3	EDO	B	516	-	3,3,3	0.43	0	2,2,2	0.52	0
3	EDO	A	507	-	3,3,3	0.57	0	2,2,2	0.36	0
5	SO4	A	524	-	4,4,4	0.28	0	6,6,6	0.37	0
3	EDO	B	513	-	3,3,3	0.41	0	2,2,2	0.52	0
3	EDO	A	508	-	3,3,3	0.49	0	2,2,2	0.46	0
3	EDO	A	506	-	3,3,3	0.41	0	2,2,2	0.69	0
3	EDO	A	516	-	3,3,3	0.52	0	2,2,2	0.35	0
3	EDO	A	504	-	3,3,3	0.60	0	2,2,2	0.31	0
3	EDO	A	513	-	3,3,3	0.45	0	2,2,2	0.36	0
2	SAM	A	501	-	27,29,29	1.13	3 (11%)	34,42,42	1.88	9 (26%)
3	EDO	B	505	-	3,3,3	0.41	0	2,2,2	0.67	0
3	EDO	A	518	-	3,3,3	0.49	0	2,2,2	0.25	0
3	EDO	A	519	-	3,3,3	0.46	0	2,2,2	0.47	0
3	EDO	B	502	-	3,3,3	0.44	0	2,2,2	0.52	0
3	EDO	B	510	-	3,3,3	0.52	0	2,2,2	0.29	0
3	EDO	B	511	-	3,3,3	0.43	0	2,2,2	0.54	0
4	GOL	A	522	-	5,5,5	1.17	0	5,5,5	0.96	0
3	EDO	A	505	-	3,3,3	0.44	0	2,2,2	0.31	0
5	SO4	B	517	-	4,4,4	0.21	0	6,6,6	0.28	0
3	EDO	B	514	-	3,3,3	0.55	0	2,2,2	0.32	0

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
3	EDO	A	502	-	-	1/1/1/1	-
3	EDO	A	511	-	-	1/1/1/1	-
3	EDO	B	504	-	-	0/1/1/1	-
3	EDO	A	520	-	-	0/1/1/1	-
3	EDO	A	514	-	-	0/1/1/1	-
4	GOL	B	508	-	-	1/4/4/4	-
3	EDO	A	517	-	-	0/1/1/1	-
3	EDO	B	509	-	-	0/1/1/1	-
3	EDO	A	523	-	-	0/1/1/1	-
3	EDO	B	512	-	-	0/1/1/1	-
4	GOL	A	512	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	509	-	-	1/1/1/1	-
3	EDO	A	515	-	-	0/1/1/1	-
3	EDO	B	515	-	-	1/1/1/1	-
3	EDO	B	503	-	-	0/1/1/1	-
4	GOL	A	521	-	-	2/4/4/4	-
3	EDO	B	507	-	-	0/1/1/1	-
4	GOL	A	503	-	-	0/4/4/4	-
2	SAM	B	501	-	-	3/17/33/33	0/3/3/3
3	EDO	A	510	-	-	1/1/1/1	-
3	EDO	A	528	-	-	0/1/1/1	-
3	EDO	B	506	-	-	0/1/1/1	-
3	EDO	B	516	-	-	0/1/1/1	-
3	EDO	A	507	-	-	0/1/1/1	-
3	EDO	B	513	-	-	0/1/1/1	-
3	EDO	A	508	-	-	1/1/1/1	-
3	EDO	A	506	-	-	0/1/1/1	-
3	EDO	A	516	-	-	0/1/1/1	-
3	EDO	A	504	-	-	0/1/1/1	-
3	EDO	A	513	-	-	1/1/1/1	-
2	SAM	A	501	-	-	1/17/33/33	0/3/3/3
3	EDO	B	505	-	-	0/1/1/1	-
3	EDO	A	518	-	-	0/1/1/1	-
3	EDO	A	519	-	-	0/1/1/1	-
3	EDO	B	502	-	-	0/1/1/1	-
3	EDO	B	510	-	-	0/1/1/1	-
3	EDO	B	511	-	-	0/1/1/1	-
4	GOL	A	522	-	-	2/4/4/4	-
3	EDO	A	505	-	-	0/1/1/1	-
3	EDO	B	514	-	-	0/1/1/1	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	SAM	C2-N1	2.78	1.38	1.33
2	B	501	SAM	C2-N1	2.74	1.38	1.33
2	B	501	SAM	C2-N3	2.69	1.38	1.33
2	A	501	SAM	C2-N3	2.55	1.38	1.33
2	A	501	SAM	OXT-C	-2.51	1.22	1.30
2	B	501	SAM	OXT-C	-2.20	1.23	1.30
2	B	501	SAM	C8-N7	2.18	1.35	1.31

