



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 11, 2026 – 06:08 PM EDT

PDB ID : 9NVB / pdb_00009nvb
Title : Co-crystal structure of human SMYD1 in complex with MYH2 peptide and SAH
Authors : Zeng, H.; Dong, A.; Arrowsmith, C.H.; Edwards, A.M.; Halabelian, L.; Structural Genomics Consortium (SGC)
Deposited on : 2025-03-20
Resolution : 2.76 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

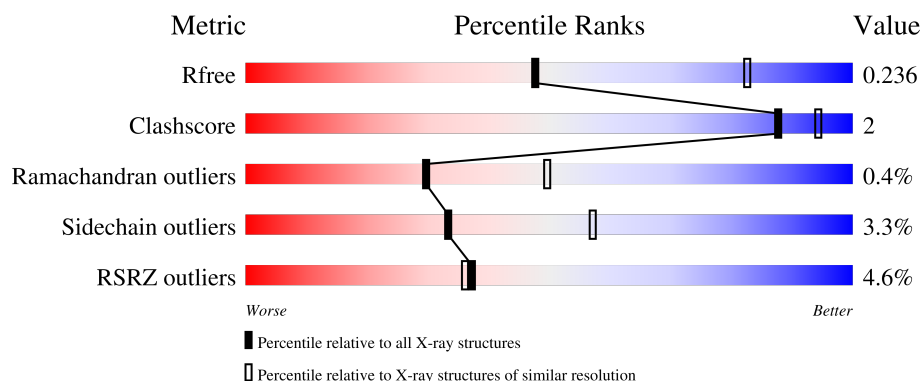
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.76 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	482	
1	B	482	
1	C	482	
2	D	15	

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Mol	Chain	Length	Quality of chain
2	E	15	
2	F	15	
2	G	15	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11252 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 Histone-lysine N-methyltransferase SMYD1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	1	0
			3585	2276	622	654	33			
1	B	454	Total	C	N	O	S	0	3	0
			3576	2269	622	653	32			
1	C	453	Total	C	N	O	S	0	0	0
			3533	2245	611	645	32			

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	initiating methionine	UNP Q8NB12
A	-11	GLY	-	expression tag	UNP Q8NB12
A	-10	SER	-	expression tag	UNP Q8NB12
A	-9	SER	-	expression tag	UNP Q8NB12
A	-8	HIS	-	expression tag	UNP Q8NB12
A	-7	HIS	-	expression tag	UNP Q8NB12
A	-6	HIS	-	expression tag	UNP Q8NB12
A	-5	HIS	-	expression tag	UNP Q8NB12
A	-4	HIS	-	expression tag	UNP Q8NB12
A	-3	HIS	-	expression tag	UNP Q8NB12
A	-2	SER	-	expression tag	UNP Q8NB12
A	-1	SER	-	expression tag	UNP Q8NB12
A	0	GLY	-	expression tag	UNP Q8NB12
A	1	LEU	-	expression tag	UNP Q8NB12
A	2	VAL	-	expression tag	UNP Q8NB12
A	3	PRO	-	expression tag	UNP Q8NB12
A	4	ARG	-	expression tag	UNP Q8NB12
A	5	GLY	-	expression tag	UNP Q8NB12
A	6	SER	-	expression tag	UNP Q8NB12
B	-12	MET	-	initiating methionine	UNP Q8NB12
B	-11	GLY	-	expression tag	UNP Q8NB12
B	-10	SER	-	expression tag	UNP Q8NB12
B	-9	SER	-	expression tag	UNP Q8NB12

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	HIS	-	expression tag	UNP Q8NB12
B	-7	HIS	-	expression tag	UNP Q8NB12
B	-6	HIS	-	expression tag	UNP Q8NB12
B	-5	HIS	-	expression tag	UNP Q8NB12
B	-4	HIS	-	expression tag	UNP Q8NB12
B	-3	HIS	-	expression tag	UNP Q8NB12
B	-2	SER	-	expression tag	UNP Q8NB12
B	-1	SER	-	expression tag	UNP Q8NB12
B	0	GLY	-	expression tag	UNP Q8NB12
B	1	LEU	-	expression tag	UNP Q8NB12
B	2	VAL	-	expression tag	UNP Q8NB12
B	3	PRO	-	expression tag	UNP Q8NB12
B	4	ARG	-	expression tag	UNP Q8NB12
B	5	GLY	-	expression tag	UNP Q8NB12
B	6	SER	-	expression tag	UNP Q8NB12
C	-12	MET	-	initiating methionine	UNP Q8NB12
C	-11	GLY	-	expression tag	UNP Q8NB12
C	-10	SER	-	expression tag	UNP Q8NB12
C	-9	SER	-	expression tag	UNP Q8NB12
C	-8	HIS	-	expression tag	UNP Q8NB12
C	-7	HIS	-	expression tag	UNP Q8NB12
C	-6	HIS	-	expression tag	UNP Q8NB12
C	-5	HIS	-	expression tag	UNP Q8NB12
C	-4	HIS	-	expression tag	UNP Q8NB12
C	-3	HIS	-	expression tag	UNP Q8NB12
C	-2	SER	-	expression tag	UNP Q8NB12
C	-1	SER	-	expression tag	UNP Q8NB12
C	0	GLY	-	expression tag	UNP Q8NB12
C	1	LEU	-	expression tag	UNP Q8NB12
C	2	VAL	-	expression tag	UNP Q8NB12
C	3	PRO	-	expression tag	UNP Q8NB12
C	4	ARG	-	expression tag	UNP Q8NB12
C	5	GLY	-	expression tag	UNP Q8NB12
C	6	SER	-	expression tag	UNP Q8NB12

- Molecule 2 is a protein called Myosin-8 peptide.

