



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:32 PM UTC

PDB ID : 7PD7 / pdb_00007pd7
Title : Crocagin methyl transferase CgnL
Authors : Zheng, D.; Koehnke, J.
Deposited on : 2021-08-04
Resolution : 1.96 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

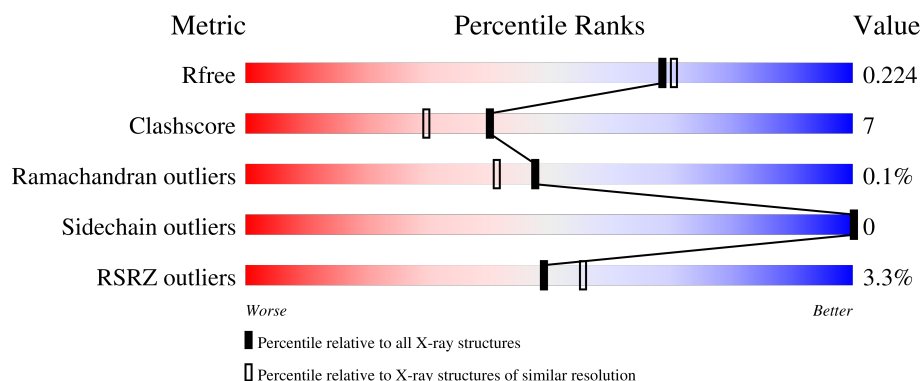
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	255	2% 86% 10% .
1	B	255	4% 87% 10% ..
1	C	255	3% 89% 8% .
1	D	255	4% 85% 12% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15740 atoms, of which 7573 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 Methyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	247	Total	C	H	N	O	S	0	0	0
			3750	1190	1854	344	351	11			
1	B	250	Total	C	H	N	O	S	0	0	0
			3788	1201	1873	347	356	11			
1	C	248	Total	C	H	N	O	S	0	0	0
			3758	1192	1858	345	352	11			
1	D	249	Total	C	H	N	O	S	0	0	0
			3770	1196	1862	346	355	11			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP A0A0K1EC20
A	-4	ALA	-	expression tag	UNP A0A0K1EC20
A	-3	MET	-	expression tag	UNP A0A0K1EC20
A	-2	GLY	-	expression tag	UNP A0A0K1EC20
A	-1	GLY	-	expression tag	UNP A0A0K1EC20
A	0	GLY	-	expression tag	UNP A0A0K1EC20
A	1	GLY	-	expression tag	UNP A0A0K1EC20
B	-5	GLY	-	expression tag	UNP A0A0K1EC20
B	-4	ALA	-	expression tag	UNP A0A0K1EC20
B	-3	MET	-	expression tag	UNP A0A0K1EC20
B	-2	GLY	-	expression tag	UNP A0A0K1EC20
B	-1	GLY	-	expression tag	UNP A0A0K1EC20
B	0	GLY	-	expression tag	UNP A0A0K1EC20
B	1	GLY	-	expression tag	UNP A0A0K1EC20
C	-5	GLY	-	expression tag	UNP A0A0K1EC20
C	-4	ALA	-	expression tag	UNP A0A0K1EC20
C	-3	MET	-	expression tag	UNP A0A0K1EC20
C	-2	GLY	-	expression tag	UNP A0A0K1EC20
C	-1	GLY	-	expression tag	UNP A0A0K1EC20
C	0	GLY	-	expression tag	UNP A0A0K1EC20
C	1	GLY	-	expression tag	UNP A0A0K1EC20

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	GLY	-	expression tag	UNP A0A0K1EC20
D	-4	ALA	-	expression tag	UNP A0A0K1EC20
D	-3	MET	-	expression tag	UNP A0A0K1EC20
D	-2	GLY	-	expression tag	UNP A0A0K1EC20
D	-1	GLY	-	expression tag	UNP A0A0K1EC20
D	0	GLY	-	expression tag	UNP A0A0K1EC20
D	1	GLY	-	expression tag	UNP A0A0K1EC20

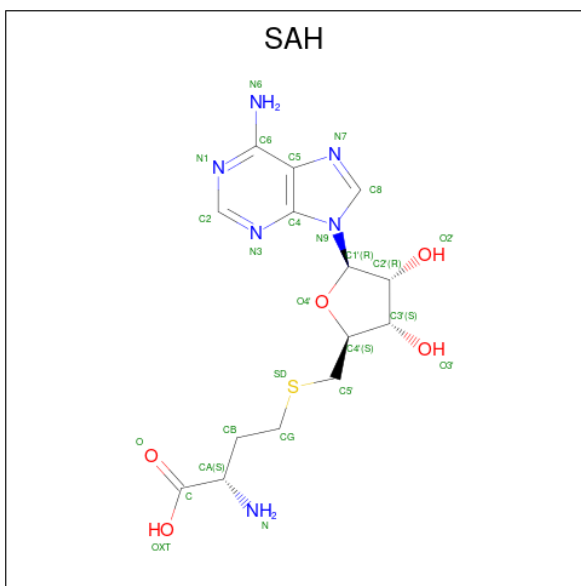
- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	A	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		
2	B	1	Total	C	H	O	0	0
			12	3	6	3		
2	C	1	Total	C	H	O	0	0
			13	3	7	3		
2	C	1	Total	C	H	O	0	0
			13	3	7	3		

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

(labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 43	C 14	H 17	N 6	O 5	S 1	0	0
3	B	1	Total 45	C 14	H 19	N 6	O 5	S 1	0	0
3	C	1	Total 45	C 14	H 19	N 6	O 5	S 1	0	0
3	D	1	Total 45	C 14	H 19	N 6	O 5	S 1	0	0

