



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 06:05 PM EDT

PDB ID : 3X0D / pdb_00003x0d
Title : Crystal structure of C.elegans PRMT7 in complex with SAH (P43212)
Authors : Hasegawa, M.; Toma-Fukai, S.; Shimizu, T.
Deposited on : 2014-10-10
Resolution : 2.15 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

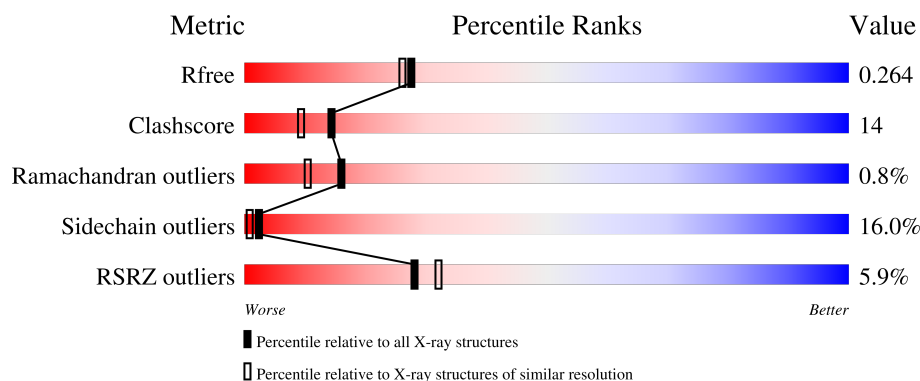
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	655	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5082 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.

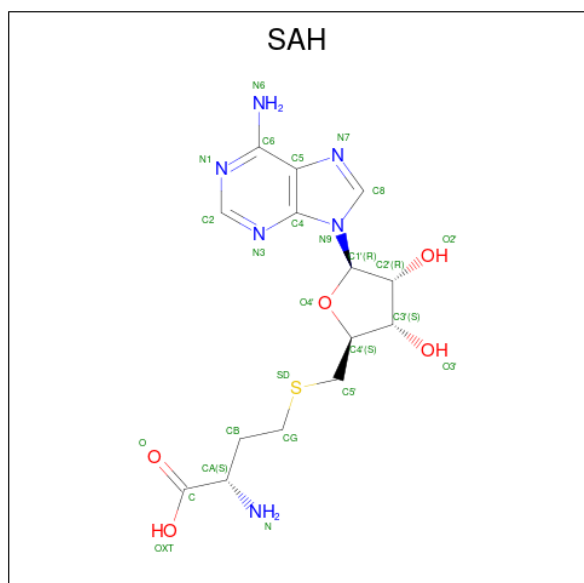
- Molecule 1 is a protein called Protein arginine N-methyltransferase 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	624	4964	3156	834	945	29	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	expression tag	UNP Q9XW42
A	-6	PRO	-	expression tag	UNP Q9XW42
A	-5	LEU	-	expression tag	UNP Q9XW42
A	-4	GLY	-	expression tag	UNP Q9XW42
A	-3	SER	-	expression tag	UNP Q9XW42
A	-2	GLY	-	expression tag	UNP Q9XW42
A	-1	ILE	-	expression tag	UNP Q9XW42
A	0	PRO	-	expression tag	UNP Q9XW42

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: C₁₄H₂₀N₆O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

