



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 02:30 AM UTC

PDB ID : 5ZQK / pdb_00005zqk
Title : Dengue Virus Non Structural Protein 5
Authors : El Sahili, A.; Soh, T.S.; Schiltz, J.; Gharbi-Ayachi, A.; Goh, B.C.; Seh, C.C.;
Dedon, P.C.; Shi, P.Y.; Lim, S.P.; Lescar, J.
Deposited on : 2018-04-19
Resolution : 2.30 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

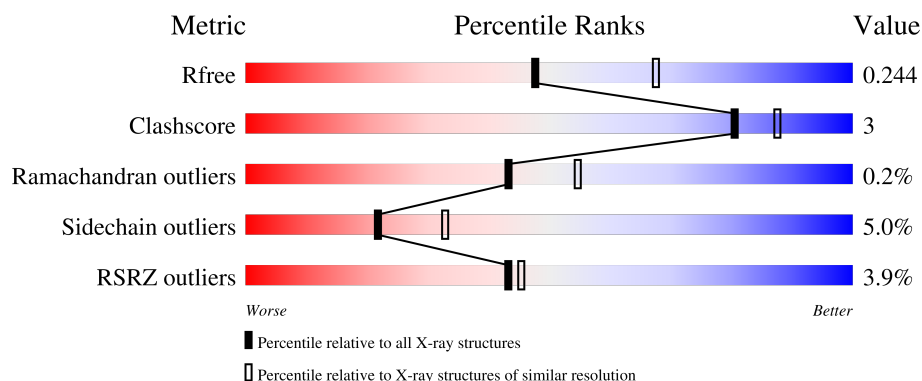
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	923	4% 83% 11% • 5%
1	B	923	3% 81% 12% • 5%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15082 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 Non Structural Protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	874	Total	C	N	O	S	0	1	0
			7044	4428	1264	1307	45			
1	B	875	Total	C	N	O	S	0	3	0
			7065	4442	1268	1310	45			

There are 46 discrepancies between the modelled and reference sequences:

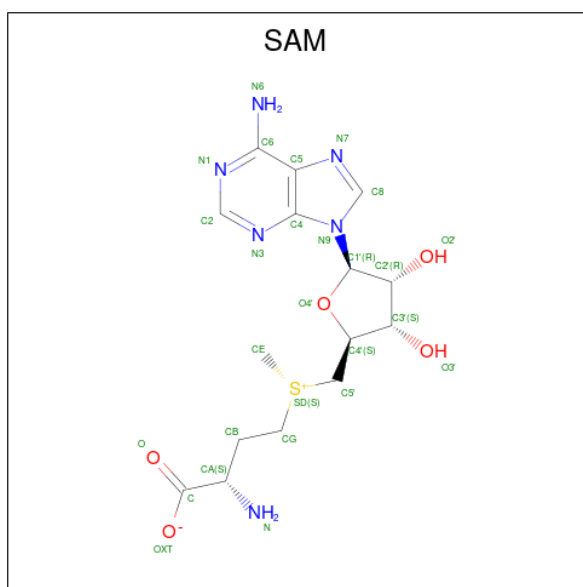
Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	expression tag	UNP H9M652
A	-21	HIS	-	expression tag	UNP H9M652
A	-20	HIS	-	expression tag	UNP H9M652
A	-19	HIS	-	expression tag	UNP H9M652
A	-18	HIS	-	expression tag	UNP H9M652
A	-17	HIS	-	expression tag	UNP H9M652
A	-16	HIS	-	expression tag	UNP H9M652
A	-15	SER	-	expression tag	UNP H9M652
A	-14	SER	-	expression tag	UNP H9M652
A	-13	GLY	-	expression tag	UNP H9M652
A	-12	VAL	-	expression tag	UNP H9M652
A	-11	ASP	-	expression tag	UNP H9M652
A	-10	LEU	-	expression tag	UNP H9M652
A	-9	GLY	-	expression tag	UNP H9M652
A	-8	THR	-	expression tag	UNP H9M652
A	-7	GLU	-	expression tag	UNP H9M652
A	-6	ASN	-	expression tag	UNP H9M652
A	-5	LEU	-	expression tag	UNP H9M652
A	-4	TYR	-	expression tag	UNP H9M652
A	-3	PHE	-	expression tag	UNP H9M652
A	-2	GLN	-	expression tag	UNP H9M652
A	-1	SER	-	expression tag	UNP H9M652
A	0	MET	-	expression tag	UNP H9M652
B	-22	MET	-	expression tag	UNP H9M652
B	-21	HIS	-	expression tag	UNP H9M652

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	HIS	-	expression tag	UNP H9M652
B	-19	HIS	-	expression tag	UNP H9M652
B	-18	HIS	-	expression tag	UNP H9M652
B	-17	HIS	-	expression tag	UNP H9M652
B	-16	HIS	-	expression tag	UNP H9M652
B	-15	SER	-	expression tag	UNP H9M652
B	-14	SER	-	expression tag	UNP H9M652
B	-13	GLY	-	expression tag	UNP H9M652
B	-12	VAL	-	expression tag	UNP H9M652
B	-11	ASP	-	expression tag	UNP H9M652
B	-10	LEU	-	expression tag	UNP H9M652
B	-9	GLY	-	expression tag	UNP H9M652
B	-8	THR	-	expression tag	UNP H9M652
B	-7	GLU	-	expression tag	UNP H9M652
B	-6	ASN	-	expression tag	UNP H9M652
B	-5	LEU	-	expression tag	UNP H9M652
B	-4	TYR	-	expression tag	UNP H9M652
B	-3	PHE	-	expression tag	UNP H9M652
B	-2	GLN	-	expression tag	UNP H9M652
B	-1	SER	-	expression tag	UNP H9M652
B	0	MET	-	expression tag	UNP H9M652