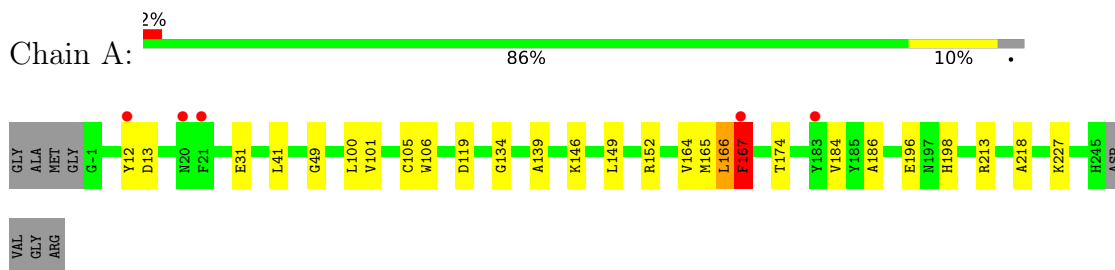
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	112	Total	O	0	0
			112	112		
4	B	98	Total	O	0	0
			98	98		
4	C	91	Total	O	0	0
			91	91		
4	D	101	Total	O	0	0
			101	101		

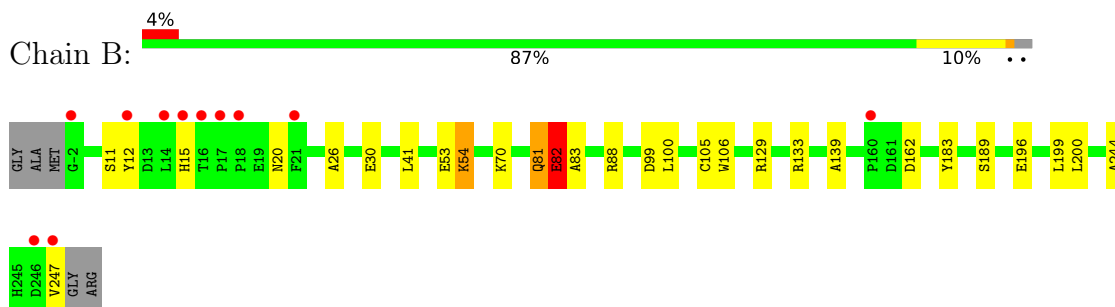
3 Residue-property plots [i](#)

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.

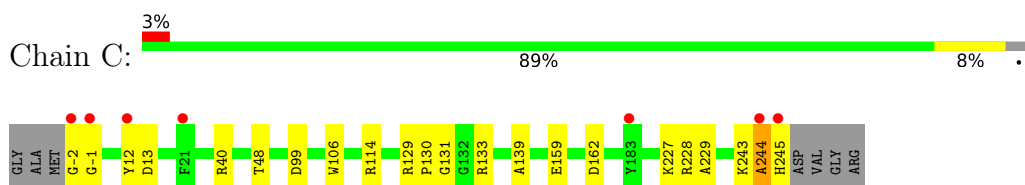
- Molecule 1: Methyltransferase



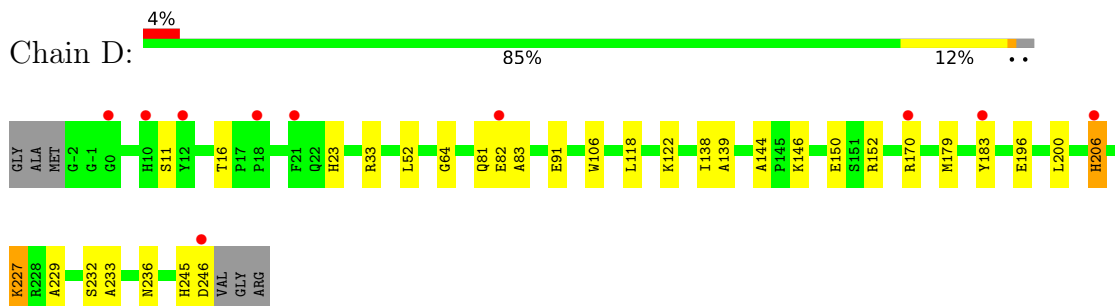
- Molecule 1: Methyltransferase



- Molecule 1: Methyltransferase



- Molecule 1: Methyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	40.95Å 128.12Å 94.30Å 90.00° 90.39° 90.00°	Depositor
Resolution (Å)	47.15 – 1.96 47.15 – 1.96	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.15-1.96) 90.1 (47.15-1.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 1.97Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.185 , 0.223 0.187 , 0.224	Depositor DCC
R_{free} test set	3542 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.055 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15740	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.01% 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, GOL

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	0.35	0/1941	0.68	4/2635 (0.2%)
1	B	0.81	11/1960 (0.6%)	0.89	11/2661 (0.4%)
1	C	0.25	0/1945	0.40	0/2640
1	D	0.42	1/1953 (0.1%)	0.74	6/2651 (0.2%)
All	All	0.50	12/7799 (0.2%)	0.70	21/10587 (0.2%)

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	1
1	B	0	2
1	D	0	1
All	All	0	4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	82	GLU	CB-CG	17.10	2.03	1.52
1	B	54	LYS	CG-CD	11.59	1.87	1.52
1	B	81	GLN	C-N	10.21	1.48	1.33
1	B	54	LYS	CB-CG	-10.11	1.22	1.52
1	B	81	GLN	CA-C	9.48	1.65	1.52
1	B	82	GLU	CA-C	9.07	1.65	1.52
1	B	82	GLU	N-CA	8.79	1.57	1.46
1	B	82	GLU	CG-CD	7.74	1.71	1.52
1	D	227	LYS	CE-NZ	7.44	1.71	1.49
1	B	82	GLU	CA-CB	7.18	1.65	1.53
1	B	54	LYS	CA-C	-6.71	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	82	GLU	CD-OE1	6.09	1.36	1.25

