



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:35 PM UTC

PDB ID : 5UNA / pdb_00005una
Title : Fragment of 7SK snRNA methylphosphate capping enzyme
Authors : Wu, H.; Tempel, W.; Dombrovski, L.; McCarthy, A.A.; Loppnau, P.; Bountra, C.; Arrowsmith, C.H.; Edwards, A.M.; Park, H.; Structural Genomics Consortium (SGC)
Deposited on : 2017-01-30
Resolution : 2.55 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

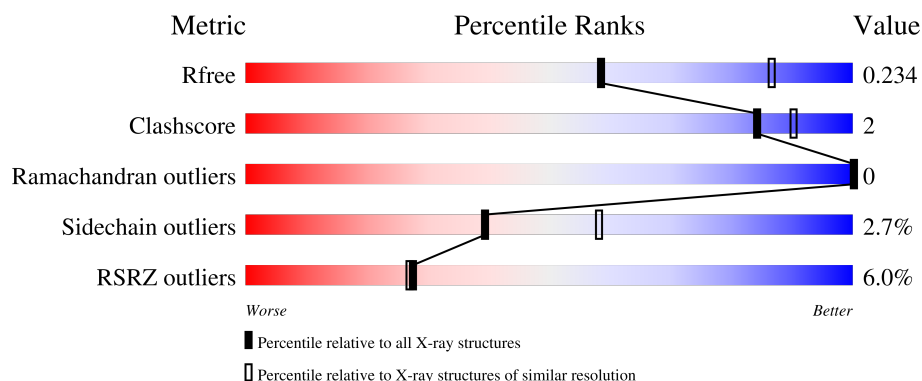
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	292	4% 63% 9% 29%
1	B	292	4% 62% 9% 29%
1	C	292	7% 66% 5% 28%
1	D	292	3% 64% 8% 28%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	292	
1	F	292	
2	M	6	
2	N	6	
2	O	6	
2	Q	6	
2	R	6	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9632 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 7SK snRNA methylphosphate capping enzyme.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	Se	0	0	1
			1567	1013	271	277	4	2			
1	B	208	Total	C	N	O	S	Se	0	0	3
			1573	1014	274	279	4	2			
1	C	210	Total	C	N	O	S	Se	0	0	3
			1555	1007	273	269	4	2			
1	D	210	Total	C	N	O	S	Se	0	0	3
			1578	1019	271	282	4	2			
1	E	211	Total	C	N	O	S	Se	0	0	2
			1590	1030	272	282	4	2			
1	F	209	Total	C	N	O	S	Se	0	0	2
			1521	973	270	272	4	2			

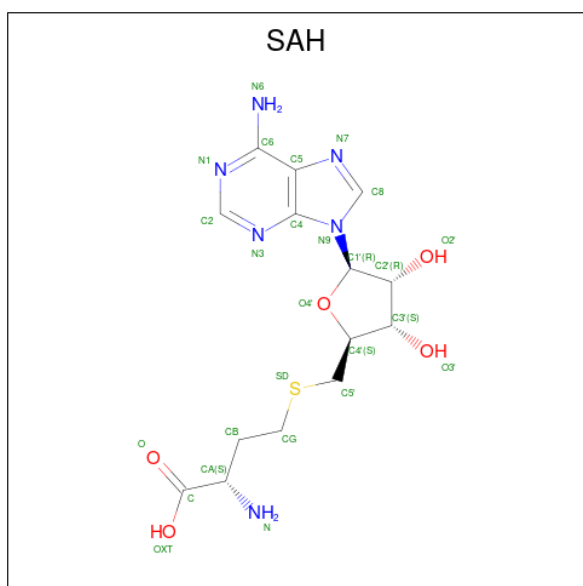
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	398	GLY	-	expression tag	UNP Q7L2J0
A	399	SER	-	expression tag	UNP Q7L2J0
B	398	GLY	-	expression tag	UNP Q7L2J0
B	399	SER	-	expression tag	UNP Q7L2J0
C	398	GLY	-	expression tag	UNP Q7L2J0
C	399	SER	-	expression tag	UNP Q7L2J0
D	398	GLY	-	expression tag	UNP Q7L2J0
D	399	SER	-	expression tag	UNP Q7L2J0
E	398	GLY	-	expression tag	UNP Q7L2J0
E	399	SER	-	expression tag	UNP Q7L2J0
F	398	GLY	-	expression tag	UNP Q7L2J0
F	399	SER	-	expression tag	UNP Q7L2J0

- Molecule 2 is a protein called unidentified peptide section/fragment.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	M	4	Total	C	N	O	0	4	1
			17	10	4	3			
2	N	5	Total	C	N	O	0	5	1
			22	13	5	4			
2	O	6	Total	C	N	O	0	0	0
			30	18	6	6			
2	Q	4	Total	C	N	O	0	2	1
			16	9	4	3			
2	R	2	Total	C	N	O	0	0	1
			7	4	2	1			

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).

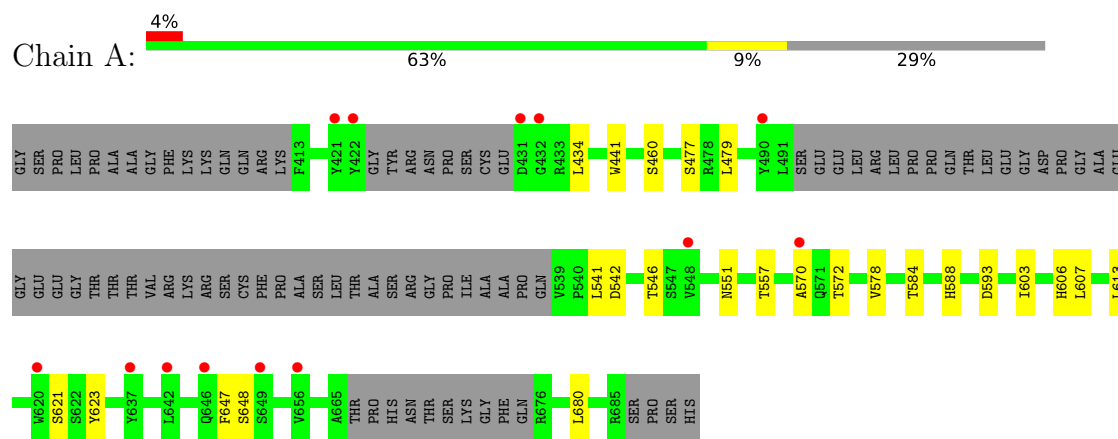


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	E	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
3	F	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

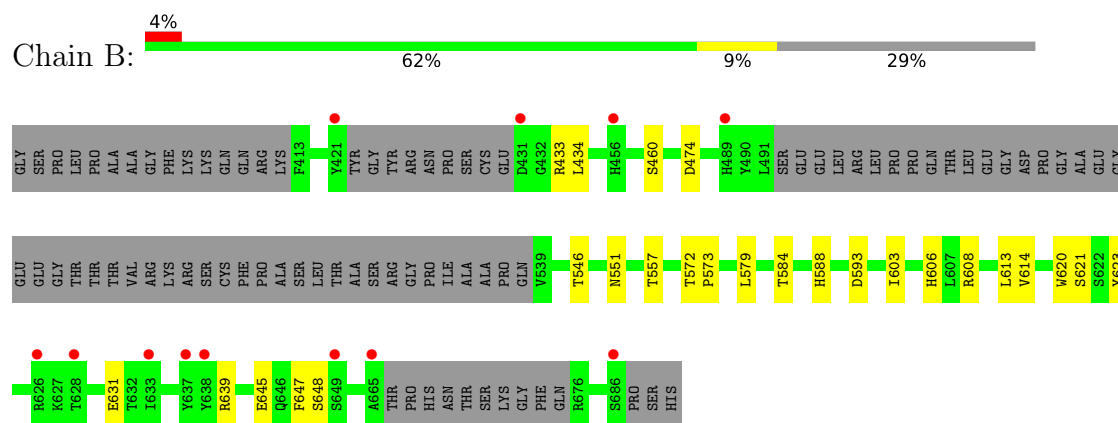
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