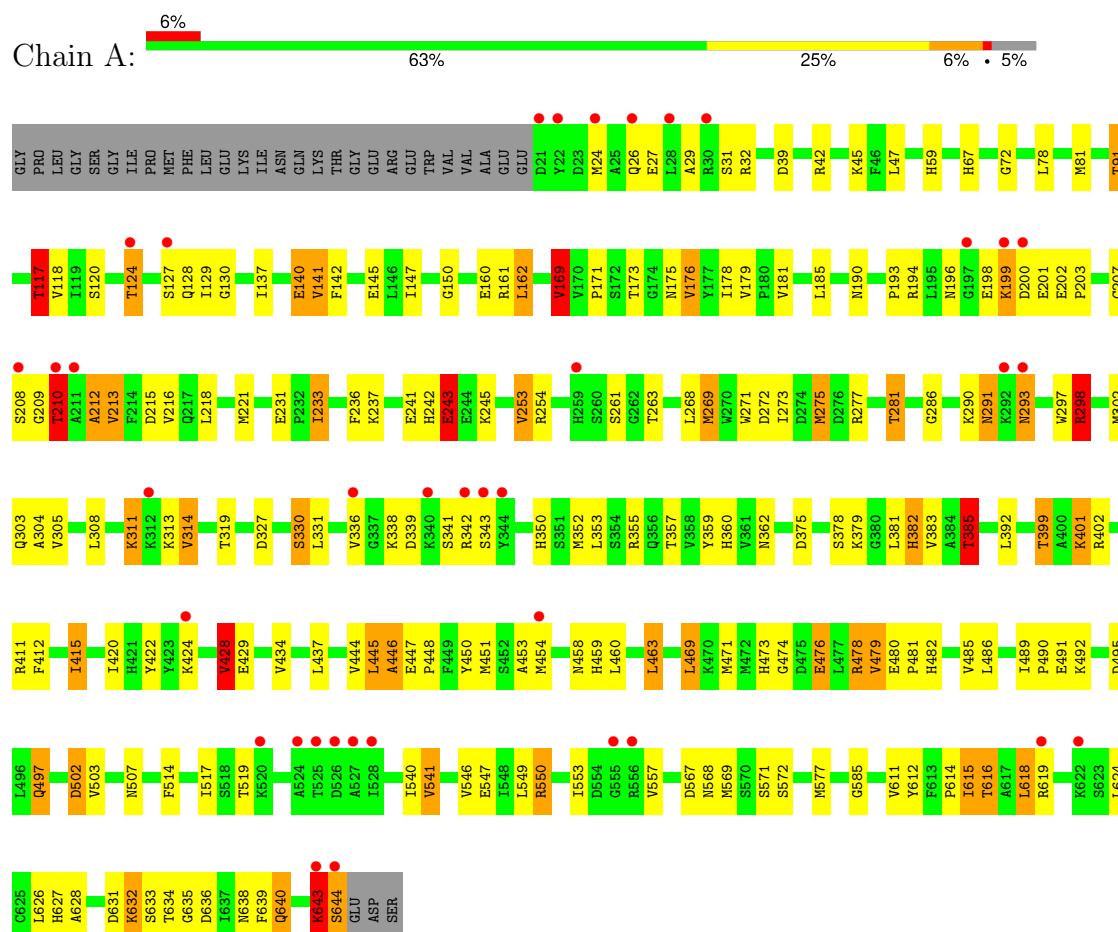
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	91	Total	O	0	0
			91	91		

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: Protein arginine N-methyltransferase 7



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	114.18Å 114.18Å 184.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.12 – 2.15 31.12 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.3 (31.12-2.15) 99.3 (31.12-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.220 , 0.266 0.218 , 0.264	Depositor DCC
R_{free} test set	3355 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	55.1	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 30.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5082	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.27% 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: SAH, 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	1.34	20/5074 (0.4%)	1.37	39/6855 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	382	HIS	CG-CD2	8.21	1.44	1.35
1	A	179	VAL	N-CA	-6.76	1.40	1.45
1	A	381	LEU	N-CA	6.67	1.53	1.45
1	A	502	ASP	C-O	-6.47	1.16	1.23
1	A	382	HIS	CE1-NE2	6.33	1.38	1.32
1	A	281	THR	CA-C	6.17	1.59	1.52
1	A	474	GLY	N-CA	5.99	1.51	1.45
1	A	117	THR	CA-C	5.90	1.59	1.52
1	A	360	HIS	CG-CD2	5.77	1.42	1.35
1	A	142	PHE	CA-C	-5.77	1.45	1.52
1	A	429	GLU	CA-C	5.70	1.59	1.52
1	A	350	HIS	CE1-NE2	5.57	1.38	1.32
1	A	263	THR	CA-C	5.43	1.59	1.52
1	A	385	THR	CB-CG2	-5.41	1.34	1.52
1	A	59	HIS	ND1-CE1	5.32	1.37	1.32
1	A	59	HIS	CG-CD2	5.16	1.41	1.35
1	A	422	TYR	N-CA	-5.15	1.40	1.46
1	A	242	HIS	CG-CD2	5.13	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	150	GLY	N-CA	5.11	1.52	1.45