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



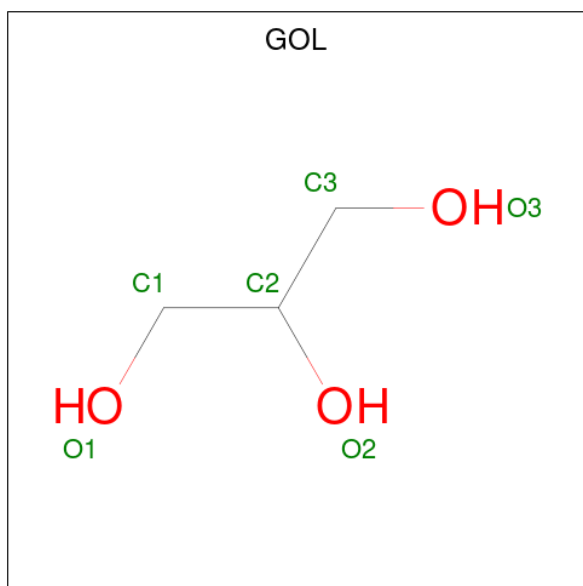
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

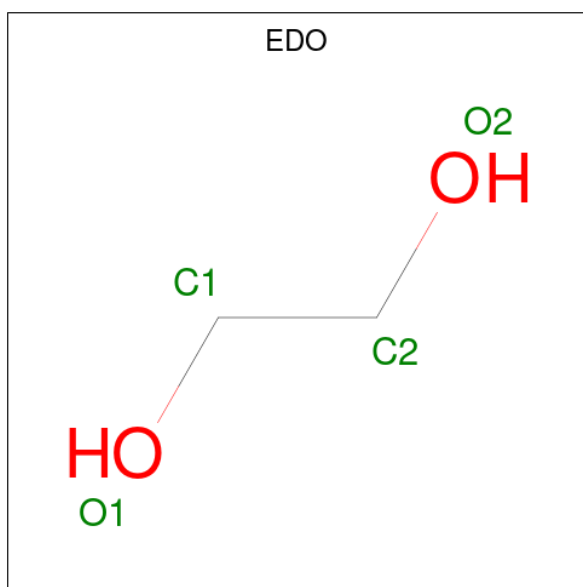


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Zn	0	0
			2	2		
4	B	2	Total	Zn	0	0
			2	2		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	2	Total	Mg	0	0
			2	2		

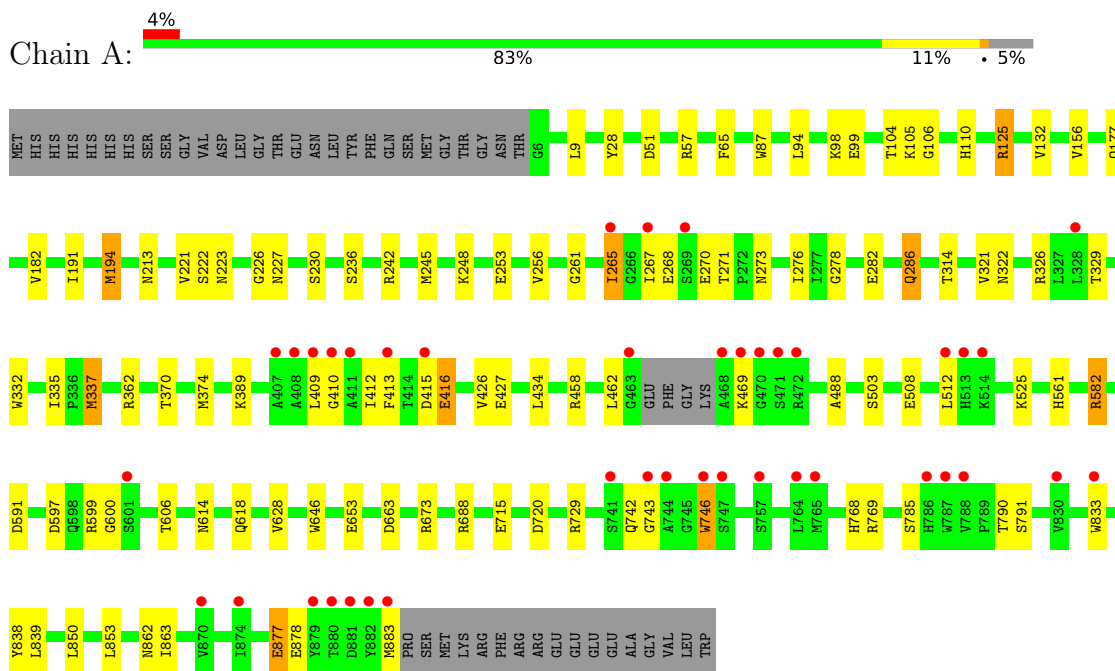
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	457	Total	O	0	0
			457	457		
7	B	436	Total	O	0	0
			436	436		