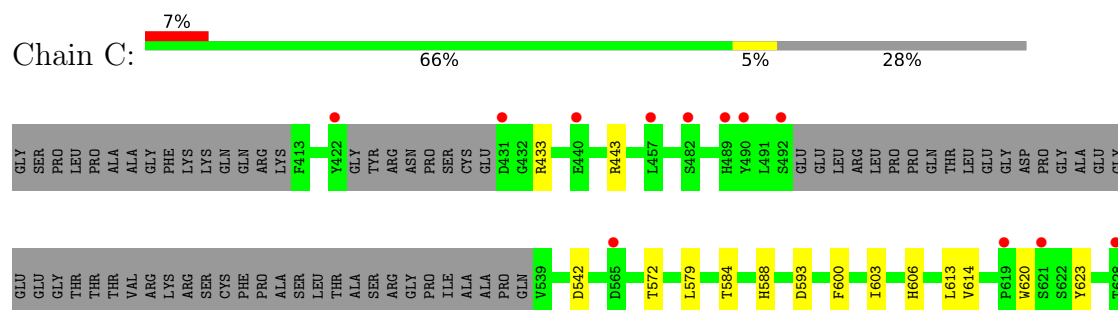
- Molecule 1: 7SK snRNA methylphosphate capping enzyme

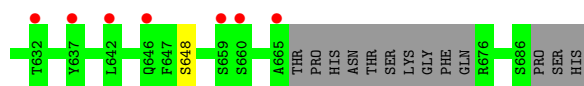


- Molecule 1: 7SK snRNA methylphosphate capping enzyme

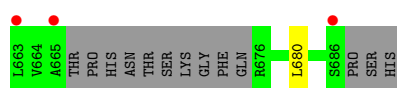
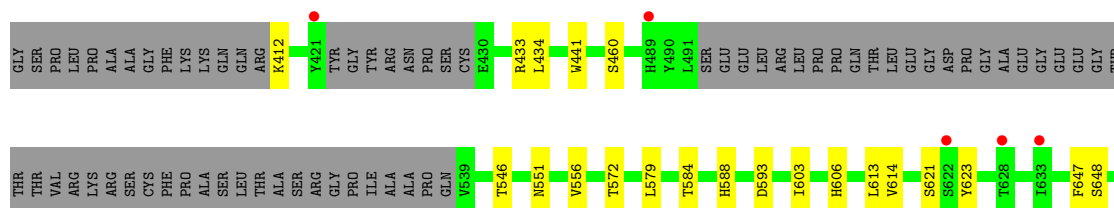


- Molecule 1: 7SK snRNA methylphosphate capping enzyme

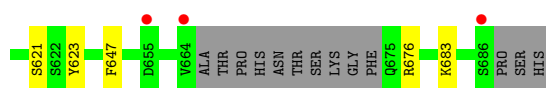
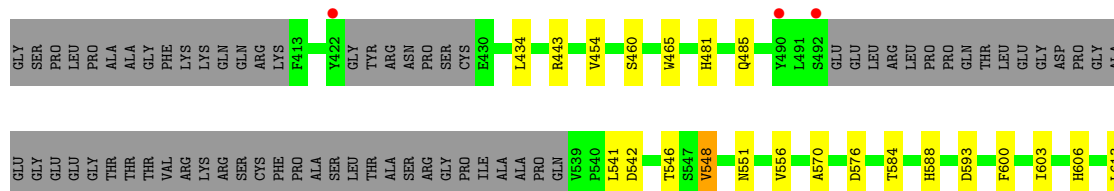




- Molecule 1: 7SK snRNA methylphosphate capping enzyme



- Molecule 1: 7SK snRNA methylphosphate capping enzyme

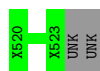


- Molecule 1: 7SK snRNA methylphosphate capping enzyme



- Molecule 2: unidentified peptide section/fragment





- Molecule 2: unidentified peptide section/fragment

Chain N:  83% 17%



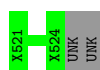
- Molecule 2: unidentified peptide section/fragment

Chain O:  83% 17%



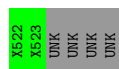
- Molecule 2: unidentified peptide section/fragment

Chain Q:  67% 33%



- Molecule 2: unidentified peptide section/fragment

Chain R:  33% 67%



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	183.24Å 183.24Å 151.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	25.70 – 2.55 25.70 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.6 (25.70-2.55) 99.5 (25.70-2.55)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.73 (at 2.51Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.204 , 0.217 (Not available) , 0.234	Depositor DCC
R_{free} test set	2018 reflections (3.08%)	wwPDB-VP
Wilson B-factor (Å ²)	67.8	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 87.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9632	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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

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	0.84	0/1605	1.33	8/2188 (0.4%)
1	B	0.85	0/1611	1.33	9/2195 (0.4%)
1	C	0.86	0/1593	1.30	6/2172 (0.3%)
1	D	0.83	0/1618	1.32	7/2206 (0.3%)
1	E	0.97	2/1630 (0.1%)	1.36	11/2223 (0.5%)
1	F	0.85	1/1556 (0.1%)	1.37	8/2122 (0.4%)
All	All	0.87	3/9613 (0.0%)	1.33	49/13106 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	454	VAL	CA-C	6.14	1.60	1.52
1	F	453	ASN	CA-C	5.14	1.57	1.53
1	E	676	ARG	CA-C	5.04	1.57	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	412	LYS	CA-C-N	6.56	134.07	121.54
1	D	412	LYS	C-N-CA	6.56	134.07	121.54
1	B	593	ASP	CA-CB-CG	6.16	118.76	112.60
1	B	620	TRP	CA-C-N	5.96	129.09	120.38
1	B	620	TRP	C-N-CA	5.96	129.09	120.38
1	E	593	ASP	CA-CB-CG	5.88	118.48	112.60
1	F	593	ASP	CA-CB-CG	5.79	118.39	112.60
1	A	593	ASP	CA-CB-CG	5.73	118.33	112.60
1	F	623	TYR	CA-C-N	5.69	126.42	119.99
1	F	623	TYR	C-N-CA	5.69	126.42	119.99
1	C	593	ASP	CA-CB-CG	5.64	118.24	112.60
1	B	631	GLU	CA-C-N	5.58	127.70	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	631	GLU	C-N-CA	5.58	127.70	120.44
1	D	572	THR	CB-CA-C	5.57	117.13	108.61
1	E	623	TYR	CA-C-N	5.47	126.17	119.99
1	E	623	TYR	C-N-CA	5.47	126.17	119.99
1	E	542	ASP	CA-CB-CG	5.46	118.06	112.60
1	D	623	TYR	CA-C-N	5.43	126.13	119.99
1	D	623	TYR	C-N-CA	5.43	126.13	119.99
1	D	593	ASP	CA-CB-CG	5.43	118.03	112.60
1	E	647	PHE	CA-CB-CG	5.41	119.21	113.80
1	D	647	PHE	CA-CB-CG	5.39	119.19	113.80
1	F	431	ASP	CA-C-N	5.39	126.92	120.13
1	F	431	ASP	C-N-CA	5.39	126.92	120.13
1	A	542	ASP	CA-CB-CG	5.39	117.99	112.60
1	A	623	TYR	CA-C-N	5.35	126.04	119.99
1	A	623	TYR	C-N-CA	5.35	126.04	119.99
1	E	683	LYS	CA-C-N	5.31	128.76	120.75
1	E	683	LYS	C-N-CA	5.31	128.76	120.75
1	E	600	PHE	CA-CB-CG	5.29	119.09	113.80
1	C	623	TYR	CA-C-N	5.28	125.96	119.99
1	C	623	TYR	C-N-CA	5.28	125.96	119.99
1	C	542	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	479	LEU	CA-C-N	5.27	127.67	120.46
1	A	479	LEU	C-N-CA	5.27	127.67	120.46
1	A	572	THR	CB-CA-C	5.27	116.67	108.61
1	C	600	PHE	CA-CB-CG	5.26	119.06	113.80
1	B	623	TYR	CA-C-N	5.24	125.92	119.99
1	B	623	TYR	C-N-CA	5.24	125.92	119.99
1	B	572	THR	CB-CA-C	5.20	116.56	108.61
1	E	548	VAL	CA-C-N	5.15	128.20	120.83
1	E	548	VAL	C-N-CA	5.15	128.20	120.83
1	C	572	THR	CB-CA-C	5.10	116.79	109.09
1	F	600	PHE	CA-CB-CG	5.06	118.86	113.80
1	E	576	ASP	N-CA-C	-5.05	107.25	113.41
1	A	647	PHE	CA-CB-CG	5.02	118.82	113.80
1	B	647	PHE	CA-CB-CG	5.01	118.81	113.80
1	F	620	TRP	CA-C-N	5.00	127.69	120.38
1	F	620	TRP	C-N-CA	5.00	127.69	120.38