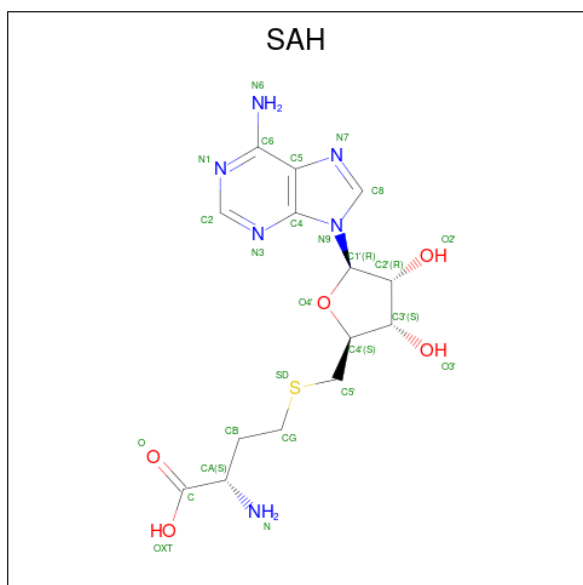
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	12	Total	C	N	O	0	1	0
			118	85	17	16			
2	F	11	Total	C	N	O	0	0	0
			96	68	14	14			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	13	Total	C	N	O	0	1	0
			122	87	18	17			
2	D	15	Total	C	N	O	0	0	0
			125	88	18	19			

- 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		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Zn	0	0
			3	3		
4	B	3	Total	Zn	0	0
			3	3		
4	C	3	Total	Zn	0	0
			3	3		

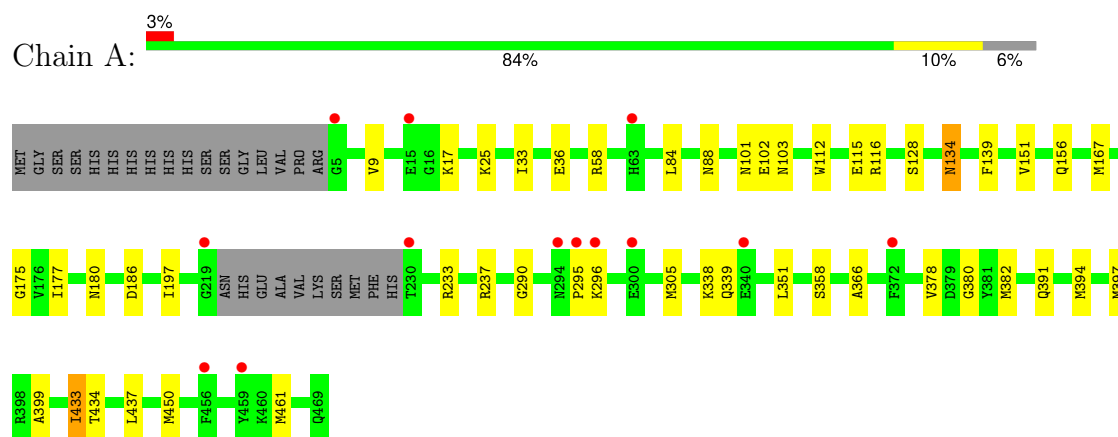
- Molecule 5 is water.

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

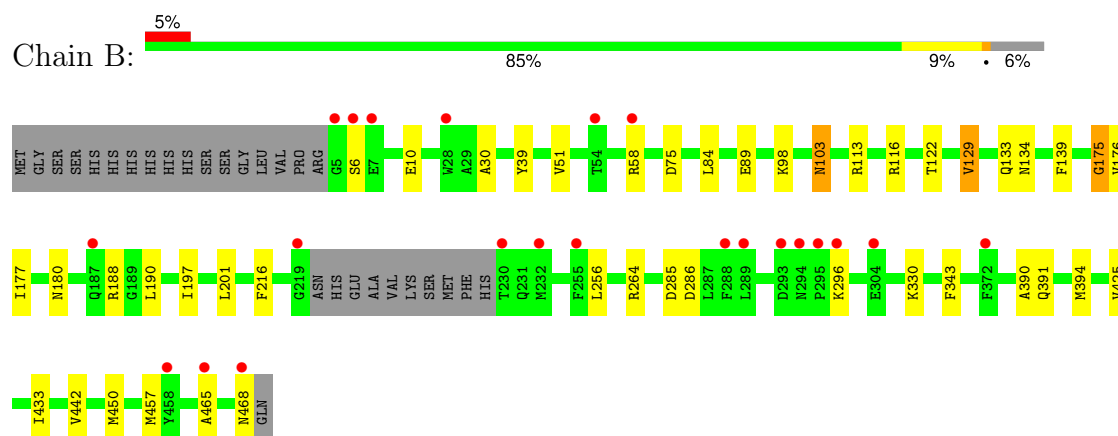
3 Residue-property plots [i](#)

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.

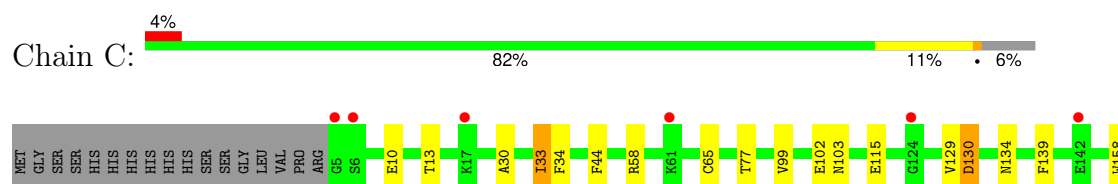
- Molecule 1: Histone-lysine N-methyltransferase SMYD1