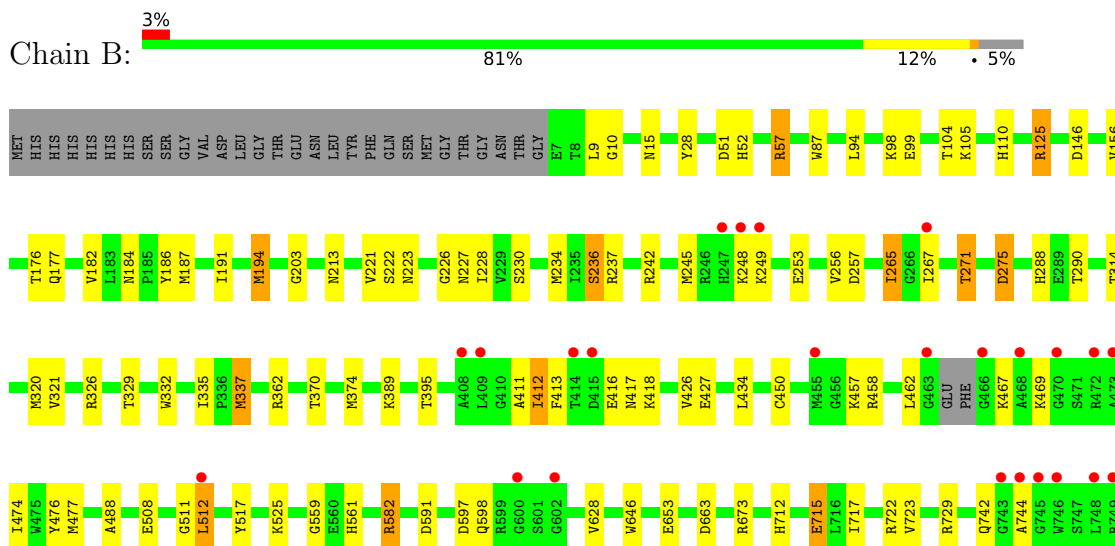
3 Residue-property plots [i](#)

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: Non Structural Protein 5



• Molecule 1: Non Structural Protein 5





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.68Å 146.10Å 97.24Å 90.00° 105.45° 90.00°	Depositor
Resolution (Å)	46.00 – 2.30 46.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.00-2.30) 99.7 (46.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.29Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.196 , 0.235 0.202 , 0.244	Depositor DCC
R_{free} test set	5152 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	49.7	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15082	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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: MG, SAM, EDO, GOL, ZN

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	0.88	1/7204 (0.0%)	1.39	43/9731 (0.4%)
1	B	0.88	2/7228 (0.0%)	1.40	49/9761 (0.5%)
All	All	0.88	3/14432 (0.0%)	1.39	92/19492 (0.5%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	194	MET	SD-CE	-11.45	1.50	1.79
1	B	194	MET	SD-CE	-9.48	1.55	1.79
1	B	234	MET	SD-CE	5.86	1.94	1.79