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	1567	0	1424	9	0
1	B	1573	0	1443	8	0
1	C	1555	0	1386	4	0
1	D	1578	0	1420	6	0
1	E	1590	0	1451	8	0
1	F	1521	0	1324	7	0
2	M	17	0	5	0	0
2	N	22	0	6	0	0
2	O	30	0	9	1	0
2	Q	16	0	5	0	0
2	R	7	0	3	0	0
3	A	26	0	19	0	0
3	B	26	0	19	0	0
3	C	26	0	19	0	0
3	D	26	0	19	0	0
3	E	26	0	19	1	0
3	F	26	0	19	0	0
All	All	9632	0	8590	41	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 2.

All (41) 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:F:433:ARG:NH1	1:F:457:LEU:HD11	1.97	0.80
1:B:434:LEU:HD11	1:B:460:SER:HB3	1.82	0.61
1:D:441:TRP:CZ2	1:D:680:LEU:HD11	2.36	0.60
1:A:441:TRP:CZ2	1:A:680:LEU:HD11	2.39	0.57
1:A:434:LEU:HD11	1:A:460:SER:HB3	1.87	0.56
1:E:434:LEU:HD11	1:E:460:SER:HB3	1.89	0.55
1:B:645:GLU:H	1:B:645:GLU:CD	2.17	0.52
1:F:645:GLU:H	1:F:645:GLU:CD	2.17	0.52
1:E:481:HIS:O	1:E:485:GLN:HG2	2.10	0.52
1:D:434:LEU:HD11	1:D:460:SER:HB3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:603:ILE:HG21	1:E:613:LEU:HD13	1.93	0.49
1:B:584:THR:O	1:B:588:HIS:HB2	2.13	0.48
1:A:578:VAL:HG23	1:A:607:LEU:HD21	1.98	0.45
1:E:584:THR:O	1:E:588:HIS:HB2	2.16	0.45
1:A:584:THR:O	1:A:588:HIS:HB2	2.17	0.45
1:A:603:ILE:HG21	1:A:613:LEU:HD13	1.99	0.44
1:D:603:ILE:HG21	1:D:613:LEU:HD13	1.99	0.44
1:F:603:ILE:HG21	1:F:613:LEU:HD13	1.99	0.44
1:A:570:ALA:HB3	1:E:541:LEU:HD21	1.99	0.44
1:D:546:THR:HA	1:D:551:ASN:HB3	2.00	0.44
1:C:579:LEU:HD23	1:C:614:VAL:HB	2.00	0.43
3:E:701:SAH:H4'	3:E:701:SAH:HB1	2.01	0.43
1:D:579:LEU:HD23	1:D:614:VAL:HB	2.00	0.43
1:B:579:LEU:HD23	1:B:614:VAL:HB	2.00	0.43
1:A:541:LEU:HD21	1:E:570:ALA:HB3	2.01	0.42
1:D:584:THR:O	1:D:588:HIS:HB2	2.19	0.42
1:B:474:ASP:O	1:B:557:THR:HA	2.19	0.42
1:F:546:THR:HA	1:F:551:ASN:HB3	2.02	0.42
1:B:603:ILE:HG21	1:B:613:LEU:HD13	2.01	0.42
1:C:603:ILE:HG21	1:C:613:LEU:HD13	2.01	0.42
1:B:573:PRO:HB2	1:B:608:ARG:HG2	2.02	0.41
1:A:546:THR:HA	1:A:551:ASN:HB3	2.03	0.41
1:F:579:LEU:HD23	1:F:614:VAL:HB	2.02	0.41
1:F:584:THR:O	1:F:588:HIS:HB2	2.20	0.41
1:E:546:THR:HA	1:E:551:ASN:HB3	2.03	0.41
1:F:645:GLU:CD	1:F:645:GLU:N	2.79	0.41
1:C:584:THR:O	1:C:588:HIS:HB2	2.21	0.40
1:B:546:THR:HA	1:B:551:ASN:HB3	2.03	0.40
1:A:477:SER:HB3	1:A:557:THR:HG21	2.04	0.40
1:C:443:ARG:HD3	2:O:525:UNK:CB	2.51	0.40
1:E:443:ARG:HG2	1:E:465:TRP:O	2.22	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	200/292 (68%)	194 (97%)	6 (3%)	0	100	100
1	B	200/292 (68%)	193 (96%)	7 (4%)	0	100	100
1	C	202/292 (69%)	193 (96%)	9 (4%)	0	100	100
1	D	202/292 (69%)	194 (96%)	8 (4%)	0	100	100
1	E	203/292 (70%)	195 (96%)	8 (4%)	0	100	100
1	F	201/292 (69%)	193 (96%)	8 (4%)	0	100	100
All	All	1208/1752 (69%)	1162 (96%)	46 (4%)	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	150/253 (59%)	147 (98%)	3 (2%)	48	67
1	B	152/253 (60%)	147 (97%)	5 (3%)	33	50
1	C	143/253 (56%)	139 (97%)	4 (3%)	38	57
1	D	150/253 (59%)	145 (97%)	5 (3%)	33	50
1	E	153/253 (60%)	149 (97%)	4 (3%)	40	59
1	F	137/253 (54%)	134 (98%)	3 (2%)	45	64
All	All	885/1518 (58%)	861 (97%)	24 (3%)	39	58