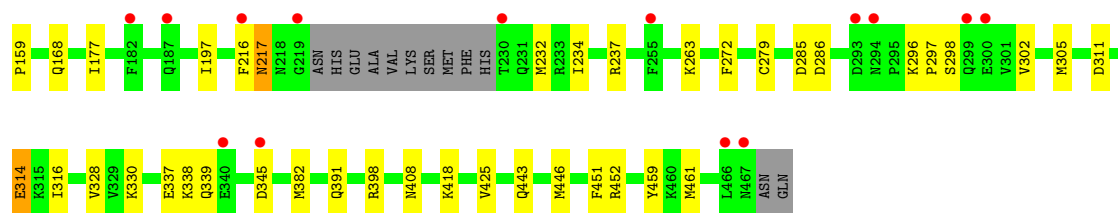


- Molecule 1: Histone-lysine N-methyltransferase SMYD1

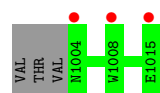
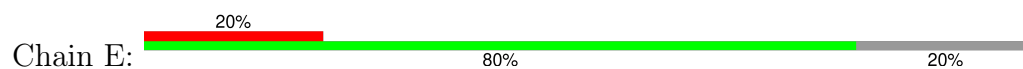


- Molecule 1: Histone-lysine N-methyltransferase SMYD1

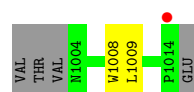




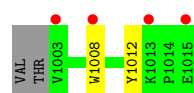
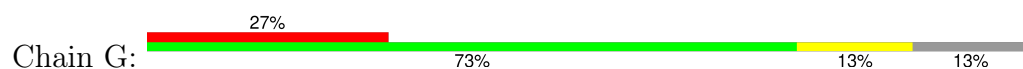
● Molecule 2: Myosin-8 peptide



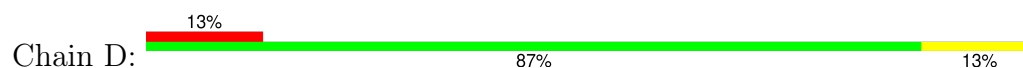
● Molecule 2: Myosin-8 peptide



● Molecule 2: Myosin-8 peptide



● Molecule 2: Myosin-8 peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	88.08Å 154.43Å 181.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.55 – 2.76 47.55 – 2.76	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.55-2.76) 99.6 (47.55-2.76)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.77Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.194 , 0.230 0.199 , 0.236	Depositor DCC
R_{free} test set	3305 reflections (4.45%)	wwPDB-VP
Wilson B-factor (Å ²)	70.4	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 50.8	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	0.94	EDS
Total number of atoms	11252	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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	0.89	1/3661 (0.0%)	1.40	22/4948 (0.4%)
1	B	0.86	0/3653	1.38	19/4941 (0.4%)
1	C	0.87	1/3609 (0.0%)	1.41	32/4882 (0.7%)
2	D	1.13	0/131	1.19	0/182
2	E	0.81	0/126	1.05	0/175
2	F	1.00	0/102	1.10	0/142
2	G	0.92	0/130	1.14	0/181
All	All	0.88	2/11412 (0.0%)	1.39	73/15451 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	461	MET	SD-CE	6.47	1.95	1.79
1	C	99	VAL	CA-C	5.10	1.57	1.53