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	418	LYS	N-CA-C	-12.16	100.76	114.62
1	B	673	ARG	CA-C-N	7.53	130.37	120.28
1	B	673	ARG	C-N-CA	7.53	130.37	120.28
1	B	275	ASP	CA-CB-CG	7.39	119.99	112.60
1	A	673	ARG	CA-C-N	7.33	130.11	120.28
1	A	673	ARG	C-N-CA	7.33	130.11	120.28
1	A	663	ASP	N-CA-C	-7.22	104.47	113.28
1	B	57	ARG	CA-C-N	7.19	127.92	119.94
1	B	57	ARG	C-N-CA	7.19	127.92	119.94
1	A	597	ASP	CA-CB-CG	6.63	119.23	112.60
1	B	271	THR	CB-CA-C	6.52	116.98	110.33
1	A	413	PHE	CA-CB-CG	6.45	120.25	113.80
1	B	663	ASP	CA-CB-CG	6.29	118.89	112.60
1	A	28	TYR	CA-C-N	6.16	128.82	120.38
1	A	28	TYR	C-N-CA	6.16	128.82	120.38
1	B	288	HIS	CA-C-N	6.05	128.67	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	288	HIS	C-N-CA	6.05	128.67	120.38
1	B	830	VAL	N-CA-CB	5.92	117.17	110.72
1	A	51	ASP	CA-CB-CG	5.90	118.50	112.60
1	B	28	TYR	CA-C-N	5.79	128.31	120.38
1	B	28	TYR	C-N-CA	5.79	128.31	120.38
1	B	87	TRP	CA-C-N	5.72	127.87	120.44
1	B	87	TRP	C-N-CA	5.72	127.87	120.44
1	B	511	GLY	CA-C-N	5.62	128.13	120.54
1	B	511	GLY	C-N-CA	5.62	128.13	120.54
1	B	329	THR	CA-C-N	5.59	127.08	120.09
1	B	329	THR	C-N-CA	5.59	127.08	120.09
1	B	156	VAL	CA-C-N	5.58	127.76	120.28
1	B	156	VAL	C-N-CA	5.58	127.76	120.28
1	A	503	SER	N-CA-C	-5.53	100.27	109.46
1	B	105	LYS	CA-C-N	-5.45	115.77	122.75
1	B	105	LYS	C-N-CA	-5.45	115.77	122.75
1	A	329	THR	CA-C-N	5.41	126.85	120.09
1	A	329	THR	C-N-CA	5.41	126.85	120.09
1	A	862	ASN	CA-CB-CG	5.39	117.99	112.60
1	B	236	SER	CA-C-N	5.38	127.43	120.44
1	B	236	SER	C-N-CA	5.38	127.43	120.44
1	B	843	GLU	CA-C-N	5.37	127.47	120.28
1	B	843	GLU	C-N-CA	5.37	127.47	120.28
1	A	839	LEU	N-CA-C	-5.37	103.81	110.41
1	A	226	GLY	CA-C-N	5.36	128.38	120.82
1	A	226	GLY	C-N-CA	5.36	128.38	120.82
1	A	222	SER	N-CA-C	5.31	117.07	111.28
1	A	322	ASN	CA-C-N	5.29	125.85	119.98
1	A	322	ASN	C-N-CA	5.29	125.85	119.98
1	B	450	CYS	CA-C-N	5.27	130.04	123.14
1	B	450	CYS	C-N-CA	5.27	130.04	123.14
1	B	434	LEU	CA-C-N	5.27	127.19	120.56
1	B	434	LEU	C-N-CA	5.27	127.19	120.56
1	A	286	GLN	CB-CG-CD	5.26	121.55	112.60
1	B	758	TYR	CA-C-N	5.26	127.28	120.44
1	B	758	TYR	C-N-CA	5.26	127.28	120.44
1	B	51	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	833	TRP	CA-C-N	5.26	127.33	120.28
1	A	833	TRP	C-N-CA	5.26	127.33	120.28
1	A	278	GLY	N-CA-C	5.25	119.23	112.83
1	A	156	VAL	CA-C-N	5.24	127.30	120.28
1	A	156	VAL	C-N-CA	5.24	127.30	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	663	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	248	LYS	N-CA-C	-5.23	101.18	109.96
1	A	87	TRP	CA-C-N	5.22	127.54	120.44
1	A	87	TRP	C-N-CA	5.22	127.54	120.44
1	B	808	ASP	CA-CB-CG	5.22	117.82	112.60
1	B	191	ILE	CA-C-N	5.22	127.22	120.44
1	B	191	ILE	C-N-CA	5.22	127.22	120.44
1	A	94	LEU	CA-C-N	5.21	128.63	120.82
1	A	94	LEU	C-N-CA	5.21	128.63	120.82
1	A	191	ILE	CA-C-N	5.17	127.16	120.44
1	A	191	ILE	C-N-CA	5.17	127.16	120.44
1	A	688	ARG	CA-C-N	5.17	128.81	121.42
1	A	688	ARG	C-N-CA	5.17	128.81	121.42
1	A	512	LEU	CA-C-N	5.17	128.16	120.31
1	A	512	LEU	C-N-CA	5.17	128.16	120.31
1	B	15	ASN	CA-C-N	5.14	127.12	120.44
1	B	15	ASN	C-N-CA	5.14	127.12	120.44
1	A	65	PHE	CA-C-N	5.14	127.03	120.56
1	A	65	PHE	C-N-CA	5.14	127.03	120.56
1	A	434	LEU	CA-C-N	5.14	127.03	120.56
1	A	434	LEU	C-N-CA	5.14	127.03	120.56
1	B	839	LEU	N-CA-C	-5.13	104.10	110.41
1	B	395	THR	CA-C-N	5.11	127.13	120.28
1	B	395	THR	C-N-CA	5.11	127.13	120.28
1	B	94	LEU	CA-C-N	5.09	128.45	120.82
1	B	94	LEU	C-N-CA	5.09	128.45	120.82
1	A	261	GLY	N-CA-C	5.08	117.98	112.29
1	B	413	PHE	CA-CB-CG	5.07	118.87	113.80
1	B	559	GLY	CA-C-N	5.07	127.07	120.28
1	B	559	GLY	C-N-CA	5.07	127.07	120.28
1	A	236	SER	CA-C-N	5.05	127.00	120.44
1	A	236	SER	C-N-CA	5.05	127.00	120.44
1	B	226	GLY	CA-C-N	5.03	128.24	121.05
1	B	226	GLY	C-N-CA	5.03	128.24	121.05

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	7044	0	6943	31	0
1	B	7065	0	6973	43	0
2	A	27	0	22	1	0
2	B	27	0	22	2	0
3	A	6	0	8	1	0
3	B	6	0	8	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	4	0	6	0	0
5	B	4	0	6	3	0
6	B	2	0	0	0	0
7	A	457	0	0	2	0
7	B	436	0	0	3	0
All	All	15082	0	13988	74	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 3.