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	606	HIS
1	A	621	SER
1	A	648	SER
1	B	433	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	606	HIS
1	B	621	SER
1	B	639	ARG
1	B	648	SER
1	C	433	ARG
1	C	606	HIS
1	C	620	TRP
1	C	648	SER
1	D	433	ARG
1	D	556	VAL
1	D	606	HIS
1	D	621	SER
1	D	648	SER
1	E	548	VAL
1	E	556	VAL
1	E	606	HIS
1	E	621	SER
1	F	556	VAL
1	F	606	HIS
1	F	621	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	414	GLN
1	B	590	ASN
1	C	456	HIS
1	C	486	ASN
1	D	485	GLN
1	D	489	HIS
1	D	682	HIS
1	E	456	HIS
1	F	590	ASN
1	F	682	HIS

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](#)

6 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	SAH	F	701	-	27,28,28	0.48	1 (3%)	36,40,40	0.79	2 (5%)
3	SAH	A	701	-	27,28,28	0.83	2 (7%)	36,40,40	0.92	2 (5%)
3	SAH	E	701	-	27,28,28	0.85	2 (7%)	36,40,40	1.10	2 (5%)
3	SAH	B	701	-	27,28,28	0.44	1 (3%)	36,40,40	0.90	2 (5%)
3	SAH	D	701	-	27,28,28	0.78	2 (7%)	36,40,40	0.84	2 (5%)
3	SAH	C	701	-	27,28,28	0.42	1 (3%)	36,40,40	0.77	2 (5%)

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	SAH	F	701	-	-	0/15/31/31	0/3/3/3
3	SAH	A	701	-	-	1/15/31/31	0/3/3/3
3	SAH	E	701	-	-	0/15/31/31	0/3/3/3
3	SAH	B	701	-	-	2/15/31/31	0/3/3/3
3	SAH	D	701	-	-	2/15/31/31	0/3/3/3
3	SAH	C	701	-	-	1/15/31/31	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	701	SAH	O-C	3.34	1.32	1.22
3	D	701	SAH	OXT-C	-2.85	1.21	1.30
3	A	701	SAH	O-C	2.72	1.30	1.22
3	A	701	SAH	OXT-C	-2.71	1.22	1.30
3	D	701	SAH	O-C	2.50	1.29	1.22
3	E	701	SAH	OXT-C	-2.50	1.22	1.30
3	F	701	SAH	CB-CA	2.28	1.58	1.53
3	B	701	SAH	CB-CA	2.16	1.57	1.53
3	C	701	SAH	CB-CA	2.02	1.57	1.53

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	701	SAH	CB-CG-SD	-4.54	103.32	113.45
3	B	701	SAH	CB-CG-SD	-3.67	105.25	113.45
3	E	701	SAH	CB-CA-N	3.66	119.65	110.12
3	A	701	SAH	CB-CG-SD	-3.65	105.31	113.45
3	D	701	SAH	CB-CG-SD	-3.29	106.11	113.45
3	F	701	SAH	CB-CG-SD	-3.10	106.54	113.45
3	A	701	SAH	CB-CA-N	2.88	117.62	110.12
3	C	701	SAH	CB-CA-N	2.77	117.33	110.12
3	B	701	SAH	CB-CA-N	2.76	117.32	110.12
3	F	701	SAH	CB-CA-N	2.75	117.29	110.12
3	C	701	SAH	CB-CG-SD	-2.64	107.56	113.45
3	D	701	SAH	CB-CA-N	2.45	116.52	110.12

There are no chirality outliers.

All (6) torsion outliers are listed below:

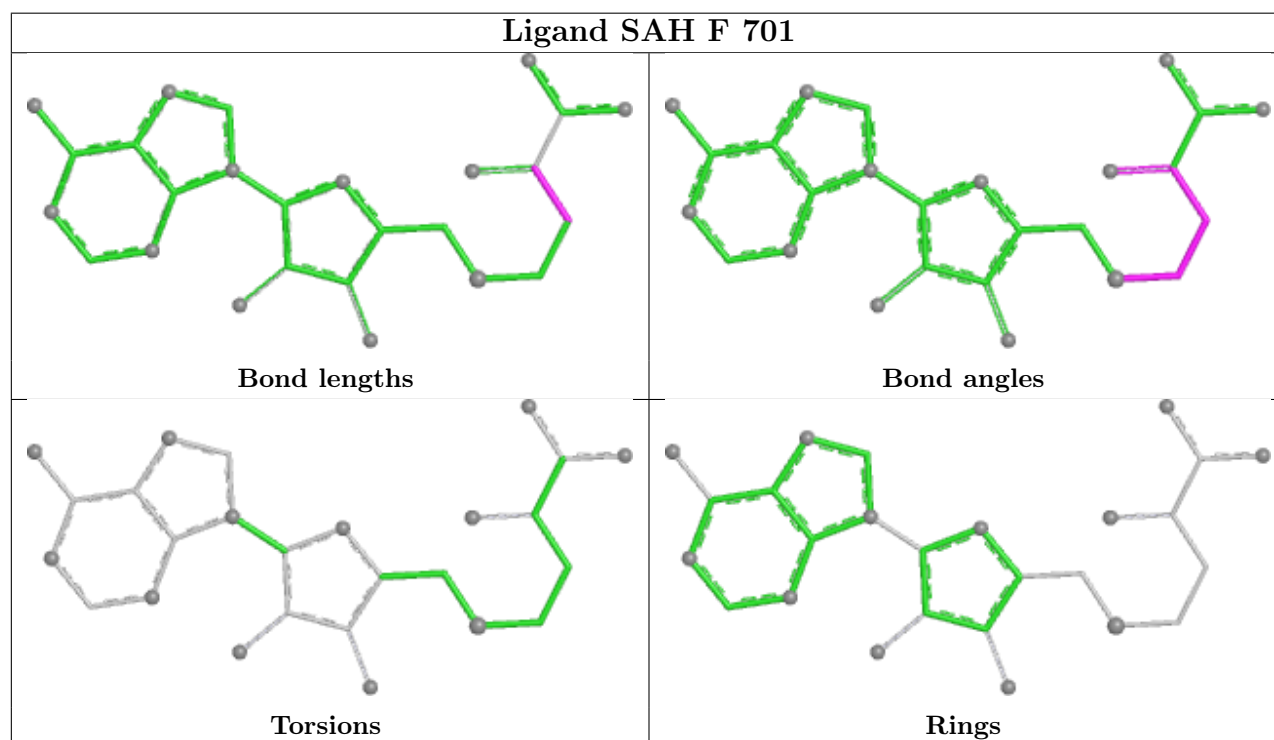
Mol	Chain	Res	Type	Atoms
3	B	701	SAH	O4'-C4'-C5'-SD
3	D	701	SAH	O4'-C4'-C5'-SD
3	D	701	SAH	CB-CG-SD-C5'
3	A	701	SAH	CB-CG-SD-C5'
3	B	701	SAH	CB-CG-SD-C5'
3	C	701	SAH	CB-CG-SD-C5'

There are no ring outliers.