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	SAM	N3-C2-N1	-5.70	119.96	128.58
2	A	501	SAM	N3-C2-N1	-5.33	120.51	128.58
2	B	501	SAM	C5-C4-N3	-4.25	120.87	126.72
2	B	501	SAM	N9-C8-N7	-4.17	108.02	113.94
2	A	501	SAM	C5-C4-N3	-4.08	121.10	126.72
2	A	501	SAM	N9-C8-N7	-3.81	108.53	113.94
2	B	501	SAM	C5-N7-C8	3.46	108.89	103.45
2	B	501	SAM	C2-N3-C4	3.44	120.22	111.83
2	A	501	SAM	C5-N7-C8	3.28	108.61	103.45
2	A	501	SAM	C2-N3-C4	3.19	119.62	111.83
2	B	501	SAM	OXT-C-O	-3.14	116.95	124.08
2	B	501	SAM	N3-C4-N9	3.03	132.32	127.17
2	A	501	SAM	N3-C4-N9	2.76	131.86	127.17
2	A	501	SAM	OXT-C-O	-2.67	118.02	124.08
2	B	501	SAM	C4-N9-C8	2.46	108.32	105.74
4	A	503	GOL	C3-C2-C1	-2.46	102.77	111.80
2	A	501	SAM	C4-C5-N7	-2.35	107.89	110.58
2	B	501	SAM	C4-C5-N7	-2.29	107.96	110.58
4	A	521	GOL	C3-C2-C1	-2.13	104.00	111.80
2	A	501	SAM	C4-N9-C8	2.08	107.93	105.74

There are no chirality outliers.

All (17) torsion outliers are listed below:

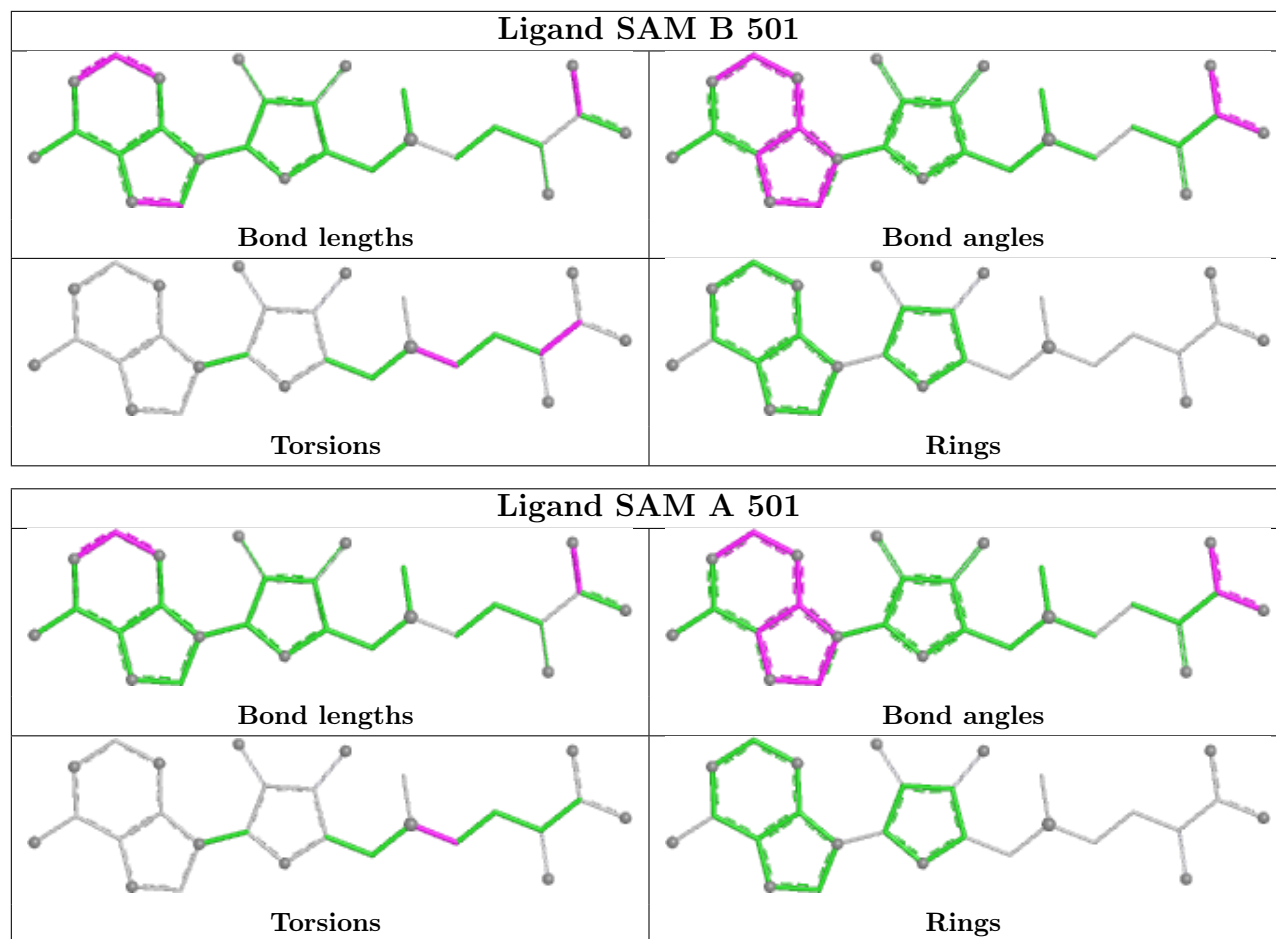
Mol	Chain	Res	Type	Atoms
4	A	522	GOL	O1-C1-C2-C3
4	A	522	GOL	O1-C1-C2-O2
3	A	509	EDO	O1-C1-C2-O2
3	A	502	EDO	O1-C1-C2-O2
3	B	515	EDO	O1-C1-C2-O2
4	A	521	GOL	O1-C1-C2-C3
3	A	511	EDO	O1-C1-C2-O2
2	B	501	SAM	OXT-C-CA-CB
2	A	501	SAM	CB-CG-SD-C5'
2	B	501	SAM	O-C-CA-CB
3	A	510	EDO	O1-C1-C2-O2
4	B	508	GOL	O1-C1-C2-O2
4	A	521	GOL	O1-C1-C2-O2
3	A	508	EDO	O1-C1-C2-O2
4	A	512	GOL	O1-C1-C2-C3
3	A	513	EDO	O1-C1-C2-O2
2	B	501	SAM	CB-CG-SD-C5'

There are no ring outliers.

27 monomers are involved in 65 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	EDO	3	0
3	A	511	EDO	3	0
3	A	514	EDO	4	0
4	B	508	GOL	5	0
3	B	509	EDO	5	0
3	A	523	EDO	9	0
3	B	512	EDO	1	0
4	A	512	GOL	5	0
3	A	509	EDO	2	0
3	B	503	EDO	5	0
4	A	521	GOL	2	0
5	A	527	SO4	1	0
3	B	507	EDO	1	0
2	B	501	SAM	1	0
3	A	510	EDO	1	0
3	A	528	EDO	4	0
3	B	506	EDO	1	0
3	B	516	EDO	2	0
3	A	508	EDO	1	0
3	A	506	EDO	2	0
3	A	504	EDO	1	0
2	A	501	SAM	1	0
3	A	518	EDO	1	0
3	A	519	EDO	1	0
3	B	511	EDO	1	0
4	A	522	GOL	1	0
5	B	517	SO4	1	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