All (74) 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:182:VAL:HG21	1:B:194:MET:HE3	1.69	0.75
1:B:227:ASN:HD22	1:B:230:SER:H	1.35	0.72
1:A:227:ASN:HD22	1:A:230:SER:H	1.37	0.72
1:B:290:THR:HG22	7:B:1304:HOH:O	1.89	0.72
1:A:213:ASN:HD21	1:A:242:ARG:HH11	1.38	0.71
1:B:213:ASN:HD21	1:B:242:ARG:HH11	1.36	0.71
1:B:237:ARG:HH12	5:B:1007:EDO:H12	1.56	0.70
1:A:177:GLN:HE22	1:A:223:ASN:HD21	1.42	0.67
1:A:582:ARG:HD3	1:A:591:ASP:OD2	1.94	0.67
1:B:582:ARG:HD3	1:B:591:ASP:OD2	1.94	0.67
1:A:282:GLU:O	1:A:286:GLN:HG2	1.97	0.65
1:A:99:GLU:HG3	1:A:125:ARG:HH21	1.64	0.63
1:B:177:GLN:HE22	1:B:223:ASN:HD21	1.44	0.62
1:B:754:LEU:HD13	1:B:791:SER:HB3	1.83	0.60
1:B:457:LYS:HB2	1:B:474:ILE:HG12	1.84	0.60
1:B:99:GLU:HG3	1:B:125:ARG:HH21	1.67	0.59
1:A:106:GLY:O	1:A:110:HIS:HB2	2.03	0.58
1:A:321:VAL:HG11	1:A:326:ARG:HD2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:TRP:HA	1:A:335:ILE:HD12	1.87	0.57
1:B:332:TRP:HA	1:B:335:ILE:HD12	1.87	0.56
1:A:769:ARG:HH11	1:A:769:ARG:HG2	1.70	0.55
1:B:769:ARG:HH11	1:B:769:ARG:HG2	1.70	0.55
1:A:182:VAL:HG21	1:A:194:MET:HE3	1.88	0.55
1:A:273:ASN:HD22	1:A:276:ILE:HG12	1.72	0.55
1:B:321:VAL:HG11	1:B:326:ARG:HD2	1.88	0.54
1:A:458:ARG:HH21	1:A:743:GLY:HA2	1.73	0.54
1:A:242:ARG:HA	1:A:245:MET:HG2	1.89	0.54
1:B:597:ASP:O	1:B:598:GLN:HB2	2.07	0.53
1:A:746:TRP:HA	1:A:746:TRP:CE3	2.44	0.53
1:B:337:MET:HB3	7:B:1494:HOH:O	2.08	0.52
1:A:335:ILE:HG23	1:A:337:MET:HE2	1.92	0.52
1:B:512:LEU:HD22	1:B:765:MET:HE3	1.92	0.52
1:B:768:HIS:HA	1:B:838:TYR:HA	1.93	0.51
1:B:320:MET:HE3	1:B:744:ALA:HB2	1.93	0.51
1:A:488:ALA:O	1:A:561:HIS:HE1	1.94	0.50
1:A:768:HIS:HA	1:A:838:TYR:HA	1.94	0.50
1:B:146:ASP:HB3	2:B:1001:SAM:HG1	1.94	0.49
1:B:9:LEU:HB3	1:B:236:SER:HB3	1.92	0.49
1:B:52:HIS:HD2	1:B:257:ASP:OD1	1.95	0.48
1:B:335:ILE:HG23	1:B:337:MET:HE2	1.94	0.48
1:B:488:ALA:O	1:B:561:HIS:HE1	1.96	0.48
1:A:410:GLY:HA3	7:A:1196:HOH:O	2.15	0.46
1:B:412:ILE:HA	1:B:477:MET:O	2.16	0.45
1:B:411:ALA:HB1	1:B:476:TYR:CD2	2.53	0.44
1:A:614:ASN:O	1:A:618:GLN:HG2	2.17	0.44
1:B:628:VAL:HG21	1:B:646:TRP:CD1	2.53	0.44
1:A:877:GLU:HA	7:A:1391:HOH:O	2.17	0.42
1:B:411:ALA:HB1	1:B:476:TYR:CG	2.54	0.42
1:A:132:VAL:HG13	2:A:1001:SAM:H2	2.01	0.42
1:B:98:LYS:HA	1:B:265:ILE:HG12	2.01	0.42
1:B:863:ILE:HG21	1:B:883:MET:HE2	2.01	0.42
1:A:599:ARG:HG2	1:A:606:THR:HG23	2.00	0.42
1:A:600:GLY:HA2	3:A:1002:GOL:O3	2.19	0.42
1:A:370:THR:HG22	1:A:374:MET:HE2	2.02	0.42
1:B:850:LEU:O	1:B:853:LEU:HB2	2.20	0.42
1:A:227:ASN:ND2	1:A:230:SER:H	2.12	0.42
1:B:203:GLY:HA3	1:B:221:VAL:O	2.20	0.41
1:B:370:THR:HG22	1:B:374:MET:HE2	2.00	0.41
1:B:517:TYR:HB3	1:B:823:TRP:CE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:712:HIS:HD2	7:B:1493:HOH:O	2.03	0.41
1:A:628:VAL:HG21	1:A:646:TRP:CD1	2.54	0.41
1:A:863:ILE:HG21	1:A:883:MET:HE2	2.02	0.41
1:B:457:LYS:HD2	1:B:474:ILE:HD11	2.03	0.41
1:B:184:ASN:OD1	1:B:187:MET:HG2	2.20	0.41
1:B:237:ARG:HH22	5:B:1007:EDO:H12	1.86	0.41
1:B:715:GLU:HG2	1:B:723:VAL:CG1	2.50	0.41
1:A:98:LYS:HA	1:A:265:ILE:HG12	2.03	0.41
1:A:850:LEU:O	1:A:853:LEU:HB2	2.21	0.41
1:B:227:ASN:ND2	1:B:230:SER:H	2.10	0.41
1:B:237:ARG:NH1	5:B:1007:EDO:H12	2.32	0.41
1:A:182:VAL:CG2	1:A:194:MET:HE3	2.50	0.41
1:B:10:GLY:HA3	1:B:186:TYR:CG	2.56	0.40
1:B:722:ARG:HD2	1:B:824:MET:SD	2.61	0.40
1:B:110:HIS:HD2	2:B:1001:SAM:O2'	2.04	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	871/923 (94%)	840 (96%)	29 (3%)	2 (0%)	43	55
1	B	874/923 (95%)	843 (96%)	30 (3%)	1 (0%)	48	60
All	All	1745/1846 (94%)	1683 (96%)	59 (3%)	3 (0%)	43	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	416	GLU
1	B	467	LYS
1	A	791	SER