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	82	GLU	CB-CG-CD	-21.25	76.48	112.60
1	A	166	LEU	CA-C-N	-16.35	95.73	122.21
1	A	166	LEU	C-N-CA	-16.35	95.73	122.21
1	B	54	LYS	N-CA-C	-13.75	96.37	111.36
1	B	82	GLU	CA-CB-CG	-13.01	88.09	114.10
1	B	82	GLU	CG-CD-OE1	12.73	147.69	118.40
1	D	206	HIS	CB-CA-C	-10.28	94.67	110.90
1	D	227	LYS	CG-CD-CE	-10.08	88.11	111.30
1	B	54	LYS	CD-CE-NZ	-9.89	80.24	111.90
1	B	82	GLU	CG-CD-OE2	-8.42	99.03	118.40
1	B	81	GLN	CA-C-O	-8.12	108.90	120.51
1	A	167	PHE	N-CA-C	-7.98	97.19	109.24
1	B	82	GLU	OE1-CD-OE2	-7.51	104.86	122.90
1	B	82	GLU	O-C-N	-6.81	113.53	122.59
1	A	167	PHE	N-CA-CB	6.73	123.40	111.69
1	D	206	HIS	N-CA-CB	6.71	119.80	110.07
1	B	54	LYS	CB-CA-C	6.61	122.09	110.85
1	B	83	ALA	N-CA-CB	-5.80	102.05	110.47
1	D	206	HIS	CB-CG-CD2	-5.58	123.94	131.20
1	D	206	HIS	N-CA-C	-5.44	105.27	111.14
1	D	81	GLN	CB-CG-CD	-5.41	103.40	112.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	PHE	Sidechain
1	B	81	GLN	Peptide
1	B	82	GLU	Sidechain
1	D	206	HIS	Sidechain

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	1896	1854	1856	24	1
1	B	1915	1873	1873	26	0
1	C	1900	1858	1860	19	0
1	D	1908	1862	1864	29	1
2	A	18	24	24	1	0
2	B	12	14	16	2	0
2	C	12	14	16	3	0
3	A	26	17	17	2	0
3	B	26	19	19	1	0
3	C	26	19	19	3	0
3	D	26	19	19	1	0
4	A	112	0	0	6	1
4	B	98	0	0	3	0
4	C	91	0	0	6	4
4	D	101	0	0	11	2
All	All	8167	7573	7583	101	5

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 7.