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	GLU	CA-C-N	8.22	131.64	120.54
1	A	102	GLU	C-N-CA	8.22	131.64	120.54
1	A	103	ASN	CA-CB-CG	7.76	120.36	112.60
1	C	234	ILE	N-CA-CB	7.58	120.08	110.99
1	C	102	GLU	CA-C-N	6.89	129.39	120.44
1	C	102	GLU	C-N-CA	6.89	129.39	120.44
1	C	130	ASP	CA-CB-CG	6.78	119.38	112.60
1	A	186	ASP	CA-CB-CG	6.78	119.38	112.60
1	C	408	ASN	CA-C-N	6.65	129.91	120.53
1	C	408	ASN	C-N-CA	6.65	129.91	120.53
1	C	103	ASN	CA-CB-CG	6.58	119.18	112.60
1	A	139	PHE	CA-CB-CG	6.47	120.27	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	139	PHE	CA-CB-CG	6.32	120.12	113.80
1	A	115	GLU	CA-C-N	6.27	129.00	120.54
1	A	115	GLU	C-N-CA	6.27	129.00	120.54
1	C	33	ILE	N-CA-C	-6.26	104.65	110.53
1	C	217	ASN	CA-C-N	6.19	130.66	120.94
1	C	217	ASN	C-N-CA	6.19	130.66	120.94
1	C	134	ASN	CA-CB-CG	6.08	118.68	112.60
1	C	338	LYS	CA-C-N	6.04	128.29	120.44
1	C	338	LYS	C-N-CA	6.04	128.29	120.44
1	A	36	GLU	CA-C-N	6.01	130.01	121.42
1	A	36	GLU	C-N-CA	6.01	130.01	121.42
1	C	115	GLU	CA-C-N	5.94	128.56	120.54
1	C	115	GLU	C-N-CA	5.94	128.56	120.54
1	C	217	ASN	CA-CB-CG	5.93	118.53	112.60
1	A	101	ASN	CA-C-N	5.92	128.50	120.38
1	A	101	ASN	C-N-CA	5.92	128.50	120.38
1	C	452	ARG	CA-C-N	5.90	128.10	120.44
1	C	452	ARG	C-N-CA	5.90	128.10	120.44
1	C	129	VAL	CA-C-N	5.77	128.58	120.28
1	C	129	VAL	C-N-CA	5.77	128.58	120.28
1	A	156	GLN	CA-C-N	5.76	128.47	120.29
1	A	156	GLN	C-N-CA	5.76	128.47	120.29
1	B	6	SER	CA-C-N	5.68	128.47	120.28
1	B	6	SER	C-N-CA	5.68	128.47	120.28
1	A	33	ILE	N-CA-C	-5.61	105.26	110.53
1	B	39	TYR	N-CA-C	-5.60	105.08	111.07
1	C	314	GLU	CA-C-N	5.60	127.78	120.28
1	C	314	GLU	C-N-CA	5.60	127.78	120.28
1	C	139	PHE	CA-CB-CG	5.59	119.39	113.80
1	C	345	ASP	CA-CB-CG	5.58	118.18	112.60
1	C	216	PHE	CA-CB-CG	5.52	119.32	113.80
1	A	134	ASN	N-CA-C	-5.43	101.02	109.72
1	B	129	VAL	CA-C-N	5.42	128.54	120.31
1	B	129	VAL	C-N-CA	5.42	128.54	120.31
1	B	442	VAL	CA-C-N	5.34	127.44	120.28
1	B	442	VAL	C-N-CA	5.34	127.44	120.28
1	B	175	GLY	CA-C-N	5.27	127.20	120.56
1	B	175	GLY	C-N-CA	5.27	127.20	120.56
1	B	103	ASN	CA-CB-CG	5.24	117.84	112.60
1	A	134	ASN	CA-CB-CG	5.24	117.84	112.60
1	A	338	LYS	CA-C-N	5.24	127.72	120.29
1	A	338	LYS	C-N-CA	5.24	127.72	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	286	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	285	ASP	CA-CB-CG	5.20	117.80	112.60
1	B	216	PHE	CA-CB-CG	5.18	118.98	113.80
1	B	264	ARG	CA-C-N	5.17	127.21	120.28
1	B	264	ARG	C-N-CA	5.17	127.21	120.28
1	C	44	PHE	CA-CB-CG	5.16	118.96	113.80
1	A	366	ALA	N-CA-C	-5.15	104.16	110.65
1	C	34	PHE	CA-CB-CG	5.13	118.93	113.80
1	B	343	PHE	N-CA-C	5.13	116.72	110.41
1	A	103	ASN	N-CA-CB	-5.12	102.32	109.94
1	C	272	PHE	CA-CB-CG	5.11	118.91	113.80
1	A	399	ALA	CA-C-N	5.11	125.61	119.94
1	A	399	ALA	C-N-CA	5.11	125.61	119.94
1	C	65	CYS	CA-C-N	5.10	126.55	120.13
1	C	65	CYS	C-N-CA	5.10	126.55	120.13
1	B	89	GLU	CA-C-N	5.09	127.38	120.65
1	B	89	GLU	C-N-CA	5.09	127.38	120.65
1	C	285	ASP	CA-C-N	5.02	127.50	120.28
1	C	285	ASP	C-N-CA	5.02	127.50	120.28

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	3585	0	3388	13	0
1	B	3576	0	3363	16	0
1	C	3533	0	3317	17	0
2	D	125	0	122	1	0
2	E	118	0	106	0	0
2	F	96	0	89	2	0
2	G	122	0	106	3	0
3	A	26	0	19	0	0
3	B	26	0	19	0	0
3	C	26	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
5	A	6	0	0	0	0
5	B	1	0	0	0	0
5	C	3	0	0	0	0
All	All	11252	0	10548	43	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 (43) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:MET:HE2	1:C:339:GLN:HG2	1.67	0.76
2:D:1001:VAL:HG12	2:D:1002:THR:HG23	1.71	0.73
1:B:450:MET:HE1	1:C:451:PHE:HA	1.73	0.70
1:B:465:ALA:HA	1:C:459:TYR:HD1	1.67	0.60
1:C:391:GLN:HG2	2:G:1008[B]:TRP:HZ2	1.67	0.59
1:B:84:LEU:HD11	1:B:116:ARG:HD2	1.85	0.58
1:A:397:MET:HG3	1:A:437:LEU:HD21	1.93	0.51
1:B:51:VAL:HG22	1:B:58[B]:ARG:HG2	1.93	0.51
1:B:391:GLN:HG2	2:F:1008:TRP:HZ2	1.75	0.50
1:B:176:VAL:O	1:B:180:ASN:HB2	2.12	0.50
1:A:88:ASN:HD22	1:A:112:TRP:CD1	2.29	0.50
1:C:382:MET:HE2	1:C:418:LYS:HE2	1.94	0.49
1:B:450:MET:HE2	1:B:457:MET:HE3	1.95	0.48
1:A:305:MET:HE2	1:A:339:GLN:HG3	1.94	0.48
1:C:30:ALA:HB2	1:C:425:VAL:HA	1.96	0.48
1:B:134:ASN:HB2	1:B:175:GLY:HA3	1.96	0.47
1:C:297:PRO:HB2	1:C:302:VAL:HG23	1.96	0.47
1:B:177:ILE:HA	1:B:197:ILE:HD11	1.97	0.46
1:B:30:ALA:HB2	1:B:425:VAL:HA	1.97	0.46
1:A:394:MET:CE	1:A:433:ILE:HD12	2.45	0.46
1:A:378:VAL:O	1:A:382:MET:HG2	2.16	0.45
1:A:177:ILE:HA	1:A:197:ILE:HD11	1.98	0.45
1:A:351:LEU:HD21	1:A:380:GLY:HA3	1.97	0.45
1:B:113:ARG:NH2	1:B:122:THR:HG21	2.33	0.43
1:A:167:MET:HG3	1:C:330:LYS:HG2	2.00	0.43
1:B:468:ASN:HA	1:C:459:TYR:HE1	1.84	0.43
1:B:391:GLN:HG2	2:F:1008:TRP:CZ2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:391:GLN:HG2	2:G:1008[B]:TRP:CZ2	2.53	0.43
1:C:217:ASN:HA	1:C:232:MET:HE3	2.01	0.42
1:A:394:MET:HE2	1:A:433:ILE:HD12	2.02	0.41
1:C:177:ILE:HA	1:C:197:ILE:HD11	2.01	0.41
1:C:316:ILE:HG23	1:C:328:VAL:HG13	2.01	0.41
1:C:398:ARG:HB3	2:G:1012:TYR:OH	2.20	0.41
1:C:311:ASP:O	1:C:314:GLU:HB2	2.21	0.41
1:A:305:MET:HE2	1:A:339:GLN:CG	2.51	0.41
1:A:84:LEU:HD11	1:A:116:ARG:HD2	2.02	0.41
1:A:151:VAL:HG11	1:A:167:MET:HE3	2.03	0.41
1:C:263:LYS:HE3	1:C:279:CYS:HB3	2.01	0.41
1:A:134:ASN:HB2	1:A:175:GLY:HA3	2.01	0.41
1:B:394:MET:HE1	1:B:433:ILE:HD13	2.03	0.40
1:C:158:TRP:HA	1:C:159:PRO:HD3	1.98	0.40
1:B:188:ARG:HB3	1:B:190:LEU:HG	2.04	0.40
1:B:390:ALA:O	1:B:394:MET:HG3	2.21	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	452/482 (94%)	442 (98%)	7 (2%)	3 (1%)	18	34
1	B	453/482 (94%)	444 (98%)	8 (2%)	1 (0%)	43	64
1	C	449/482 (93%)	434 (97%)	14 (3%)	1 (0%)	43	64
2	D	13/15 (87%)	11 (85%)	2 (15%)	0	100	100
2	E	11/15 (73%)	11 (100%)	0	0	100	100
2	F	9/15 (60%)	9 (100%)	0	0	100	100
2	G	12/15 (80%)	11 (92%)	1 (8%)	0	100	100
All	All	1399/1506 (93%)	1362 (97%)	32 (2%)	5 (0%)	30	50