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	392/409 (95%)	-0.48	3 (0%) 82 86	15, 29, 49, 77	1 (0%)
1	B	393/409 (96%)	0.08	27 (6%) 23 26	22, 34, 83, 101	0
All	All	785/818 (95%)	-0.20	30 (3%) 44 50	15, 31, 64, 101	1 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	269	LEU	4.7
1	B	292	ILE	4.6
1	B	247	TRP	4.6
1	B	278	THR	4.3
1	B	279	VAL	4.1
1	B	209	ALA	3.8
1	B	283	ASP	3.6
1	B	207	MET	3.5
1	B	211	ALA	3.4
1	B	205	ILE	3.2
1	B	284	ILE	3.2
1	B	276	VAL	3.1
1	B	206	SER	3.0
1	B	272	VAL	3.0
1	B	273	ILE	3.0
1	A	28	GLY	2.9
1	A	30	SER	2.8
1	B	289	LEU	2.8
1	B	214	TYR	2.7
1	B	268	ASP	2.7
1	B	120	GLU	2.7
1	B	280	GLY	2.7
1	B	212	SER	2.7
1	B	282	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	30	SER	2.3
1	B	210	MET	2.3
1	A	31	THR	2.2
1	B	151	TYR	2.2
1	B	290	MET	2.1
1	B	216	HIS	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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	EDO	B	505	4/4	0.73	0.17	45,48,51,52	0
4	GOL	A	521	6/6	0.73	0.20	33,37,38,50	0
3	EDO	A	502	4/4	0.75	0.16	31,38,38,41	0
3	EDO	A	514	4/4	0.77	0.23	46,52,52,53	0
3	EDO	B	516	4/4	0.78	0.19	43,49,52,57	0
3	EDO	A	508	4/4	0.78	0.15	40,45,47,50	0
3	EDO	B	514	4/4	0.79	0.17	47,48,48,52	0
3	EDO	A	520	4/4	0.79	0.16	49,51,55,63	0
3	EDO	A	519	4/4	0.79	0.16	47,47,52,56	0
3	EDO	A	515	4/4	0.81	0.16	46,48,57,58	0
3	EDO	A	516	4/4	0.81	0.15	44,45,46,50	0
3	EDO	B	510	4/4	0.83	0.15	41,46,47,50	0
2	SAM	B	501	27/27	0.84	0.12	40,63,68,69	0
3	EDO	B	509	4/4	0.84	0.15	47,48,50,57	0
3	EDO	B	503	4/4	0.84	0.11	36,40,42,42	0
3	EDO	B	511	4/4	0.85	0.12	45,51,53,58	0
3	EDO	B	504	4/4	0.85	0.14	40,46,52,54	0