All (101) 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:D:227:LYS:NZ	1:D:227:LYS:CE	1.71	1.49
1:B:54:LYS:CD	1:B:54:LYS:CG	1.87	1.48
1:B:82:GLU:CB	1:B:82:GLU:CG	2.03	1.37
1:B:82:GLU:CB	1:B:82:GLU:CD	2.33	1.02
1:B:82:GLU:CG	1:B:82:GLU:CA	2.58	0.81
1:D:229:ALA:N	4:D:601:HOH:O	2.00	0.81
1:D:91:GLU:OE1	4:D:602:HOH:O	2.00	0.80
1:B:54:LYS:CD	1:B:54:LYS:CB	2.59	0.79
1:D:170:ARG:NH2	4:D:603:HOH:O	2.17	0.77
1:B:129:ARG:HD2	1:C:129:ARG:HD2	1.69	0.75
1:D:82:GLU:HG2	1:D:83:ALA:N	2.03	0.73
1:A:174:THR:O	4:A:501:HOH:O	2.07	0.71
1:A:41:LEU:HD12	1:A:100:LEU:HD23	1.70	0.71
1:A:31:GLU:OE1	4:A:502:HOH:O	2.09	0.69
2:B:403:GOL:H31	1:D:122:LYS:HB3	1.74	0.68
1:D:229:ALA:HB3	4:D:601:HOH:O	1.96	0.66
1:A:146:LYS:NZ	4:A:506:HOH:O	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ARG:HD3	4:B:501:HOH:O	1.98	0.63
1:D:152:ARG:NE	4:D:605:HOH:O	2.20	0.63
1:D:82:GLU:H	1:D:82:GLU:CD	2.07	0.62
1:B:20:ASN:ND2	4:B:506:HOH:O	2.32	0.61
1:A:13:ASP:OD1	2:A:401:GOL:O3	2.19	0.61
1:B:54:LYS:CG	1:B:54:LYS:CE	2.77	0.60
1:D:170:ARG:CZ	4:D:603:HOH:O	2.50	0.60
1:D:106:TRP:CE2	1:D:139:ALA:HB2	2.36	0.59
1:D:229:ALA:CB	4:D:601:HOH:O	2.51	0.59
1:A:166:LEU:C	1:A:167:PHE:HD1	2.10	0.59
1:B:82:GLU:CG	1:B:82:GLU:HA	2.32	0.59
1:B:106:TRP:CE2	1:B:139:ALA:HB2	2.38	0.58
1:B:99:ASP:OD1	1:B:129:ARG:NE	2.34	0.58
1:C:106:TRP:CE2	1:C:139:ALA:HB2	2.40	0.57
1:A:165:MET:HB3	1:A:167:PHE:CE1	2.39	0.57
1:A:166:LEU:C	1:A:167:PHE:CD1	2.85	0.55
1:D:11:SER:OG	4:D:604:HOH:O	2.18	0.54
1:D:33:ARG:NH2	4:D:608:HOH:O	2.41	0.54
1:C:129:ARG:HH22	2:C:402:GOL:H2	1.73	0.53
1:A:119:ASP:OD1	4:A:503:HOH:O	2.19	0.53
1:D:144:ALA:O	1:D:146:LYS:HD2	2.09	0.53
1:B:26:ALA:O	1:B:30:GLU:HG3	2.09	0.52
1:A:106:TRP:CE2	1:A:139:ALA:HB2	2.44	0.52
1:D:179:MET:HE2	1:D:200:LEU:HD12	1.91	0.51
1:D:23:HIS:HB2	4:D:606:HOH:O	2.10	0.51
1:D:16:THR:O	1:D:16:THR:HG22	2.09	0.51
1:D:170:ARG:NE	1:D:170:ARG:HA	2.26	0.51
1:A:166:LEU:O	1:A:167:PHE:HD1	1.94	0.50
1:C:99:ASP:OD1	1:C:129:ARG:NE	2.39	0.49
1:B:54:LYS:CG	1:B:54:LYS:NZ	2.76	0.49
1:B:129:ARG:HH12	2:B:401:GOL:H12	1.78	0.49
1:C:40:ARG:NH1	4:C:505:HOH:O	2.32	0.49
1:C:130:PRO:HB3	1:C:245:HIS:C	2.38	0.49
1:C:12:TYR:CE1	3:C:403:SAH:HB2	2.48	0.49
1:D:170:ARG:NH1	4:D:603:HOH:O	2.45	0.49
1:D:23:HIS:CE1	1:D:227:LYS:NZ	2.81	0.48
1:A:105:CYS:HB2	3:A:403:SAH:HA	1.66	0.47
1:A:227:LYS:HB2	4:A:547:HOH:O	2.13	0.47
1:B:41:LEU:C	1:B:41:LEU:HD23	2.39	0.47
1:A:165:MET:HA	1:A:184:VAL:O	2.15	0.46
1:B:244:ALA:HB3	1:B:247:VAL:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:403:SAH:H4'	3:C:403:SAH:HG2	1.72	0.46
1:C:244:ALA:O	1:C:245:HIS:HB2	2.16	0.46
1:A:213:ARG:NH1	1:A:218:ALA:O	2.49	0.45
1:C:131:GLY:O	2:C:402:GOL:H32	2.16	0.45
1:A:152:ARG:HH11	1:A:152:ARG:HG2	1.82	0.45
1:C:227:LYS:O	1:C:228:ARG:HB2	2.16	0.45
1:A:196:GLU:HG2	1:A:198:HIS:CD2	2.51	0.45
1:D:118:LEU:HG	1:D:122:LYS:HE2	1.97	0.45
1:C:114:ARG:NH2	4:C:502:HOH:O	2.25	0.45
1:C:133:ARG:NH2	2:C:402:GOL:O3	2.50	0.44
3:D:501:SAH:HB1	3:D:501:SAH:H4'	1.99	0.44
1:B:11:SER:OG	4:B:502:HOH:O	2.20	0.44
1:C:-1:GLY:N	4:C:510:HOH:O	2.50	0.44
1:B:53:GLU:O	1:B:54:LYS:C	2.57	0.44
1:B:105:CYS:O	3:B:402:SAH:HG1	2.17	0.44
1:C:243:LYS:O	1:C:244:ALA:C	2.60	0.44
1:C:229:ALA:HB3	4:C:525:HOH:O	2.16	0.44
3:A:403:SAH:HG1	3:A:403:SAH:H4'	1.83	0.43
1:D:183:TYR:CE1	1:D:196:GLU:HB2	2.53	0.43
1:B:12:TYR:HA	1:B:15:HIS:NE2	2.33	0.43
1:C:131:GLY:N	1:C:245:HIS:HA	2.34	0.43
1:B:183:TYR:CE1	1:B:196:GLU:HB3	2.54	0.43
1:B:199:LEU:C	1:B:200:LEU:HD12	2.44	0.43
1:D:33:ARG:NH2	1:D:33:ARG:HG2	2.32	0.43
1:D:245:HIS:O	1:D:246:ASP:C	2.61	0.43
1:A:149:LEU:O	1:A:166:LEU:HA	2.18	0.43
1:A:12:TYR:CD1	1:A:12:TYR:C	2.97	0.42
1:A:149:LEU:O	1:A:167:PHE:N	2.50	0.42
1:D:52:LEU:HD11	1:D:64:GLY:HA3	2.01	0.42
1:C:13:ASP:OD2	1:C:48:THR:HG21	2.19	0.42
1:D:232:SER:OG	1:D:233:ALA:N	2.53	0.42
1:C:-2:GLY:C	4:C:510:HOH:O	2.63	0.41
1:A:41:LEU:CD1	1:A:100:LEU:HD23	2.47	0.41
1:B:100:LEU:HD12	1:B:133:ARG:O	2.20	0.41
1:B:162:ASP:OD2	1:B:189:SER:OG	2.36	0.41
1:C:159:GLU:HB2	1:C:162:ASP:HB2	2.02	0.41
1:B:70:LYS:HD2	1:B:70:LYS:HA	1.93	0.41
1:D:138:ILE:O	1:D:236:ASN:HA	2.20	0.41
3:C:403:SAH:N	4:C:506:HOH:O	2.37	0.41
1:A:49:GLY:HA2	4:A:538:HOH:O	2.21	0.40
1:A:101:VAL:O	1:A:134:GLY:HA2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:VAL:CG1	1:A:186:ALA:HB3	2.52	0.40
1:D:23:HIS:CE1	1:D:227:LYS:HZ3	2.38	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:595:HOH:O	4:C:580:HOH:O[1_655]	1.86	0.34
1:A:152:ARG:HH22	1:D:150:GLU:OE2[1_554]	1.45	0.15
4:C:585:HOH:O	4:D:661:HOH:O[2_657]	2.09	0.11
4:C:582:HOH:O	4:C:583:HOH:O[1_455]	2.10	0.10
4:C:585:HOH:O	4:D:675:HOH:O[2_657]	2.15	0.05

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	245/255 (96%)	240 (98%)	5 (2%)	0	100	100
1	B	248/255 (97%)	241 (97%)	7 (3%)	0	100	100
1	C	246/255 (96%)	240 (98%)	5 (2%)	1 (0%)	30	21
1	D	247/255 (97%)	241 (98%)	6 (2%)	0	100	100
All	All	986/1020 (97%)	962 (98%)	23 (2%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	244	ALA

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	195/199 (98%)	195 (100%)	0	100	100
1	B	197/199 (99%)	197 (100%)	0	100	100
1	C	195/199 (98%)	195 (100%)	0	100	100
1	D	196/199 (98%)	196 (100%)	0	100	100
All	All	783/796 (98%)	783 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	23	HIS
1	C	6	ASN
1	D	23	HIS
1	D	143	HIS

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

11 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	B	402	-	27,28,28	1.04	3 (11%)	36,40,40	2.22	11 (30%)
2	GOL	A	401	-	5,5,5	0.76	0	5,5,5	1.07	0
3	SAH	A	403	-	27,28,28	1.08	3 (11%)	36,40,40	2.09	9 (25%)
2	GOL	B	403	-	5,5,5	0.81	0	5,5,5	1.34	1 (20%)
2	GOL	A	402	-	5,5,5	0.90	0	5,5,5	1.41	1 (20%)
2	GOL	A	404	-	5,5,5	0.48	0	5,5,5	0.87	0
2	GOL	C	401	-	5,5,5	0.77	0	5,5,5	1.16	1 (20%)
2	GOL	C	402	-	5,5,5	0.88	0	5,5,5	0.98	0
3	SAH	D	501	-	27,28,28	1.09	4 (14%)	36,40,40	2.16	11 (30%)
2	GOL	B	401	-	5,5,5	0.48	0	5,5,5	0.90	0
3	SAH	C	403	-	27,28,28	1.14	4 (14%)	36,40,40	2.12	11 (30%)