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	759/800 (95%)	721 (95%)	38 (5%)	22	33
1	B	762/800 (95%)	724 (95%)	38 (5%)	22	33
All	All	1521/1600 (95%)	1445 (95%)	76 (5%)	22	33

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	57	ARG
1	A	104	THR
1	A	105	LYS
1	A	125	ARG
1	A	221	VAL
1	A	253	GLU
1	A	256	VAL
1	A	265	ILE
1	A	267	ILE
1	A	268	GLU
1	A	270	GLU
1	A	271	THR
1	A	314	THR
1	A	337	MET
1	A	362	ARG
1	A	389	LYS
1	A	409	LEU
1	A	412	ILE
1	A	415	ASP
1	A	416	GLU
1	A	426	VAL
1	A	427	GLU
1	A	462	LEU
1	A	469	LYS
1	A	508	GLU
1	A	525	LYS

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Mol	Chain	Res	Type
1	A	582	ARG
1	A	653	GLU
1	A	715	GLU
1	A	720	ASP
1	A	729	ARG
1	A	742	GLN
1	A	746	TRP
1	A	785	SER
1	A	790	THR
1	A	877	GLU
1	A	878	GLU
1	B	57	ARG
1	B	104	THR
1	B	125	ARG
1	B	176	THR
1	B	222	SER
1	B	228	ILE
1	B	245	MET
1	B	248	LYS
1	B	249	LYS
1	B	253	GLU
1	B	256	VAL
1	B	265	ILE
1	B	267	ILE
1	B	271	THR
1	B	275	ASP
1	B	314	THR
1	B	337	MET
1	B	362	ARG
1	B	389	LYS
1	B	412	ILE
1	B	416	GLU
1	B	417	ASN
1	B	426	VAL
1	B	427	GLU
1	B	458	ARG
1	B	462	LEU
1	B	469	LYS
1	B	508	GLU
1	B	512	LEU
1	B	525	LYS
1	B	582	ARG

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Mol	Chain	Res	Type
1	B	653	GLU
1	B	715	GLU
1	B	717	ILE
1	B	729	ARG
1	B	742	GLN
1	B	785	SER
1	B	790	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	34	GLN
1	A	110	HIS
1	A	127	GLN
1	A	170	ASN
1	A	213	ASN
1	A	223	ASN
1	A	227	ASN
1	A	273	ASN
1	A	513	HIS
1	A	555	ASN
1	A	561	HIS
1	A	575	ASN
1	A	618	GLN
1	A	622	GLN
1	A	633	GLN
1	A	712	HIS
1	A	731	GLN
1	A	760	GLN
1	A	786	HIS
1	A	801	HIS
1	A	862	ASN
1	A	864	GLN
1	B	26	GLN
1	B	34	GLN
1	B	52	HIS
1	B	96	ASN
1	B	110	HIS
1	B	170	ASN
1	B	213	ASN
1	B	223	ASN

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Mol	Chain	Res	Type
1	B	227	ASN
1	B	273	ASN
1	B	288	HIS
1	B	406	ASN
1	B	417	ASN
1	B	513	HIS
1	B	555	ASN
1	B	561	HIS
1	B	575	ASN
1	B	603	GLN
1	B	622	GLN
1	B	633	GLN
1	B	712	HIS
1	B	731	GLN
1	B	801	HIS
1	B	864	GLN

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](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SAM	B	1001	-	27,29,29	0.55	0	34,42,42	0.55	1 (2%)
2	SAM	A	1001	-	27,29,29	0.45	0	34,42,42	0.55	0
3	GOL	B	1002	-	5,5,5	0.09	0	5,5,5	0.27	0
3	GOL	A	1002	-	5,5,5	0.12	0	5,5,5	0.24	0
5	EDO	A	1005	-	3,3,3	0.48	0	2,2,2	0.51	0
5	EDO	B	1007	-	3,3,3	0.69	0	2,2,2	0.23	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
2	SAM	B	1001	-	-	0/17/33/33	0/3/3/3
2	SAM	A	1001	-	-	1/17/33/33	0/3/3/3
3	GOL	B	1002	-	-	1/4/4/4	-
3	GOL	A	1002	-	-	2/4/4/4	-
5	EDO	A	1005	-	-	0/1/1/1	-
5	EDO	B	1007	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	SAM	CG-SD-C5'	-2.10	98.31	103.43

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1002	GOL	C1-C2-C3-O3
3	A	1002	GOL	O2-C2-C3-O3
3	B	1002	GOL	C1-C2-C3-O3
2	A	1001	SAM	C2'-C1'-N9-C8

There are no ring outliers.