1	A	446	ALA	CA-C	-5.05	1.46	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	473	HIS	CA-C-N	-12.71	109.69	122.27
1	A	473	HIS	C-N-CA	-12.71	109.69	122.27
1	A	428	VAL	N-CA-C	9.37	121.76	108.36
1	A	302	MET	N-CA-C	-7.54	98.46	108.19
1	A	473	HIS	N-CA-C	-7.46	97.12	109.80
1	A	179	VAL	CB-CA-C	-7.14	102.95	110.16
1	A	281	THR	CB-CA-C	6.52	120.99	110.16
1	A	209	GLY	N-CA-C	-6.17	104.86	112.33
1	A	298	ARG	NE-CZ-NH2	-6.01	113.79	119.20
1	A	196	ASN	N-CA-C	5.94	120.54	112.88
1	A	291	ASN	N-CA-C	-5.92	98.19	110.80
1	A	213	VAL	CB-CA-C	5.87	118.18	110.91
1	A	141	VAL	N-CA-CB	-5.84	101.59	111.23
1	A	81	MET	N-CA-C	-5.77	105.08	111.36
1	A	298	ARG	CB-CG-CD	-5.76	98.06	111.30
1	A	207	CYS	CA-C-N	5.66	128.19	120.54
1	A	207	CYS	C-N-CA	5.66	128.19	120.54
1	A	253	VAL	CB-CA-C	5.61	117.87	110.91
1	A	231	GLU	CA-C-N	5.59	126.83	119.84
1	A	231	GLU	C-N-CA	5.59	126.83	119.84
1	A	635	GLY	N-CA-C	-5.59	107.61	115.32
1	A	286	GLY	CA-C-N	5.51	125.81	119.92
1	A	286	GLY	C-N-CA	5.51	125.81	119.92
1	A	385	THR	N-CA-CB	-5.50	101.93	110.57
1	A	474	GLY	N-CA-C	5.50	120.66	112.41
1	A	213	VAL	N-CA-CB	-5.41	104.83	110.72
1	A	298	ARG	NE-CZ-NH1	5.36	126.86	121.50
1	A	199	LYS	N-CA-C	-5.30	101.89	110.32
1	A	169	VAL	CB-CA-C	5.22	118.85	110.82
1	A	341	SER	N-CA-C	5.21	116.81	110.41
1	A	212	ALA	N-CA-C	-5.19	102.83	110.52
1	A	634	THR	N-CA-C	-5.14	107.40	113.97
1	A	585	GLY	CA-C-N	-5.13	116.68	122.48
1	A	585	GLY	C-N-CA	-5.13	116.68	122.48
1	A	120	SER	N-CA-C	5.12	118.64	110.70
1	A	147	ILE	N-CA-C	5.11	118.67	112.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	VAL	N-CA-C	5.03	115.92	108.23
1	A	272	ASP	CA-C-N	-5.02	116.14	123.06
1	A	272	ASP	C-N-CA	-5.02	116.14	123.06