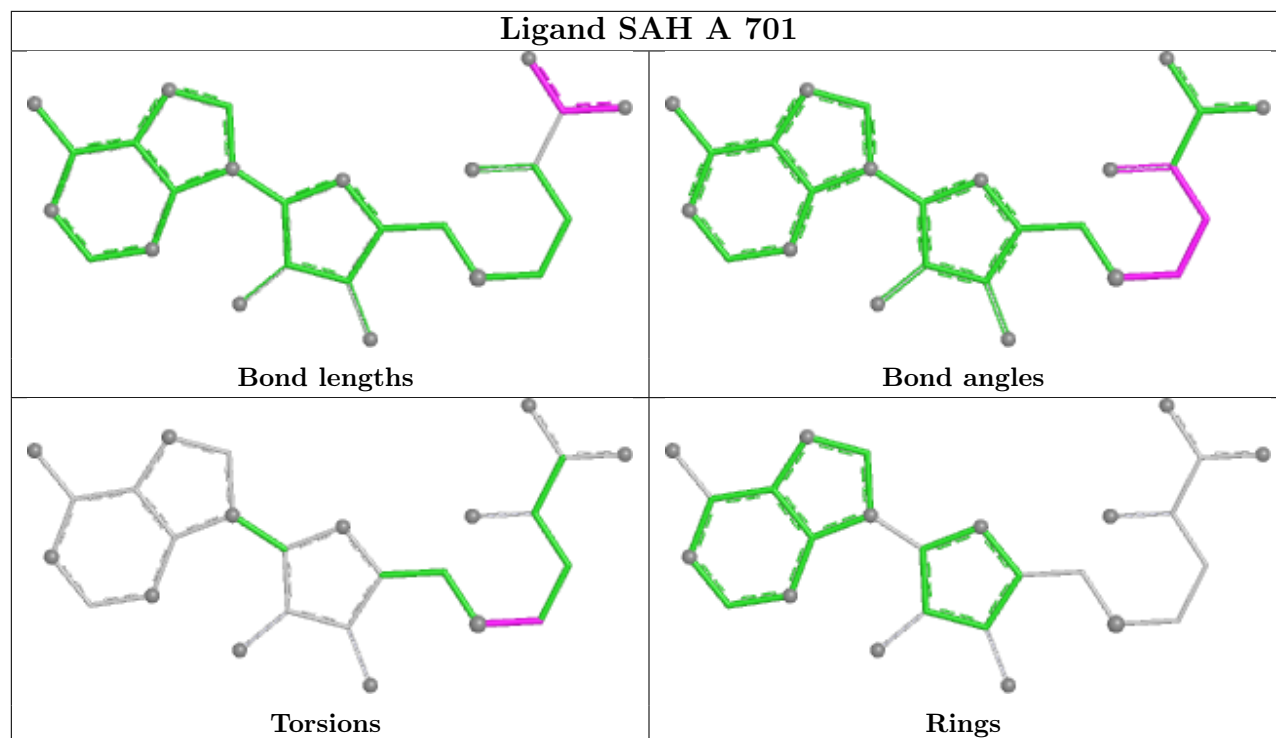
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	701	SAH	1	0

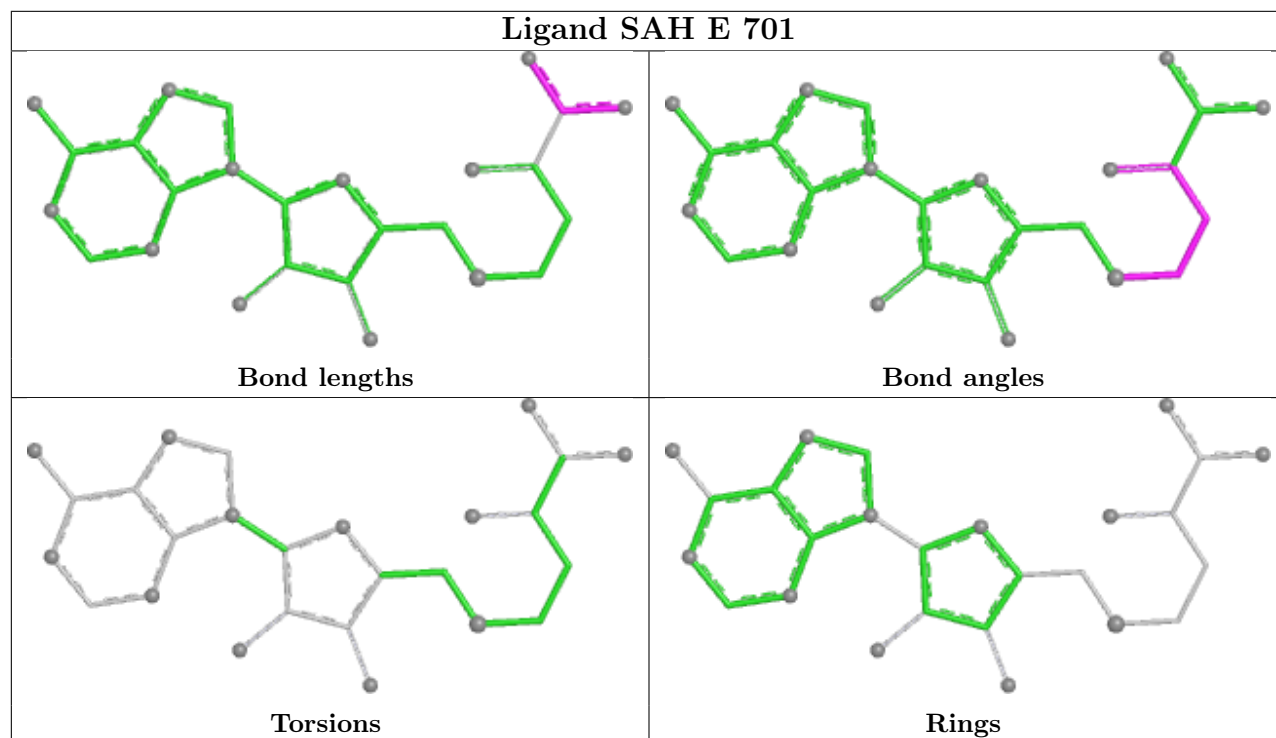
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