4 monomers are involved in 7 short contacts:

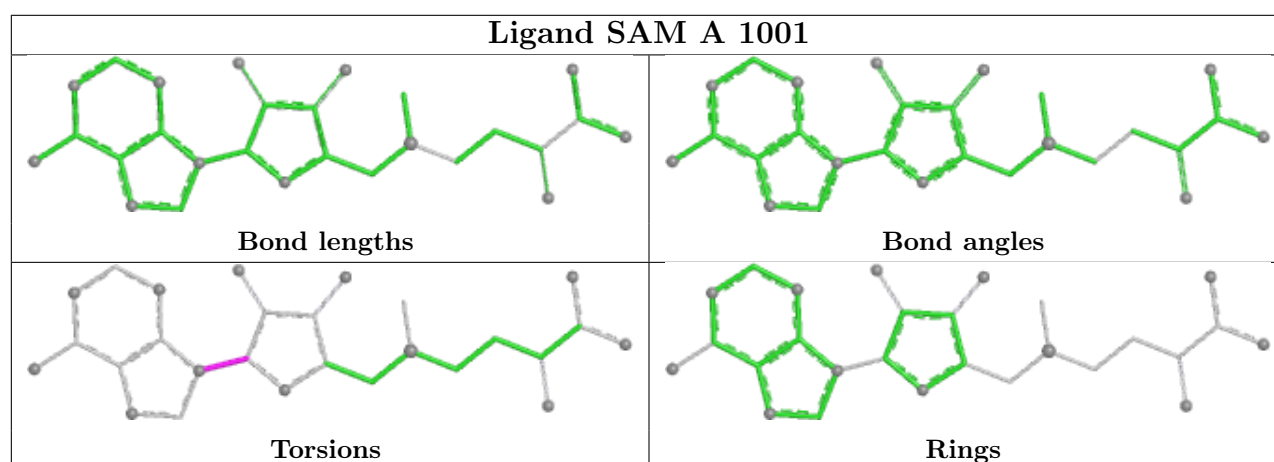
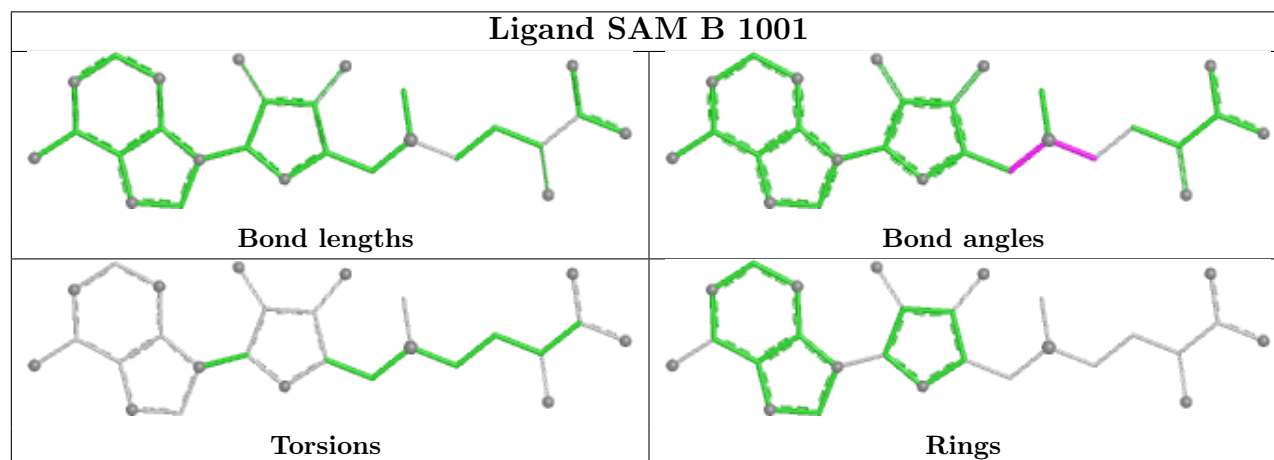
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1001	SAM	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	SAM	1	0
3	A	1002	GOL	1	0
5	B	1007	EDO	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.