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	198	GLU	Peptide
1	A	210	THR	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4964	0	4853	139	0
2	A	26	0	19	2	0
3	A	1	0	0	0	0
4	A	91	0	0	8	0
All	All	5082	0	4872	139	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 14.

All (139) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:MET:HA	1:A:275:MET:HE2	1.13	1.10
1:A:269:MET:HE2	1:A:304:ALA:HB3	1.31	1.09
1:A:199:LYS:HG2	1:A:200:ASP:HA	1.13	1.08
1:A:502:ASP:OD2	1:A:616:THR:HG21	1.58	1.04
1:A:67:HIS:HE1	1:A:91:THR:CG2	1.73	1.01
1:A:569:MET:HA	1:A:569:MET:HE2	1.40	1.00
1:A:171:PRO:HB3	1:A:275:MET:HE1	1.41	0.99
1:A:379:LYS:HA	1:A:399:THR:HG23	1.43	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:MET:HE2	1:A:275:MET:CA	1.92	0.99
1:A:269:MET:CE	1:A:304:ALA:HB3	1.92	0.98
1:A:489:ILE:HD13	1:A:541:VAL:HG21	1.42	0.96
1:A:450:TYR:H	1:A:459:HIS:HD2	1.12	0.95
1:A:490:PRO:HB3	1:A:569:MET:HE3	1.49	0.95
1:A:171:PRO:HB3	1:A:275:MET:CE	1.98	0.92
1:A:497:GLN:H	1:A:497:GLN:HE21	1.14	0.91
1:A:489:ILE:CD1	1:A:541:VAL:HG21	2.04	0.88
1:A:577:MET:HE1	1:A:639:PHE:CE1	2.09	0.88
1:A:210:THR:HB	1:A:212:ALA:H	1.38	0.87
1:A:275:MET:HA	1:A:275:MET:CE	2.02	0.87
1:A:199:LYS:CG	1:A:200:ASP:HA	2.01	0.87
1:A:190:ASN:HD22	1:A:355:ARG:HH12	1.22	0.87
1:A:67:HIS:HE1	1:A:91:THR:HG22	1.42	0.84
1:A:450:TYR:H	1:A:459:HIS:CD2	1.95	0.84
1:A:378:SER:HB2	1:A:399:THR:HG22	1.61	0.81
1:A:67:HIS:CE1	1:A:91:THR:CG2	2.61	0.81
1:A:478:ARG:HH21	1:A:478:ARG:HG2	1.45	0.80
1:A:643:LYS:O	1:A:644:SER:HB2	1.84	0.78
1:A:480:GLU:OE2	1:A:482:HIS:HD2	1.67	0.76
1:A:489:ILE:HD13	1:A:541:VAL:CG2	2.16	0.75
1:A:269:MET:HE2	1:A:304:ALA:CB	2.17	0.72
1:A:497:GLN:H	1:A:497:GLN:NE2	1.85	0.72
1:A:275:MET:CA	1:A:275:MET:CE	2.66	0.72
1:A:392:LEU:O	1:A:392:LEU:HD23	1.89	0.72
1:A:117:THR:CG2	4:A:813:HOH:O	2.39	0.70
1:A:117:THR:HG22	4:A:813:HOH:O	1.93	0.69
1:A:39:ASP:OD2	1:A:298:ARG:HD3	1.94	0.68
1:A:627:HIS:HB2	1:A:640:GLN:HG2	1.74	0.68
1:A:67:HIS:HE1	1:A:91:THR:HG23	1.58	0.67
1:A:273:ILE:HD12	1:A:275:MET:HE1	1.77	0.67
1:A:497:GLN:HE21	1:A:497:GLN:N	1.90	0.66
1:A:547:GLU:OE2	1:A:550:ARG:NH1	2.28	0.66
1:A:269:MET:CE	1:A:304:ALA:CB	2.73	0.64
1:A:454:MET:H	1:A:458:ASN:HD22	1.46	0.63
1:A:569:MET:CE	1:A:572:SER:HB2	2.27	0.63
1:A:210:THR:HB	1:A:212:ALA:N	2.12	0.63
1:A:445:LEU:HD12	1:A:480:GLU:HB2	1.81	0.62
1:A:67:HIS:CE1	1:A:91:THR:HG22	2.29	0.62
1:A:379:LYS:CA	1:A:399:THR:HG23	2.25	0.62
1:A:489:ILE:CD1	1:A:541:VAL:CG2	2.77	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:VAL:HG13	1:A:241:GLU:HG2	1.82	0.61
1:A:269:MET:C	1:A:269:MET:HE3	2.27	0.60
1:A:434:VAL:CG1	1:A:469:LEU:HD13	2.32	0.60
1:A:32:ARG:HB3	1:A:514:PHE:HZ	1.68	0.58
1:A:353:LEU:HD22	1:A:357:THR:HG21	1.84	0.58
1:A:476:GLU:H	1:A:476:GLU:CD	2.11	0.58
1:A:478:ARG:HH21	1:A:478:ARG:CG	2.15	0.58
1:A:490:PRO:HB3	1:A:569:MET:CE	2.29	0.58
1:A:631:ASP:OD1	1:A:633:SER:HB3	2.05	0.57
1:A:434:VAL:HG13	1:A:469:LEU:HD13	1.85	0.57
1:A:615:ILE:HG22	1:A:618:LEU:HD22	1.87	0.57
1:A:375:ASP:O	1:A:399:THR:HG21	2.05	0.56
1:A:171:PRO:HB3	1:A:275:MET:HE2	1.85	0.56
1:A:626:LEU:HD23	1:A:626:LEU:C	2.29	0.56
1:A:218:LEU:H	1:A:303:GLN:HE21	1.54	0.55
1:A:268:LEU:N	1:A:268:LEU:HD23	2.22	0.55
1:A:478:ARG:HG2	1:A:478:ARG:NH2	2.20	0.55