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	B	402	-	-	5/15/31/31	0/3/3/3
2	GOL	A	401	-	-	0/4/4/4	-
3	SAH	A	403	-	-	6/15/31/31	0/3/3/3
2	GOL	B	403	-	-	2/4/4/4	-
2	GOL	A	402	-	-	2/4/4/4	-
2	GOL	A	404	-	-	3/4/4/4	-
2	GOL	C	401	-	-	2/4/4/4	-
2	GOL	C	402	-	-	4/4/4/4	-
3	SAH	D	501	-	-	0/15/31/31	0/3/3/3
2	GOL	B	401	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SAH	C	403	-	-	5/15/31/31	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	501	SAH	C2-N3	2.76	1.38	1.33
3	C	403	SAH	C2-N3	2.72	1.38	1.33
3	D	501	SAH	C2-N1	2.54	1.38	1.33
3	C	403	SAH	C2-N1	2.52	1.38	1.33
3	A	403	SAH	C2-N3	2.48	1.38	1.33
3	B	402	SAH	C2-N3	2.46	1.38	1.33
3	A	403	SAH	OXT-C	-2.45	1.22	1.30
3	A	403	SAH	C2-N1	2.37	1.38	1.33
3	C	403	SAH	OXT-C	-2.30	1.23	1.30
3	B	402	SAH	C2-N1	2.25	1.37	1.33
3	D	501	SAH	C8-N7	2.13	1.35	1.31
3	C	403	SAH	C8-N7	2.07	1.35	1.31
3	D	501	SAH	OXT-C	-2.06	1.24	1.30
3	B	402	SAH	OXT-C	-2.03	1.24	1.30

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	501	SAH	N3-C2-N1	-5.95	119.57	128.58
3	A	403	SAH	N3-C2-N1	-5.87	119.69	128.58
3	C	403	SAH	N3-C2-N1	-5.76	119.86	128.58
3	B	402	SAH	N3-C2-N1	-5.73	119.90	128.58
3	B	402	SAH	N9-C8-N7	-4.96	106.90	113.94
3	A	403	SAH	N9-C8-N7	-4.78	107.15	113.94
3	D	501	SAH	N9-C8-N7	-4.69	107.28	113.94
3	C	403	SAH	N9-C8-N7	-4.66	107.33	113.94
3	B	402	SAH	C5-C4-N3	-4.23	120.89	126.72
3	C	403	SAH	C5-C4-N3	-4.20	120.94	126.72
3	D	501	SAH	C5-C4-N3	-4.19	120.95	126.72
3	B	402	SAH	C5-N7-C8	4.11	109.90	103.45
3	A	403	SAH	C4-N9-C8	3.89	109.82	105.74
3	C	403	SAH	C5-N7-C8	3.68	109.24	103.45
3	A	403	SAH	C5-C4-N3	-3.64	121.70	126.72
3	D	501	SAH	C5-N7-C8	3.57	109.06	103.45
3	C	403	SAH	C4-N9-C8	3.56	109.48	105.74
3	A	403	SAH	C5-N7-C8	3.56	109.04	103.45
3	D	501	SAH	C4-N9-C8	3.45	109.36	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	SAH	C4-N9-C8	3.43	109.34	105.74
3	C	403	SAH	N3-C4-N9	3.35	132.86	127.17
3	B	402	SAH	N3-C4-N9	3.35	132.86	127.17
3	D	501	SAH	C2-N3-C4	3.35	120.00	111.83
3	B	402	SAH	C2-N3-C4	3.32	119.95	111.83
3	D	501	SAH	N3-C4-N9	3.29	132.77	127.17
3	C	403	SAH	C2-N3-C4	3.28	119.85	111.83
3	A	403	SAH	N3-C4-N9	3.21	132.62	127.17
3	B	402	SAH	OXT-C-O	-3.20	116.81	124.08
3	A	403	SAH	C2-N3-C4	3.06	119.30	111.83
3	D	501	SAH	C5'-SD-CG	-3.02	93.31	102.26
3	B	402	SAH	C5'-SD-CG	-2.87	93.73	102.26
2	A	402	GOL	C3-C2-C1	-2.75	101.73	111.80
3	C	403	SAH	OXT-C-O	-2.64	118.09	124.08
3	D	501	SAH	C2'-C3'-C4'	2.63	107.69	102.61
3	B	402	SAH	C4-C5-N7	-2.60	107.61	110.58
3	D	501	SAH	OXT-C-O	-2.54	118.32	124.08
3	A	403	SAH	OXT-C-O	-2.51	118.38	124.08
3	C	403	SAH	C4-C5-N7	-2.48	107.74	110.58
3	A	403	SAH	C2'-C3'-C4'	2.39	107.23	102.61
2	B	403	GOL	C3-C2-C1	-2.29	103.39	111.80
3	D	501	SAH	C4-C5-N7	-2.25	108.01	110.58
3	B	402	SAH	C2'-C3'-C4'	2.22	106.90	102.61
3	C	403	SAH	C2'-C3'-C4'	2.21	106.88	102.61
2	C	401	GOL	C3-C2-C1	-2.08	104.16	111.80
3	C	403	SAH	O4'-C1'-N9	2.01	111.94	108.09

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	402	GOL	C1-C2-C3-O3
2	A	404	GOL	O1-C1-C2-C3
2	B	401	GOL	O1-C1-C2-C3
2	C	401	GOL	C1-C2-C3-O3
2	C	402	GOL	O1-C1-C2-O2
2	C	402	GOL	O1-C1-C2-C3
2	C	402	GOL	C1-C2-C3-O3
3	A	403	SAH	O-C-CA-N
3	B	402	SAH	O-C-CA-N
3	A	403	SAH	CA-CB-CG-SD
3	B	402	SAH	CA-CB-CG-SD