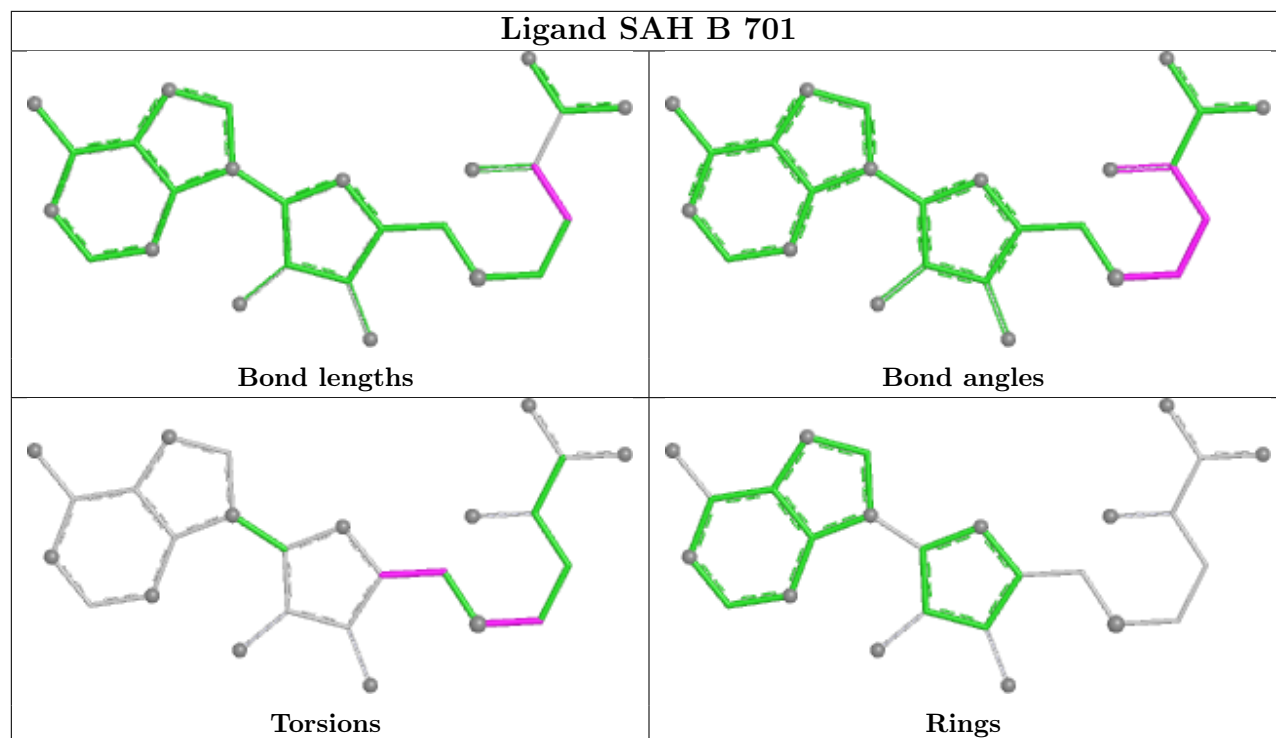
Ligand SAH A 701



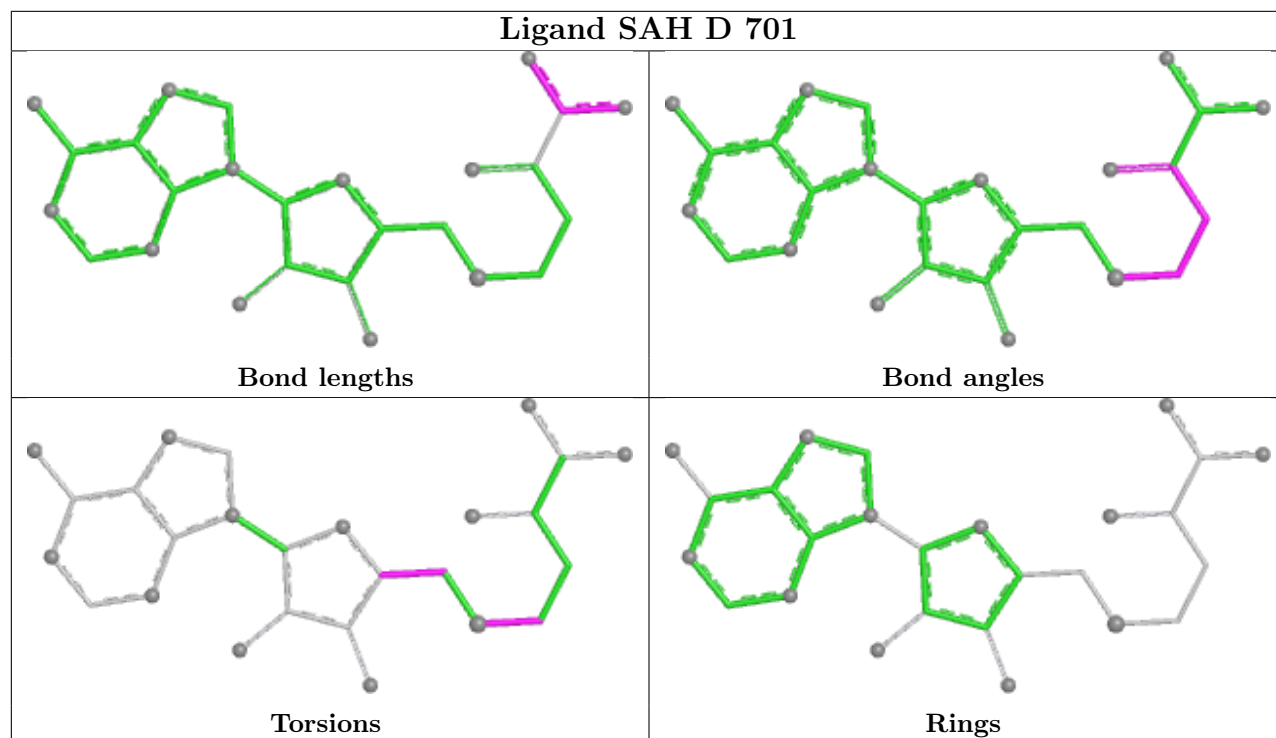
Ligand SAH E 701

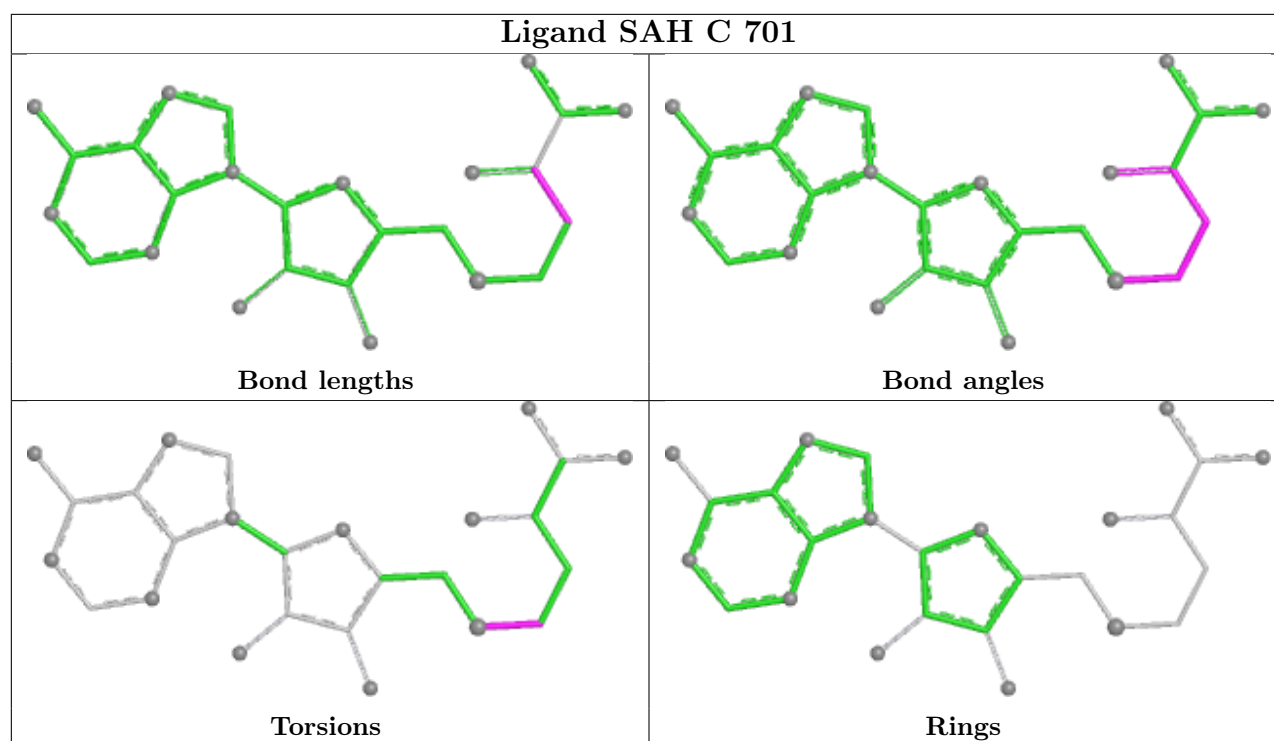


Ligand SAH B 701



Ligand SAH D 701





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	206/292 (70%)	0.49	13 (6%) 26 25	56, 91, 128, 138	0
1	B	206/292 (70%)	0.33	12 (5%) 29 28	51, 79, 118, 133	0
1	C	208/292 (71%)	0.63	19 (9%) 15 14	58, 95, 129, 140	0
1	D	208/292 (71%)	0.48	8 (3%) 44 45	59, 88, 126, 134	0
1	E	209/292 (71%)	0.48	6 (2%) 53 55	51, 81, 112, 120	0
1	F	207/292 (70%)	0.71	17 (8%) 17 17	65, 103, 141, 156	0
2	M	0/6	-	-	-	-
2	N	0/6	-	-	-	-
2	O	0/6	-	-	-	-
2	Q	0/6	-	-	-	-
2	R	0/6	-	-	-	-
All	All	1244/1782 (69%)	0.52	75 (6%) 27 27	51, 89, 130, 156	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	665	ALA	8.5
1	F	421	TYR	8.4
1	D	665	ALA	6.6
1	D	421	TYR	5.5
1	A	421	TYR	5.1
1	B	421	TYR	4.9
1	B	686	SER	4.4
1	E	686	SER	4.4
1	F	686	SER	4.4
1	A	422	TYR	4.4
1	B	431	ASP	4.0
1	D	633	ILE	3.7
1	C	492	SER	3.6
1	F	637	TYR	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	628	THR	3.5
1	A	431	ASP	3.2
1	D	686	SER	3.2
1	C	431	ASP	3.2
1	F	620	TRP	3.1
1	C	422	TYR	3.1
1	B	633	ILE	3.1
1	E	490	TYR	3.0
1	F	617	PRO	3.0
1	F	649	SER	3.0
1	E	492	SER	2.9