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	290	GLY
1	C	296	LYS
1	A	296	LYS
1	A	295	PRO
1	B	296	LYS

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	365/423 (86%)	352 (96%)	13 (4%)	31	55
1	B	365/423 (86%)	356 (98%)	9 (2%)	42	64
1	C	356/423 (84%)	342 (96%)	14 (4%)	28	51
2	D	13/15 (87%)	13 (100%)	0	100	100
2	E	11/15 (73%)	11 (100%)	0	100	100
2	F	10/15 (67%)	9 (90%)	1 (10%)	7	14
2	G	11/15 (73%)	11 (100%)	0	100	100
All	All	1131/1329 (85%)	1094 (97%)	37 (3%)	33	57

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	17	LYS
1	A	25	LYS
1	A	58	ARG
1	A	128	SER
1	A	180	ASN
1	A	233	ARG
1	A	237	ARG
1	A	358	SER
1	A	391	GLN
1	A	433	ILE

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Mol	Chain	Res	Type
1	A	434	THR
1	A	450	MET
1	B	10	GLU
1	B	75	ASP
1	B	98	LYS
1	B	103	ASN
1	B	129	VAL
1	B	133	GLN
1	B	201	LEU
1	B	256	LEU
1	B	330	LYS
2	F	1009	LEU
1	C	10	GLU
1	C	13	THR
1	C	33	ILE
1	C	58	ARG
1	C	77	THR
1	C	130	ASP
1	C	168	GLN
1	C	237	ARG
1	C	286	ASP
1	C	298	SER
1	C	337	GLU
1	C	443	GLN
1	C	446	MET
1	C	461	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	161	GLN
1	A	191	GLN
1	A	218	ASN
1	A	257	ASN
1	A	403	ASN
1	A	408	ASN
1	A	468	ASN
1	B	49	ASN
1	B	72	HIS
1	B	103	ASN
1	B	178	ASN

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Mol	Chain	Res	Type
1	B	180	ASN
1	B	217	ASN
1	C	85	ASN
1	C	133	GLN
1	C	161	GLN
1	C	218	ASN
1	C	269	GLN
1	C	278	HIS
1	C	403	ASN
1	C	453	GLN
1	C	454	ASN
2	G	1004	ASN

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, 9 are monoatomic - leaving 3 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	$\# Z > 2$
3	SAH	C	2000	-	27,28,28	0.29	0	36,40,40	0.59	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SAH	A	2000	-	27,28,28	0.30	0	36,40,40	0.76	2 (5%)
3	SAH	B	2000	-	27,28,28	0.34	0	36,40,40	0.56	1 (2%)

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	C	2000	-	-	3/15/31/31	0/3/3/3
3	SAH	A	2000	-	-	2/15/31/31	0/3/3/3
3	SAH	B	2000	-	-	3/15/31/31	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2000	SAH	CB-CA-N	2.89	117.65	110.12
3	A	2000	SAH	CB-CG-SD	-2.32	108.28	113.45
3	C	2000	SAH	CB-CA-N	2.11	115.61	110.12
3	B	2000	SAH	CB-CA-N	2.11	115.61	110.12

There are no chirality outliers.