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Mol	Chain	Res	Type	Atoms
3	A	403	SAH	OXT-C-CA-N
3	B	402	SAH	OXT-C-CA-N
2	B	401	GOL	O1-C1-C2-O2
2	B	403	GOL	C1-C2-C3-O3
2	A	402	GOL	O2-C2-C3-O3
2	A	404	GOL	O1-C1-C2-O2
2	C	401	GOL	O2-C2-C3-O3
2	C	402	GOL	O2-C2-C3-O3
3	C	403	SAH	OXT-C-CA-CB
3	C	403	SAH	O-C-CA-CB
3	C	403	SAH	OXT-C-CA-N
3	C	403	SAH	O-C-CA-N
3	A	403	SAH	O-C-CA-CB
2	B	403	GOL	O2-C2-C3-O3
3	A	403	SAH	OXT-C-CA-CB
2	A	404	GOL	C1-C2-C3-O3
3	B	402	SAH	O-C-CA-CB
3	B	402	SAH	OXT-C-CA-CB
3	A	403	SAH	C4'-C5'-SD-CG
3	C	403	SAH	C4'-C5'-SD-CG

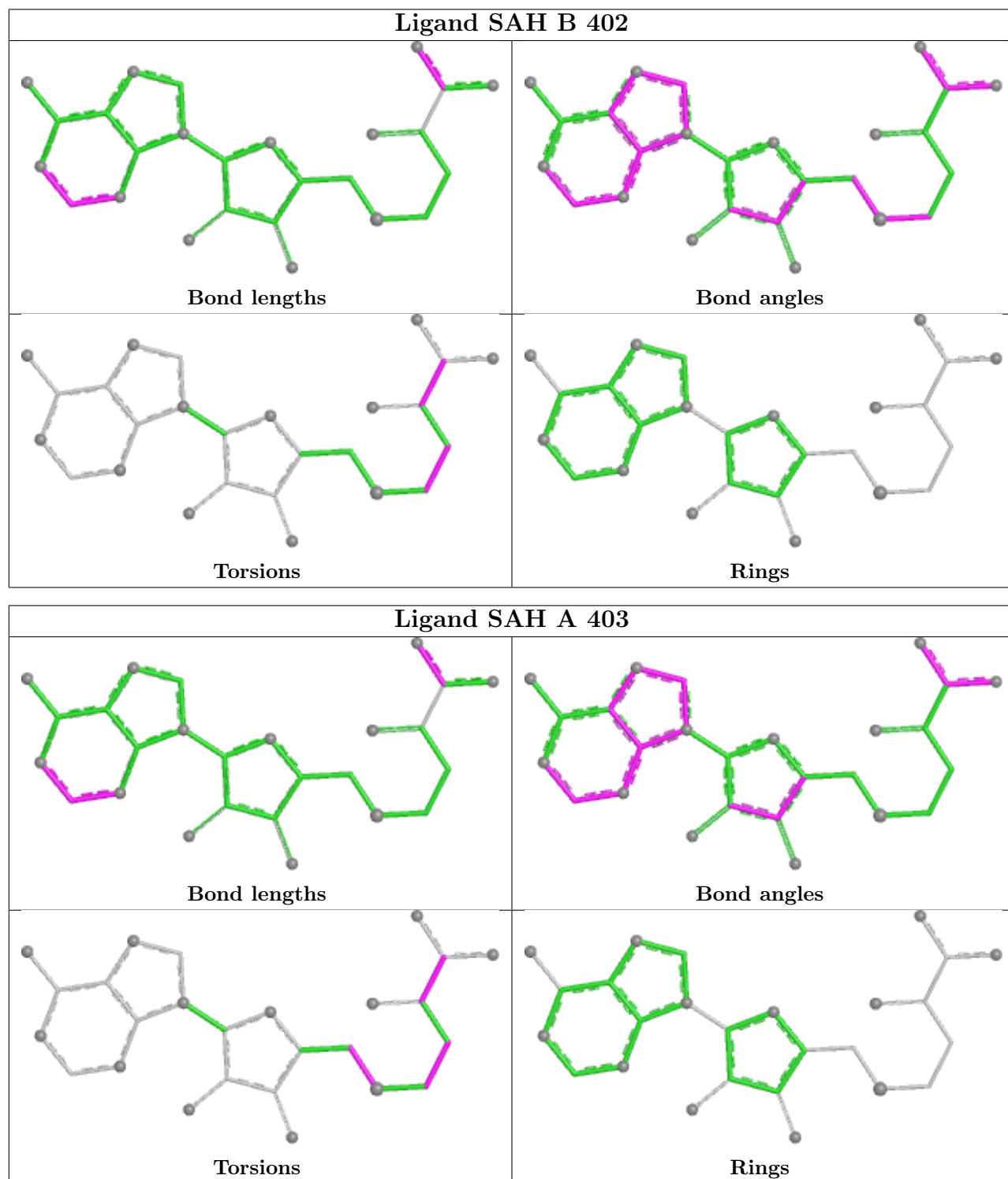
There are no ring outliers.