1:A:569:MET:HA	1:A:569:MET:CE	2.24	0.54
1:A:399:THR:HB	4:A:814:HOH:O	2.08	0.54
1:A:411:ARG:O	1:A:415:ILE:HD12	2.07	0.54
1:A:460:LEU:HD22	1:A:463:LEU:HD22	1.89	0.53
1:A:261:SER:HA	1:A:314:VAL:O	2.08	0.53
1:A:385:THR:HG21	4:A:809:HOH:O	2.09	0.53
1:A:490:PRO:CB	1:A:569:MET:HE3	2.29	0.53
1:A:497:GLN:NE2	1:A:497:GLN:N	2.54	0.52
1:A:233:ILE:CD1	1:A:254:ARG:HB3	2.40	0.52
1:A:32:ARG:HB3	1:A:514:PHE:CZ	2.44	0.52
1:A:26:GLN:O	1:A:29:ALA:HB3	2.10	0.52
1:A:269:MET:HE3	1:A:269:MET:O	2.10	0.51
1:A:479:VAL:HG22	1:A:553:ILE:HG21	1.92	0.51
1:A:569:MET:HE1	1:A:572:SER:CB	2.41	0.51
1:A:67:HIS:CE1	1:A:91:THR:HG23	2.37	0.51
1:A:117:THR:HG23	4:A:813:HOH:O	2.08	0.51
1:A:569:MET:HE1	1:A:572:SER:HB2	1.91	0.51
1:A:632:LYS:O	1:A:632:LYS:HG2	2.09	0.51
1:A:401:LYS:CB	1:A:401:LYS:HZ3	2.23	0.51
1:A:353:LEU:HD22	1:A:357:THR:CG2	2.41	0.50
1:A:297:TRP:CE3	1:A:495:ASP:HB3	2.47	0.50
1:A:420:ILE:HG21	1:A:428:VAL:HG22	1.94	0.50
1:A:479:VAL:CG2	1:A:553:ILE:HG21	2.43	0.49
1:A:193:PRO:HA	1:A:362:ASN:ND2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:PRO:HA	1:A:362:ASN:HD21	1.77	0.48
1:A:275:MET:CE	1:A:275:MET:N	2.77	0.48
1:A:160:GLU:HG3	1:A:243:GLU:HG2	1.95	0.48
1:A:612:TYR:CE2	1:A:614:PRO:HA	2.49	0.48
1:A:490:PRO:CB	1:A:569:MET:CE	2.90	0.48
1:A:218:LEU:HD22	1:A:221:MET:HE2	1.96	0.47
1:A:453:ALA:HB1	1:A:458:ASN:HB2	1.95	0.47
1:A:492:LYS:HE3	1:A:571:SER:O	2.14	0.47
1:A:42:ARG:HH11	1:A:140:GLU:HG3	1.78	0.47
1:A:124:THR:O	1:A:161:ARG:NH2	2.48	0.47
1:A:643:LYS:O	1:A:644:SER:CB	2.59	0.47
1:A:178:ILE:HA	1:A:268:LEU:O	2.15	0.47
1:A:311:LYS:HB3	1:A:311:LYS:NZ	2.30	0.47
1:A:171:PRO:CB	1:A:275:MET:CE	2.83	0.47
1:A:502:ASP:CG	1:A:616:THR:HG21	2.36	0.47
1:A:569:MET:CE	1:A:572:SER:CB	2.92	0.47
1:A:171:PRO:CB	1:A:275:MET:HE1	2.30	0.46
1:A:627:HIS:O	1:A:639:PHE:HA	2.16	0.45
1:A:275:MET:HE2	1:A:275:MET:N	2.32	0.45
1:A:446:ALA:O	1:A:481:PRO:HD3	2.16	0.45
1:A:78:LEU:HD22	2:A:701:SAH:HN2	1.82	0.45
1:A:297:TRP:CD2	1:A:495:ASP:HB3	2.52	0.45
1:A:176:VAL:HG13	1:A:236:PHE:HB2	1.99	0.44
1:A:569:MET:HE2	1:A:572:SER:HB2	1.98	0.44
1:A:399:THR:HG23	1:A:399:THR:O	2.17	0.44
1:A:327:ASP:OD1	1:A:330:SER:HB2	2.18	0.44
1:A:628:ALA:HA	1:A:638:ASN:O	2.17	0.44
1:A:378:SER:HB2	1:A:399:THR:CG2	2.40	0.44
1:A:385:THR:CG2	4:A:801:HOH:O	2.66	0.43
1:A:491:GLU:O	1:A:572:SER:HB3	2.18	0.43
1:A:161:ARG:HB3	1:A:162:LEU:HD13	2.00	0.43
1:A:175:ASN:ND2	1:A:237:LYS:HG2	2.33	0.43
1:A:385:THR:HG23	4:A:801:HOH:O	2.18	0.43
1:A:547:GLU:CD	1:A:550:ARG:HH12	2.25	0.43
1:A:72:GLY:O	2:A:701:SAH:HB1	2.19	0.43
1:A:507:ASN:ND2	4:A:848:HOH:O	2.51	0.43
1:A:567:ASP:O	1:A:568:ASN:HB2	2.19	0.43
1:A:271:TRP:CZ3	1:A:273:ILE:HG12	2.54	0.42
1:A:401:LYS:HZ2	1:A:401:LYS:HG3	1.62	0.42
1:A:194:ARG:CG	1:A:194:ARG:HH11	2.33	0.42
1:A:145:GLU:OE1	1:A:215:ASP:OD1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:GLU:C	1:A:203:PRO:HD3	2.45	0.41
1:A:447:GLU:N	1:A:448:PRO:HA	2.35	0.41
1:A:352:MET:HG2	1:A:412:PHE:CZ	2.56	0.41
1:A:359:TYR:CD1	1:A:359:TYR:C	2.99	0.41
1:A:382:HIS:CG	1:A:402:ARG:HD3	2.56	0.40
1:A:137:ILE:HB	1:A:169:VAL:HB	2.02	0.40
1:A:169:VAL:HG22	1:A:171:PRO:O	2.22	0.40
1:A:293:ASN:HD22	1:A:293:ASN:C	2.29	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	622/655 (95%)	588 (94%)	29 (5%)	5 (1%)	16 10