All (8) torsion outliers are listed below:

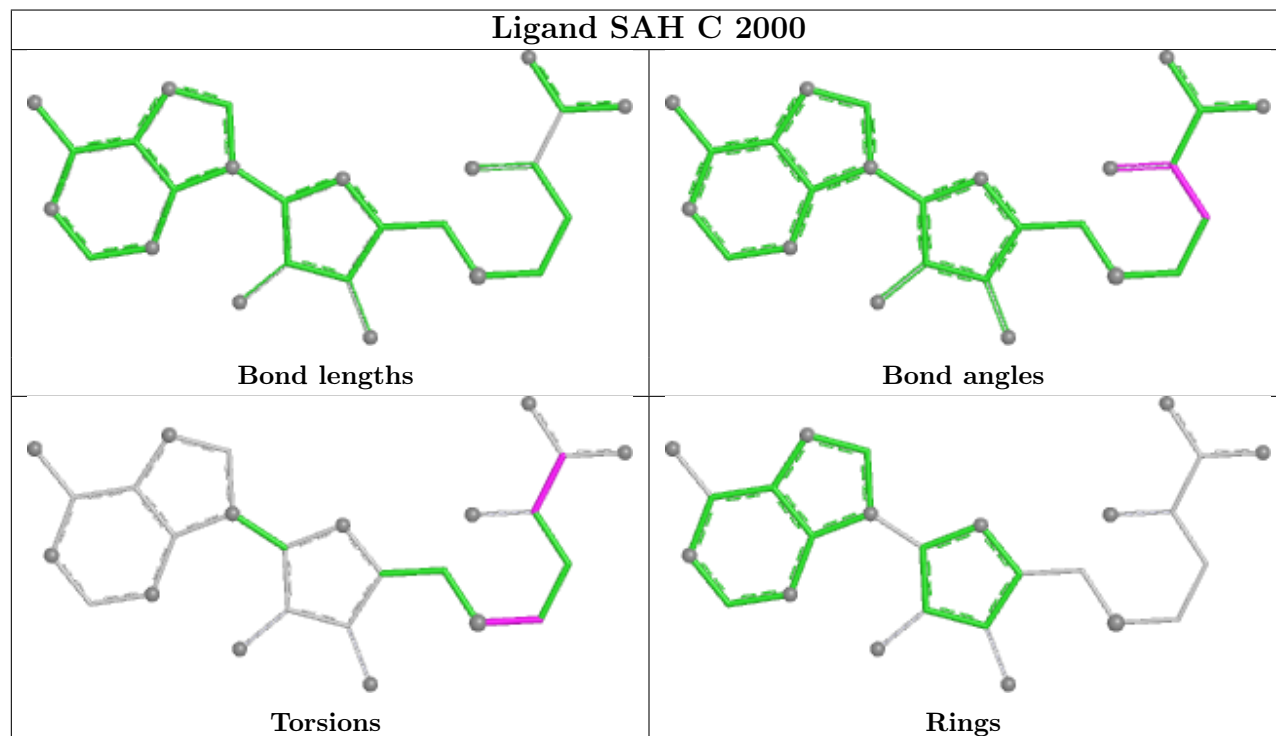
Mol	Chain	Res	Type	Atoms
3	C	2000	SAH	O-C-CA-CB
3	C	2000	SAH	OXT-C-CA-CB
3	C	2000	SAH	CB-CG-SD-C5'
3	A	2000	SAH	CB-CG-SD-C5'
3	B	2000	SAH	CB-CG-SD-C5'
3	B	2000	SAH	O-C-CA-CB
3	B	2000	SAH	OXT-C-CA-CB
3	A	2000	SAH	O-C-CA-CB

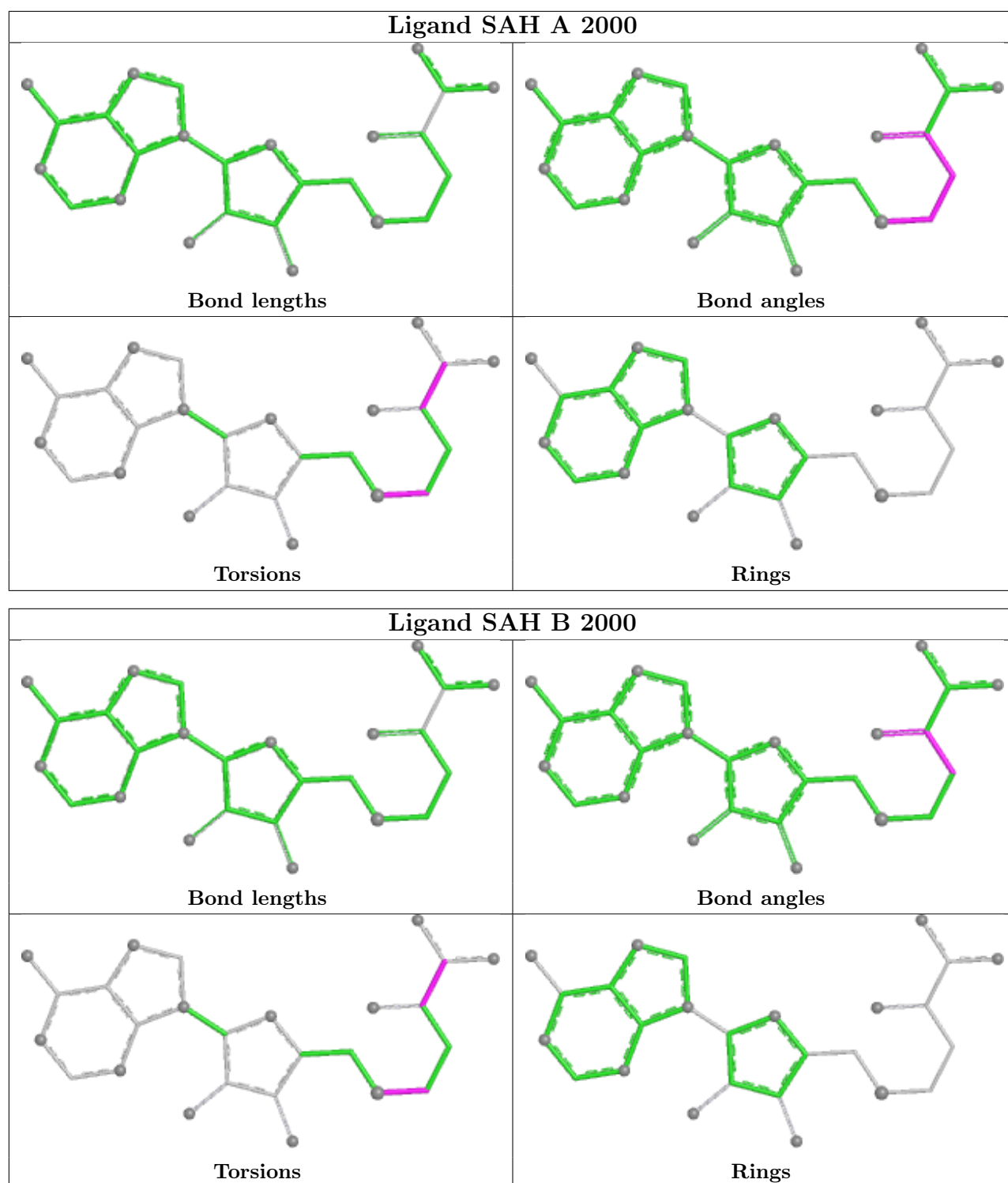
There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