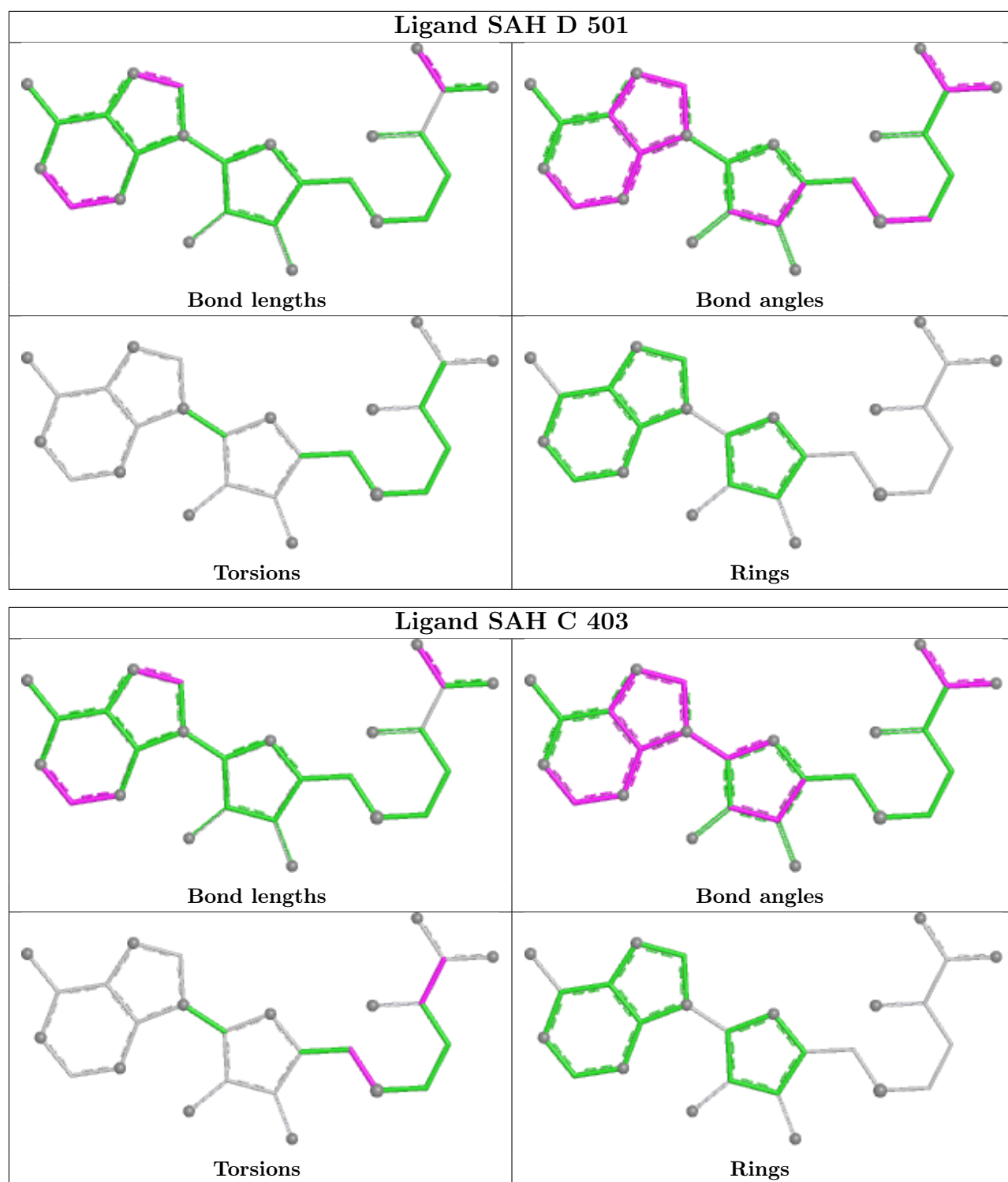
8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	SAH	1	0
2	A	401	GOL	1	0
3	A	403	SAH	2	0
2	B	403	GOL	1	0
2	C	402	GOL	3	0
3	D	501	SAH	1	0
2	B	401	GOL	1	0
3	C	403	SAH	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 ⓘ

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	247/255 (96%)	0.10	5 (2%) 65 72	28, 37, 61, 74	0
1	B	250/255 (98%)	0.24	11 (4%) 39 45	25, 40, 71, 122	0
1	C	248/255 (97%)	0.15	7 (2%) 55 62	27, 38, 62, 83	0
1	D	249/255 (97%)	0.19	10 (4%) 42 49	26, 39, 66, 84	0
All	All	994/1020 (97%)	0.17	33 (3%) 49 55	25, 38, 66, 122	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	247	VAL	7.6
1	C	-2	GLY	4.2
1	C	-1	GLY	3.9
1	D	246	ASP	3.7
1	A	167	PHE	3.7
1	B	15	HIS	3.6
1	B	246	ASP	3.5
1	C	21	PHE	3.5
1	B	18	PRO	3.4
1	B	160	PRO	3.4
1	D	82	GLU	3.4
1	A	21	PHE	3.4
1	C	244	ALA	3.3
1	C	183	TYR	3.3
1	C	245	HIS	3.1
1	C	12	TYR	2.9
1	D	21	PHE	2.9
1	B	21	PHE	2.8
1	B	16	THR	2.8
1	D	12	TYR	2.8
1	B	-2	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	0	GLY	2.8
1	B	12	TYR	2.7
1	A	183	TYR	2.7
1	D	18	PRO	2.6
1	B	17	PRO	2.5
1	D	183	TYR	2.5
1	A	12	TYR	2.4
1	D	170	ARG	2.4
1	D	10	HIS	2.2
1	B	14	LEU	2.2
1	D	206	HIS	2.2
1	A	20	ASN	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](#)