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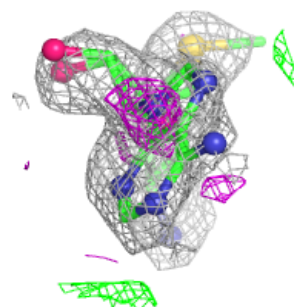
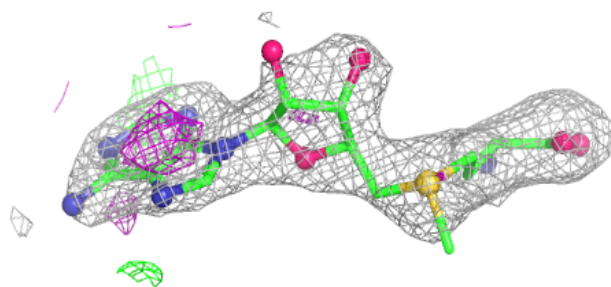
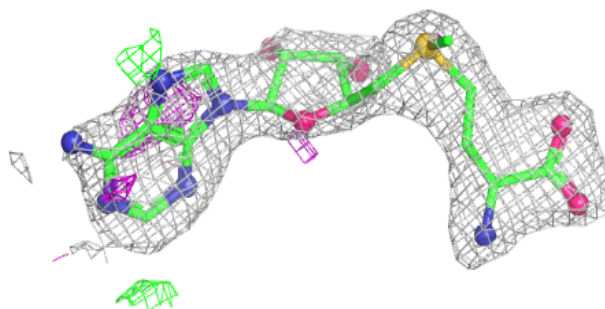
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	522	6/6	0.85	0.12	27,43,47,49	0
4	GOL	B	508	6/6	0.85	0.12	44,52,60,62	0
5	SO4	A	525	5/5	0.85	0.17	49,66,83,104	0
3	EDO	B	515	4/4	0.86	0.14	36,39,45,46	0
3	EDO	B	506	4/4	0.86	0.12	33,39,43,43	0
3	EDO	B	507	4/4	0.86	0.14	32,40,41,44	0
3	EDO	A	513	4/4	0.87	0.16	41,44,44,49	0
3	EDO	A	506	4/4	0.87	0.13	30,37,44,46	0
3	EDO	A	528	4/4	0.87	0.13	40,42,45,45	0
3	EDO	A	509	4/4	0.87	0.18	35,39,40,54	0
3	EDO	A	510	4/4	0.87	0.14	44,44,46,49	0
3	EDO	A	518	4/4	0.87	0.12	38,44,44,49	0
3	EDO	A	505	4/4	0.88	0.16	39,41,41,42	0
3	EDO	A	504	4/4	0.88	0.12	28,39,40,40	0
3	EDO	A	517	4/4	0.89	0.14	34,43,44,57	0
3	EDO	A	507	4/4	0.90	0.12	33,34,37,38	0
4	GOL	A	512	6/6	0.90	0.15	34,45,47,52	0
3	EDO	B	512	4/4	0.90	0.22	36,44,50,50	0
3	EDO	A	511	4/4	0.91	0.25	33,34,34,41	0
3	EDO	B	513	4/4	0.91	0.11	44,44,46,61	0
5	SO4	A	527	5/5	0.91	0.11	32,36,41,46	5
5	SO4	B	518	5/5	0.91	0.11	45,55,66,68	0
5	SO4	A	524	5/5	0.92	0.15	46,49,56,60	0
3	EDO	B	502	4/4	0.93	0.08	31,35,36,37	0
3	EDO	A	523	4/4	0.94	0.19	27,32,44,44	0
4	GOL	A	503	6/6	0.95	0.08	27,34,37,39	0
5	SO4	A	526	5/5	0.96	0.16	48,54,79,85	0
5	SO4	B	517	5/5	0.97	0.08	39,44,46,50	0
2	SAM	A	501	27/27	0.97	0.06	19,24,26,30	0

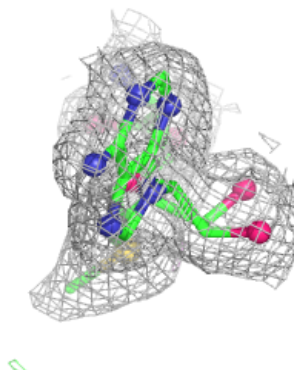
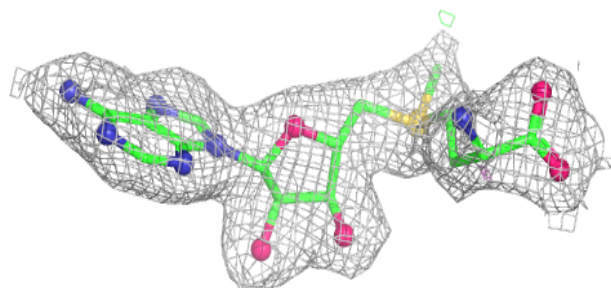
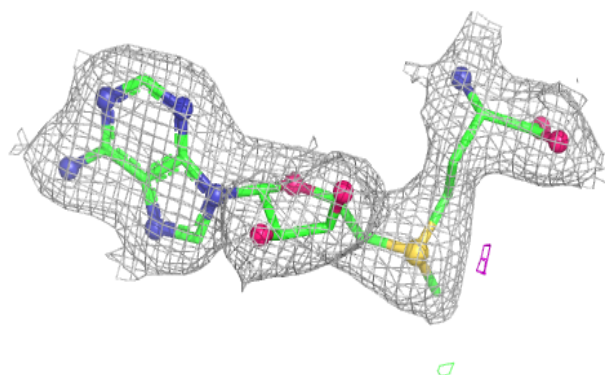
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around SAM A 501:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.