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	455/482 (94%)	-0.06	13 (2%)	53 52	27, 61, 88, 116	1 (0%)
1	B	454/482 (94%)	0.32	22 (4%)	35 35	27, 80, 111, 140	3 (0%)
1	C	453/482 (93%)	0.35	20 (4%)	39 38	54, 79, 111, 126	0
2	D	15/15 (100%)	0.61	2 (13%)	7 6	48, 57, 66, 78	0
2	E	12/15 (80%)	0.48	3 (25%)	2 1	21, 48, 61, 76	1 (8%)
2	F	11/15 (73%)	0.54	1 (9%)	15 14	64, 76, 81, 84	0
2	G	13/15 (86%)	1.16	4 (30%)	1 1	30, 70, 88, 94	1 (7%)
All	All	1413/1506 (93%)	0.22	65 (4%)	37 36	21, 74, 107, 140	6 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	372[A]	PHE	8.9
1	A	219	GLY	6.6
1	B	5	GLY	5.5
1	C	467	ASN	4.9
1	C	6	SER	4.8
1	C	219	GLY	4.8
1	C	5	GLY	4.7
1	C	230	THR	4.6
2	D	1015	GLU	4.5
1	A	230	THR	4.4
2	G	1015	GLU	4.4
2	D	1001	VAL	4.3
2	G	1003	VAL	4.1
1	A	372[A]	PHE	4.1
1	B	6	SER	4.0
1	C	187	GLN	3.7
1	B	288	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	294	ASN	3.5
1	B	54	THR	3.3
1	B	293	ASP	3.3
1	C	340	GLU	3.2
1	B	230	THR	3.2
1	C	300	GLU	3.2
1	A	459	TYR	3.1
1	B	219	GLY	3.1
1	B	58[A]	ARG	3.0
1	B	232	MET	3.0
1	B	7	GLU	2.9
1	C	216	PHE	2.9
1	B	187	GLN	2.9
1	C	294	ASN	2.9
1	B	465	ALA	2.9
1	C	124	GLY	2.8
1	B	296	LYS	2.8
1	B	304	GLU	2.8
1	B	289	LEU	2.8
1	A	340	GLU	2.8
1	B	255	PHE	2.8
1	A	300	GLU	2.7
2	F	1014	PRO	2.7
2	E	1015	GLU	2.6
2	G	1013	LYS	2.6
1	A	296	LYS	2.6
2	E	1008[A]	TRP	2.6
1	C	142	GLU	2.6
1	B	295	PRO	2.6
1	B	468	ASN	2.6
1	C	466	LEU	2.5
1	C	182	PHE	2.5
1	C	293	ASP	2.5
2	G	1008[A]	TRP	2.5
1	C	17	LYS	2.4
1	A	63	HIS	2.4
1	C	345	ASP	2.4
1	B	28	TRP	2.3
2	E	1004	ASN	2.3
1	A	295	PRO	2.3
1	B	458	TYR	2.3
1	A	15	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	456	PHE	2.2
1	C	61	LYS	2.2
1	C	255	PHE	2.2
1	A	294	ASN	2.2
1	A	5	GLY	2.1
1	C	299	GLN	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](#)

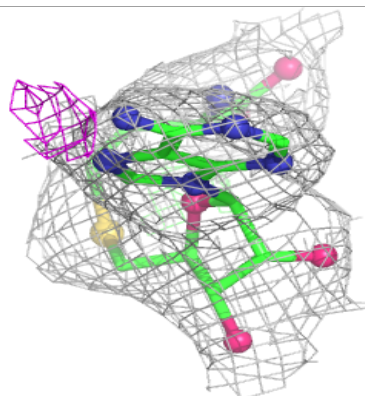
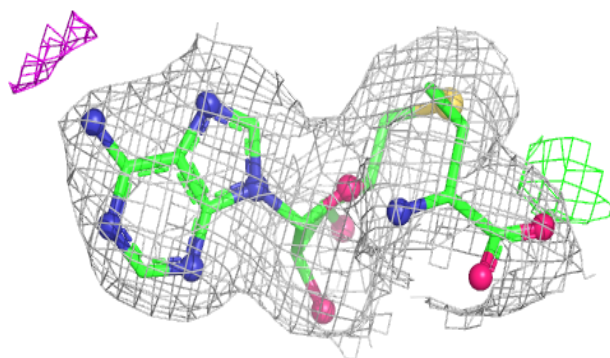
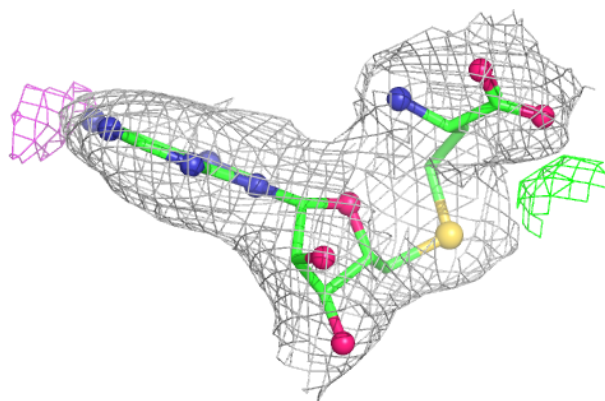
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	C	2000	26/26	0.94	0.08	73,79,91,92	0
3	SAH	B	2000	26/26	0.95	0.07	69,77,82,85	0
3	SAH	A	2000	26/26	0.96	0.08	55,61,70,73	0
4	ZN	A	2002	1/1	0.99	0.03	68,68,68,68	0
4	ZN	B	2002	1/1	0.99	0.03	81,81,81,81	0
4	ZN	B	2003	1/1	0.99	0.03	76,76,76,76	0
4	ZN	C	2002	1/1	0.99	0.06	98,98,98,98	0
4	ZN	C	2003	1/1	0.99	0.06	98,98,98,98	0
4	ZN	A	2003	1/1	1.00	0.02	70,70,70,70	0
4	ZN	C	2001	1/1	1.00	0.05	81,81,81,81	0
4	ZN	B	2001	1/1	1.00	0.04	82,82,82,82	0
4	ZN	A	2001	1/1	1.00	0.04	62,62,62,62	0