1	B	628	THR	2.9
1	C	628	THR	2.9
1	A	656	VAL	2.8
1	F	628	THR	2.8
1	C	665	ALA	2.7
1	C	659	SER	2.7
1	B	649	SER	2.6
1	C	632	THR	2.6
1	F	640	ILE	2.6
1	D	663	LEU	2.6
1	F	629	LEU	2.6
1	A	646	GLN	2.6
1	C	490	TYR	2.6
1	F	412	LYS	2.6
1	C	489	HIS	2.5
1	C	619	PRO	2.5
1	D	622	SER	2.5
1	C	637	TYR	2.5
1	F	437	LEU	2.5
1	A	649	SER	2.5
1	A	642	LEU	2.5
1	C	646	GLN	2.5
1	B	637	TYR	2.4
1	C	440	GLU	2.4
1	D	489	HIS	2.4
1	E	664	VAL	2.4
1	E	422	TYR	2.4
1	F	488	ARG	2.3
1	A	637	TYR	2.3
1	C	565	ASP	2.3
1	B	489	HIS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	655	ASP	2.3
1	C	642	LEU	2.2
1	F	619	PRO	2.2
1	B	638	TYR	2.2
1	C	621	SER	2.2
1	C	660	SER	2.2
1	B	626	ARG	2.2
1	A	620	TRP	2.1
1	B	456	HIS	2.1
1	A	490	TYR	2.1
1	F	612	ILE	2.1
1	A	570	ALA	2.1
1	F	685	ARG	2.1
1	F	664	VAL	2.0
1	A	432	GLY	2.0
1	A	548	VAL	2.0
1	C	457	LEU	2.0
1	F	636	ASN	2.0
1	C	482	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

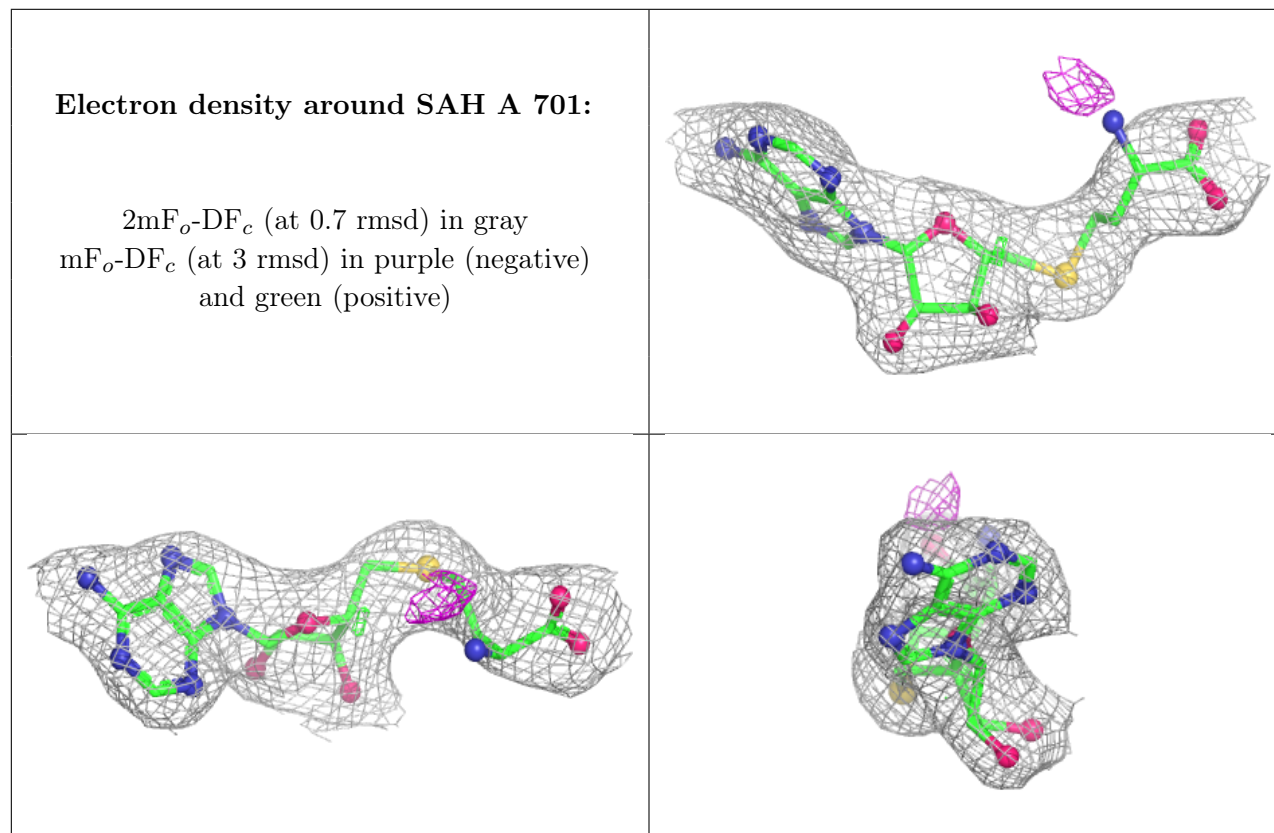
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SAH	A	701	26/26	0.95	0.09	63,71,104,107	0
3	SAH	D	701	26/26	0.95	0.09	66,78,94,100	0
3	SAH	E	701	26/26	0.95	0.08	53,63,89,92	0
3	SAH	C	701	26/26	0.96	0.08	70,76,104,109	0

Continued on next page...

Continued from previous page...