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	874/923 (94%)	0.30	41 (4%)	36 38	24, 56, 91, 125	1 (0%)
1	B	875/923 (94%)	0.23	27 (3%)	51 53	25, 56, 89, 118	3 (0%)
All	All	1749/1846 (94%)	0.26	68 (3%)	43 45	24, 56, 90, 125	4 (0%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	745	GLY	4.9
1	A	746	TRP	4.5
1	B	744	ALA	4.4
1	A	409	LEU	4.3
1	B	512	LEU	4.2
1	B	743	GLY	4.1
1	A	744	ALA	4.0
1	A	471	SER	3.8
1	B	247	HIS	3.6
1	A	883	MET	3.5
1	B	746	TRP	3.5
1	A	879	TYR	3.5
1	B	414	THR	3.5
1	B	795	TRP	3.4
1	B	765	MET	3.4
1	A	514	LYS	3.4
1	A	407	ALA	3.3
1	B	415	ASP	3.2
1	B	602	GLY	3.2
1	A	513	HIS	3.2
1	B	408	ALA	3.1
1	A	882	TYR	3.0
1	B	463	GLY	3.0
1	A	468	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	466	GLY	2.9
1	B	468	ALA	2.9
1	A	470	GLY	2.9
1	A	463	GLY	2.8
1	A	472	ARG	2.8
1	A	601	SER	2.7
1	A	786	HIS	2.7
1	A	743	GLY	2.7
1	A	765	MET	2.7
1	A	267	ILE	2.7
1	B	248	LYS	2.7
1	A	413	PHE	2.7
1	B	472	ARG	2.6
1	A	512	LEU	2.6
1	A	870	VAL	2.5
1	A	408	ALA	2.5
1	A	469	LYS	2.5
1	A	410	GLY	2.5
1	B	409	LEU	2.4
1	A	881	ASP	2.4
1	B	749	ARG	2.4
1	A	874	ILE	2.3
1	A	328	LEU	2.3
1	B	600	GLY	2.3
1	A	880	THR	2.3
1	A	269	SER	2.3
1	B	267	ILE	2.3
1	A	833	TRP	2.3
1	A	411	ALA	2.2
1	A	787	TRP	2.2
1	A	788	VAL	2.2
1	B	455	MET	2.2
1	A	747	SER	2.2
1	A	757	SER	2.2
1	A	764	LEU	2.2
1	B	249	LYS	2.1
1	B	748	LEU	2.1
1	A	415	ASP	2.1
1	A	741	SER	2.1
1	B	473	ALA	2.1
1	B	873	LEU	2.1
1	A	830	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	265	ILE	2.0
1	B	470	GLY	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](#)

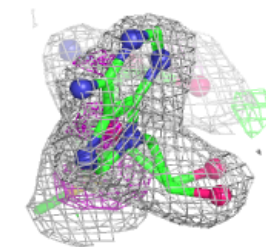
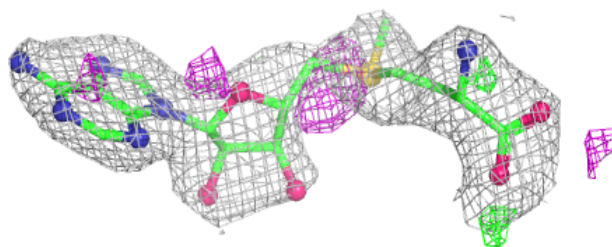
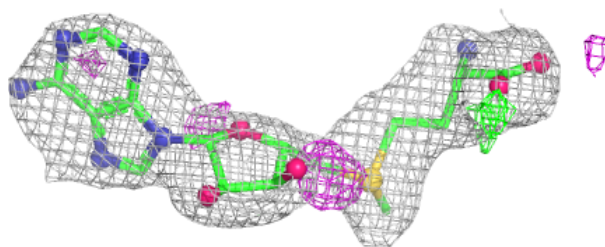
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
6	MG	B	1003	1/1	0.74	0.24	80,80,80,80	0
3	GOL	A	1002	6/6	0.84	0.13	63,65,65,66	0
6	MG	B	1004	1/1	0.84	0.17	75,75,75,75	0
5	EDO	A	1005	4/4	0.85	0.25	72,73,74,74	0
2	SAM	B	1001	27/27	0.87	0.14	60,74,79,80	0
3	GOL	B	1002	6/6	0.91	0.12	52,57,58,61	0
2	SAM	A	1001	27/27	0.92	0.10	49,57,63,66	0
5	EDO	B	1007	4/4	0.92	0.15	43,51,58,62	0
4	ZN	A	1003	1/1	0.99	0.05	55,55,55,55	0
4	ZN	B	1005	1/1	1.00	0.02	52,52,52,52	0
4	ZN	B	1006	1/1	1.00	0.05	57,57,57,57	0
4	ZN	A	1004	1/1	1.00	0.03	53,53,53,53	0

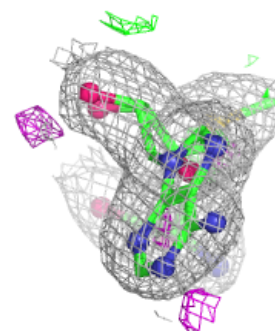
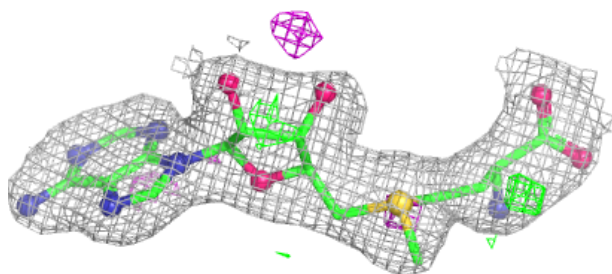
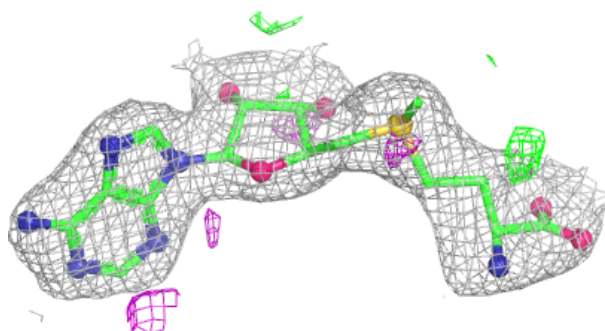
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAM B 1001:

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

**Electron density around SAM A 1001:**

$2mF_o-DF_c$ (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.