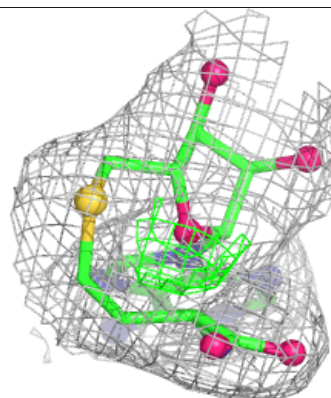
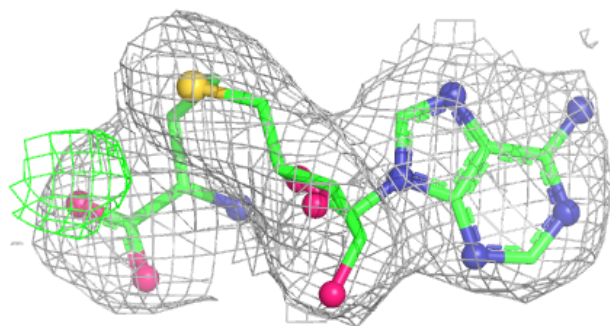
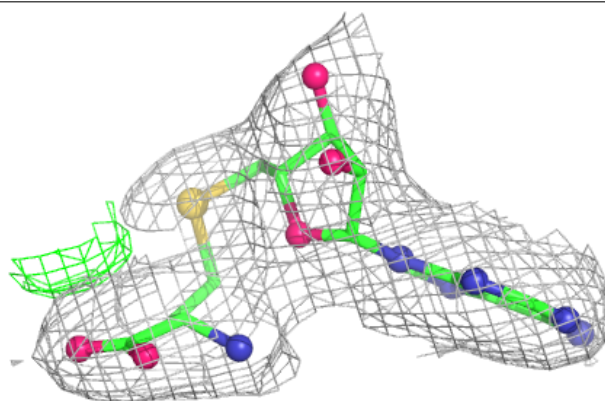
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAH C 2000:

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

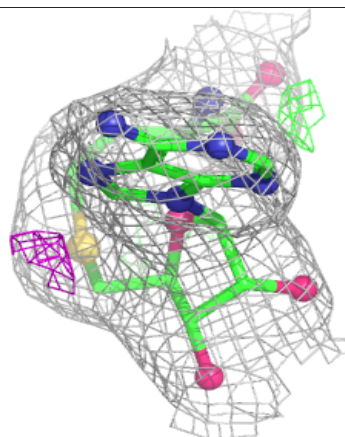
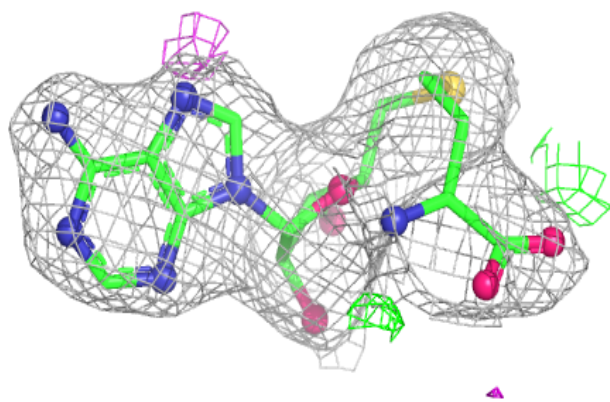
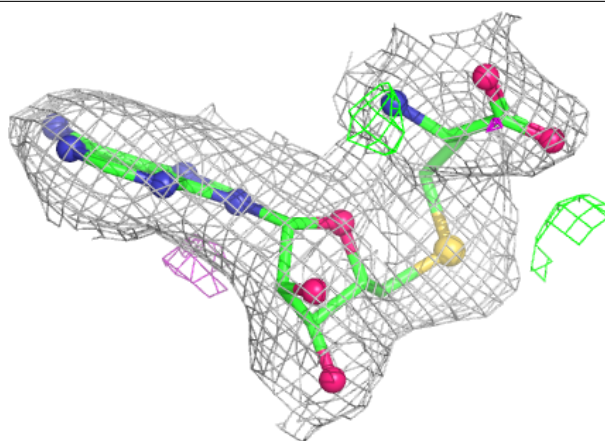
**Electron density around SAH B 2000:**

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



Electron density around SAH A 2000:

$2mF_o-DF_c$ (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.