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	643	LYS
1	A	243	GLU
1	A	619	ARG
1	A	130	GLY
1	A	291	ASN

5.3.2 Protein sidechains [i](#)

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	543/569 (95%)	456 (84%)	87 (16%)	2 1

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

Mol	Chain	Res	Type
1	A	24	MET
1	A	27	GLU
1	A	31	SER
1	A	45	LYS
1	A	47	LEU
1	A	91	THR
1	A	117	THR
1	A	124	THR
1	A	127	SER
1	A	128	GLN
1	A	129	ILE
1	A	140	GLU
1	A	141	VAL
1	A	162	LEU
1	A	169	VAL
1	A	173	THR
1	A	176	VAL
1	A	181	VAL
1	A	185	LEU
1	A	202	GLU
1	A	208	SER
1	A	210	THR
1	A	213	VAL
1	A	216	VAL
1	A	233	ILE
1	A	243	GLU
1	A	245	LYS
1	A	253	VAL
1	A	269	MET
1	A	275	MET
1	A	277	ARG
1	A	281	THR
1	A	290	LYS
1	A	293	ASN
1	A	298	ARG
1	A	305	VAL

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Mol	Chain	Res	Type
1	A	308	LEU
1	A	311	LYS
1	A	313	LYS
1	A	314	VAL
1	A	319	THR
1	A	330	SER
1	A	331	LEU
1	A	336	VAL
1	A	338	LYS
1	A	339	ASP
1	A	342	ARG
1	A	343	SER
1	A	383	VAL
1	A	385	THR
1	A	399	THR
1	A	401	LYS
1	A	415	ILE
1	A	424	LYS
1	A	428	VAL
1	A	437	LEU
1	A	444	VAL
1	A	445	LEU
1	A	451	MET
1	A	463	LEU
1	A	469	LEU
1	A	471	MET
1	A	476	GLU
1	A	478	ARG
1	A	479	VAL
1	A	485	VAL
1	A	486	LEU
1	A	497	GLN
1	A	503	VAL
1	A	517	ILE
1	A	519	THR
1	A	540	ILE
1	A	541	VAL
1	A	546	VAL
1	A	549	LEU
1	A	550	ARG
1	A	557	VAL
1	A	611	VAL

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Mol	Chain	Res	Type
1	A	615	ILE
1	A	616	THR
1	A	618	LEU
1	A	624	LEU
1	A	632	LYS
1	A	636	ASP
1	A	640	GLN
1	A	643	LYS
1	A	644	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	67	HIS
1	A	105	HIS
1	A	175	ASN
1	A	190	ASN
1	A	293	ASN
1	A	303	GLN
1	A	317	ASN
1	A	362	ASN
1	A	368	GLN
1	A	421	HIS
1	A	455	ASN
1	A	458	ASN
1	A	459	HIS
1	A	482	HIS
1	A	497	GLN
1	A	498	ASN
1	A	507	ASN
1	A	560	GLN
1	A	565	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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	SAH	A	701	-	27,28,28	1.62	4 (14%)	36,40,40	2.58	20 (55%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAH	A	701	-	-	0/15/31/31	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	SAH	C8-N7	4.71	1.40	1.31
2	A	701	SAH	C5-C4	4.46	1.47	1.39
2	A	701	SAH	C5-N7	-2.61	1.34	1.39
2	A	701	SAH	O4'-C1'	2.41	1.47	1.42