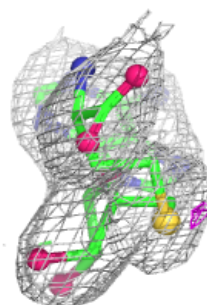
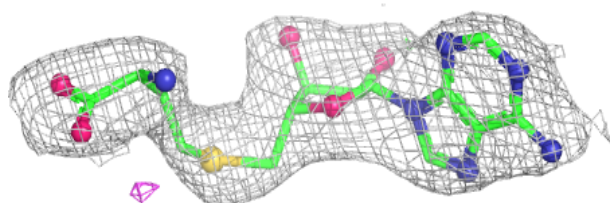
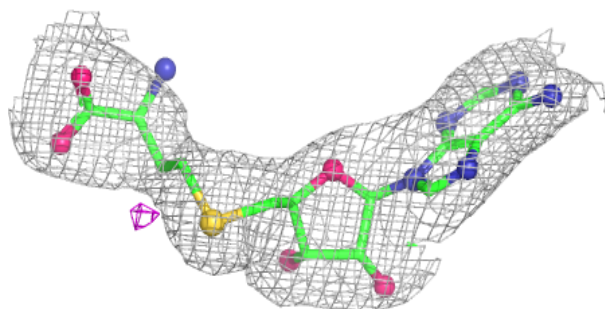
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SAH	B	701	26/26	0.97	0.08	53,65,86,89	0
3	SAH	F	701	26/26	0.97	0.08	79,86,109,114	0

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.

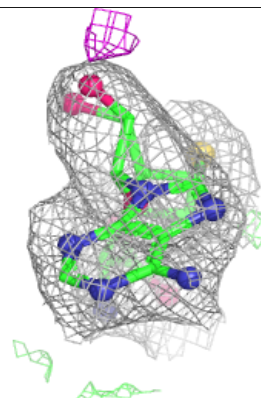
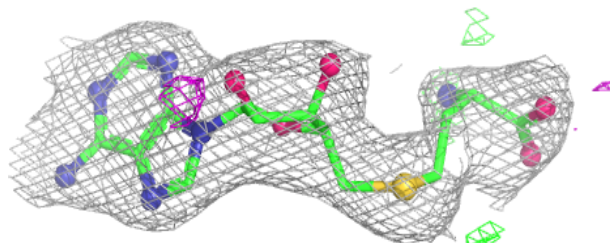
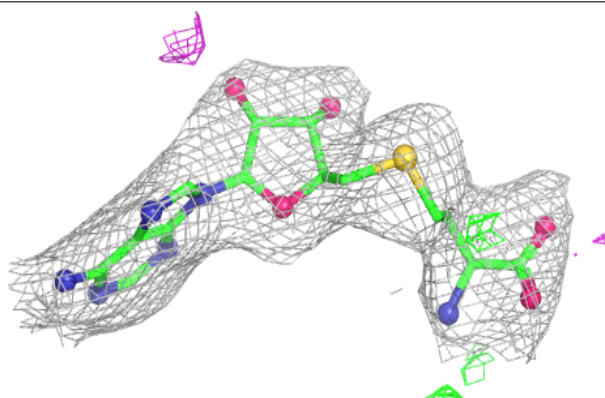


Electron density around SAH D 701:

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

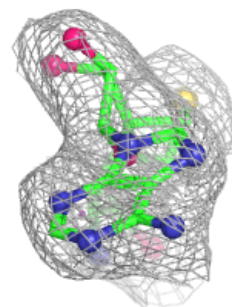
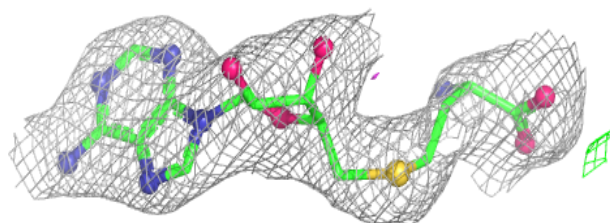
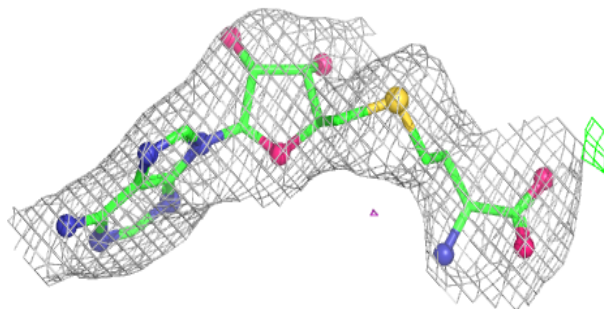
**Electron density around SAH E 701:**

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

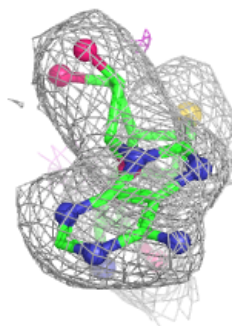
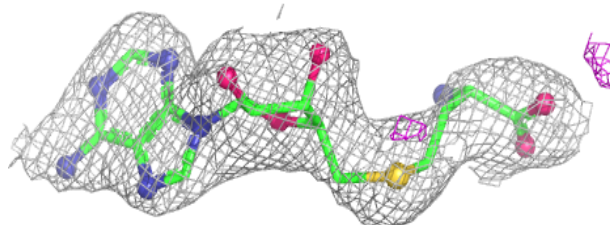
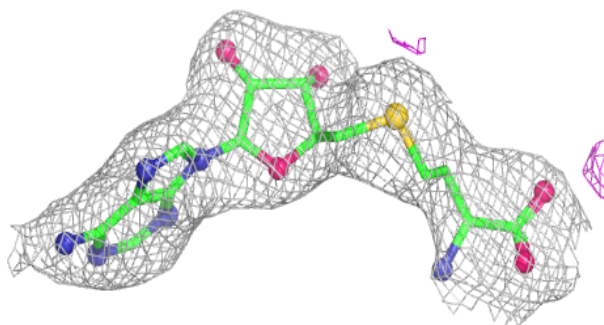


Electron density around SAH C 701:

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

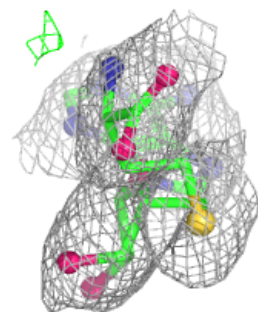
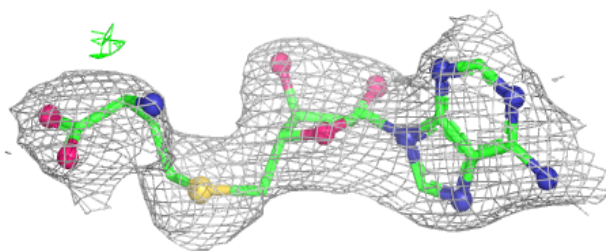
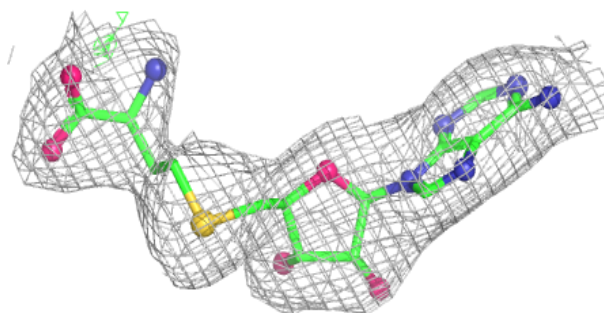
**Electron density around SAH B 701:**

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



Electron density around SAH F 701:

$2mF_o-DF_c$ (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.