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	SAH	N3-C2-N1	-4.99	121.03	128.58
2	A	701	SAH	C5-C4-N3	-4.53	120.47	126.72
2	A	701	SAH	O4'-C4'-C5'	4.47	120.34	108.83
2	A	701	SAH	O4'-C1'-N9	-4.43	99.58	108.09
2	A	701	SAH	C2-N1-C6	3.63	124.70	118.73
2	A	701	SAH	N3-C4-N9	3.48	133.08	127.17
2	A	701	SAH	O3'-C3'-C4'	-3.41	101.28	111.08
2	A	701	SAH	C4-N9-C8	3.37	109.28	105.74
2	A	701	SAH	C4-N9-C1'	-3.27	118.99	126.63
2	A	701	SAH	O2'-C2'-C1'	-3.21	99.04	110.10
2	A	701	SAH	C2-N3-C4	3.12	119.45	111.83
2	A	701	SAH	N9-C8-N7	-3.10	109.53	113.94
2	A	701	SAH	C2'-C1'-N9	2.95	120.64	113.30
2	A	701	SAH	OXT-C-O	-2.80	117.73	124.08
2	A	701	SAH	CB-CA-N	2.54	116.74	110.12
2	A	701	SAH	C4-C5-N7	-2.39	107.84	110.58
2	A	701	SAH	N6-C6-N1	2.25	123.39	118.38
2	A	701	SAH	C5-N7-C8	2.20	106.90	103.45
2	A	701	SAH	C2'-C3'-C4'	2.19	106.84	102.61
2	A	701	SAH	CB-CA-C	-2.00	105.14	110.45

There are no chirality outliers.

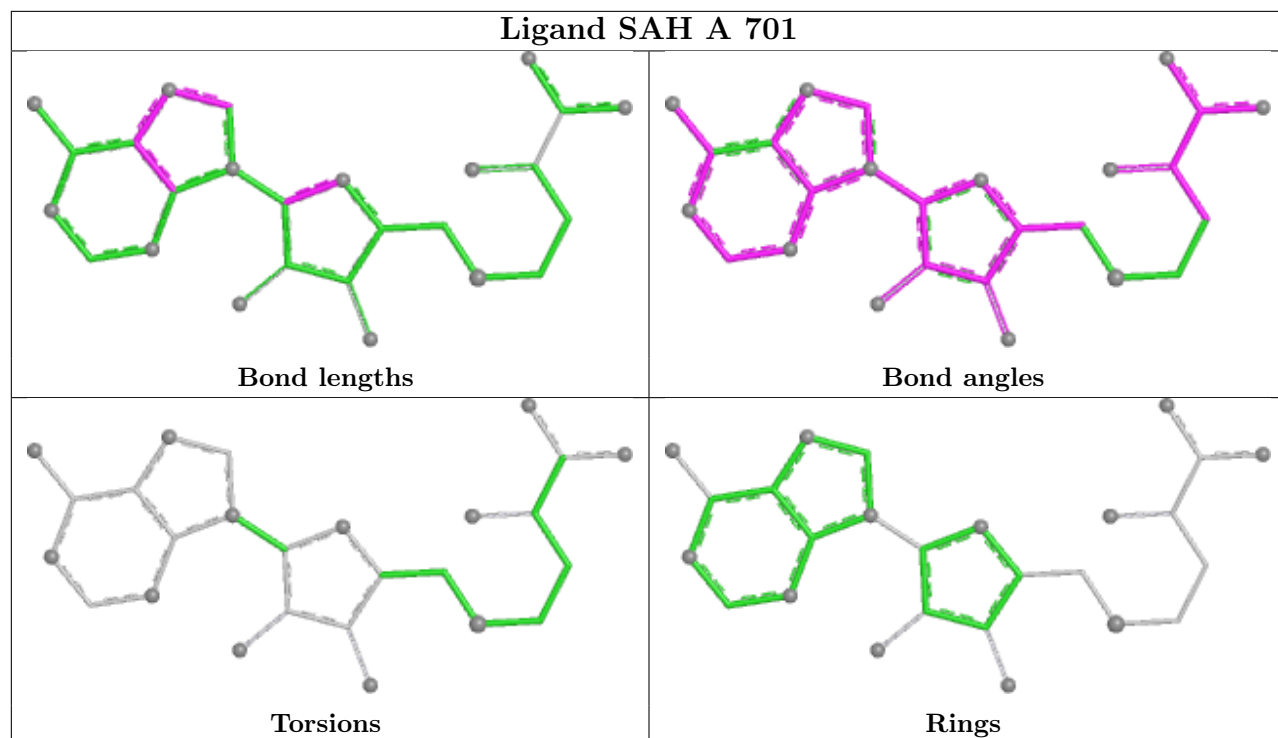
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	SAH	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 ⓘ

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	624/655 (95%)	0.30	37 (5%) 28 32	38, 58, 100, 130	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	344	TYR	5.1
1	A	24	MET	4.4
1	A	528	ILE	4.1
1	A	211	ALA	4.1
1	A	292	LYS	4.0
1	A	526	ASP	3.8
1	A	619	ARG	3.5
1	A	343	SER	3.5
1	A	22	TYR	3.4
1	A	644	SER	3.4
1	A	527	ALA	3.4
1	A	643	LYS	3.0
1	A	454	MET	3.0
1	A	199	LYS	2.9
1	A	340	LYS	2.9
1	A	555	GLY	2.9
1	A	210	THR	2.7
1	A	556	ARG	2.6
1	A	312	LYS	2.5
1	A	336	VAL	2.5
1	A	259	HIS	2.5
1	A	424	LYS	2.5
1	A	622	LYS	2.5
1	A	124	THR	2.5
1	A	524	ALA	2.3
1	A	293	ASN	2.3
1	A	127	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	342	ARG	2.3
1	A	26	GLN	2.3
1	A	30	ARG	2.3
1	A	525	THR	2.3
1	A	208	SER	2.2
1	A	28	LEU	2.2
1	A	520	LYS	2.2
1	A	197	GLY	2.1
1	A	200	ASP	2.1
1	A	21	ASP	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](#)

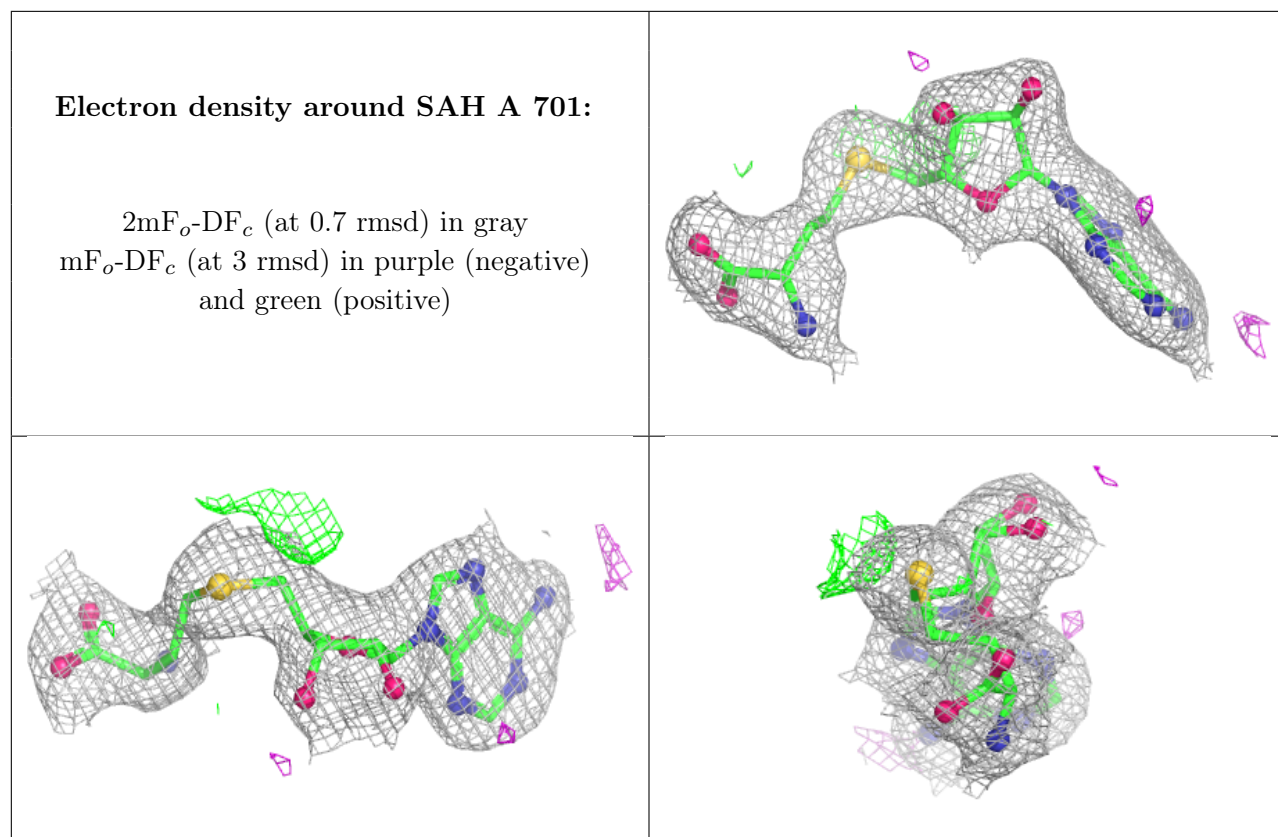
There are no oligosaccharides in this entry.

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	SAH	A	701	26/26	0.96	0.08	40,50,60,65	0
3	ZN	A	702	1/1	0.99	0.04	66,66,66,66	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.