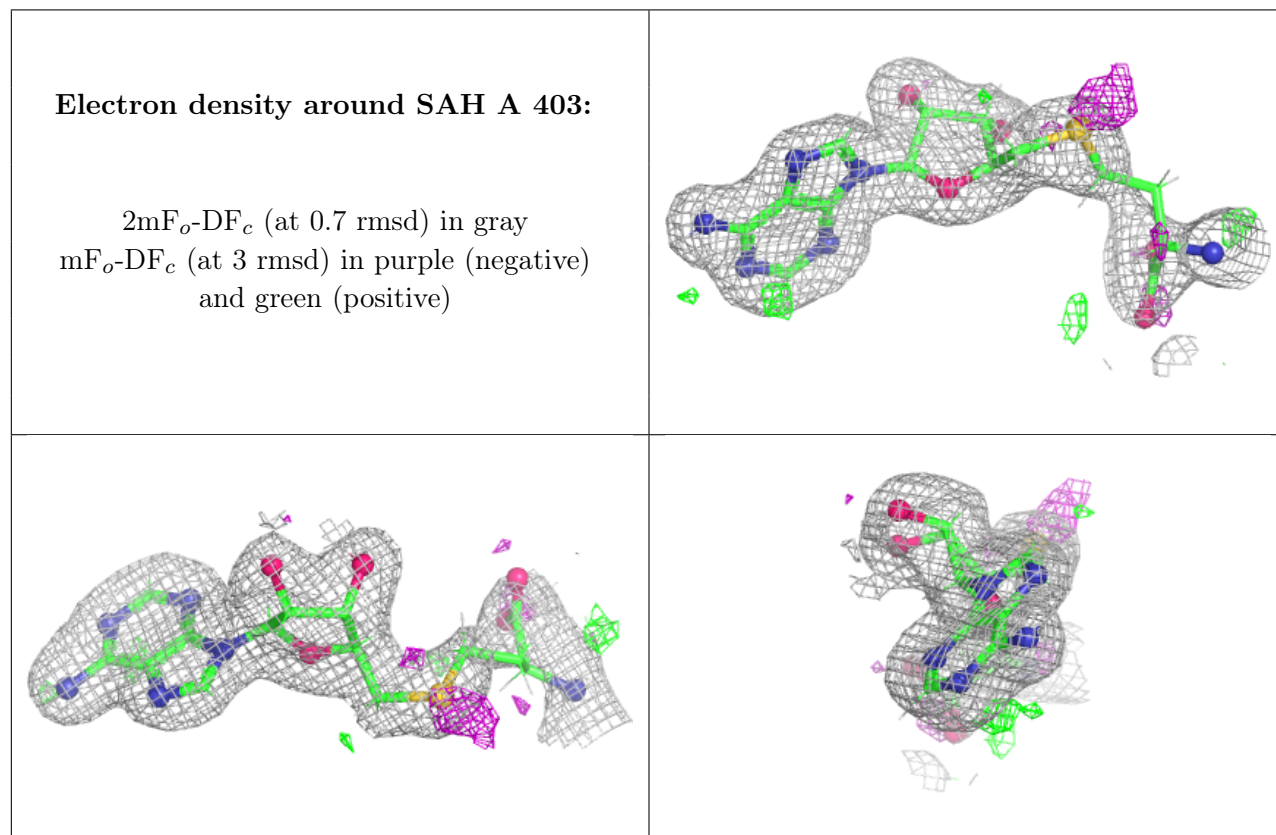
There are no oligosaccharides in this entry.

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.

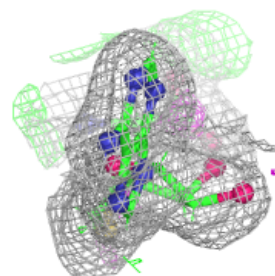
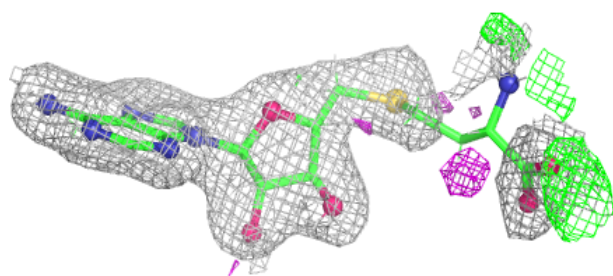
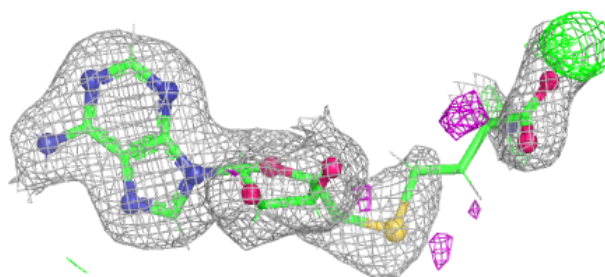
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	C	401	6/6	0.77	0.16	42,52,67,78	0
2	GOL	B	403	6/6	0.78	0.16	43,52,63,70	0
2	GOL	A	404	6/6	0.79	0.14	46,55,63,63	0
2	GOL	A	401	6/6	0.81	0.13	39,52,60,69	0
2	GOL	B	401	6/6	0.83	0.12	42,53,58,64	0
2	GOL	C	402	6/6	0.85	0.12	47,53,60,64	0
2	GOL	A	402	6/6	0.89	0.11	31,41,47,54	0
3	SAH	A	403	26/26	0.92	0.10	27,33,84,118	0
3	SAH	C	403	26/26	0.92	0.12	27,36,99,116	0
3	SAH	B	402	26/26	0.94	0.12	24,34,140,147	0
3	SAH	D	501	26/26	0.96	0.07	26,36,57,70	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.

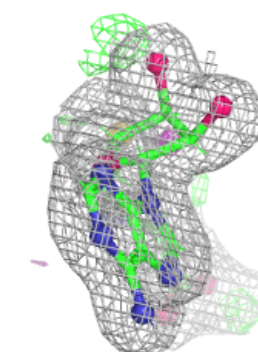
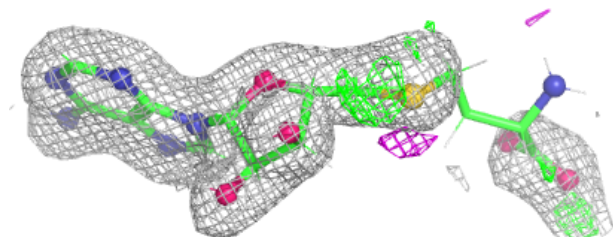
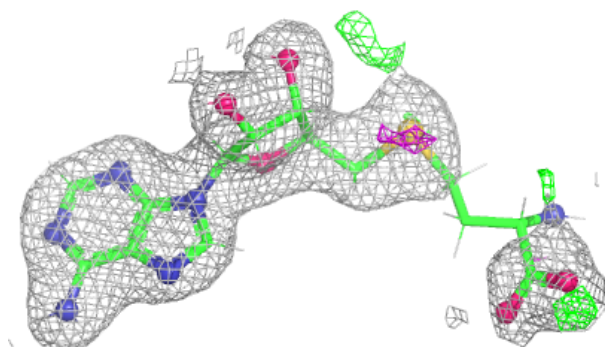


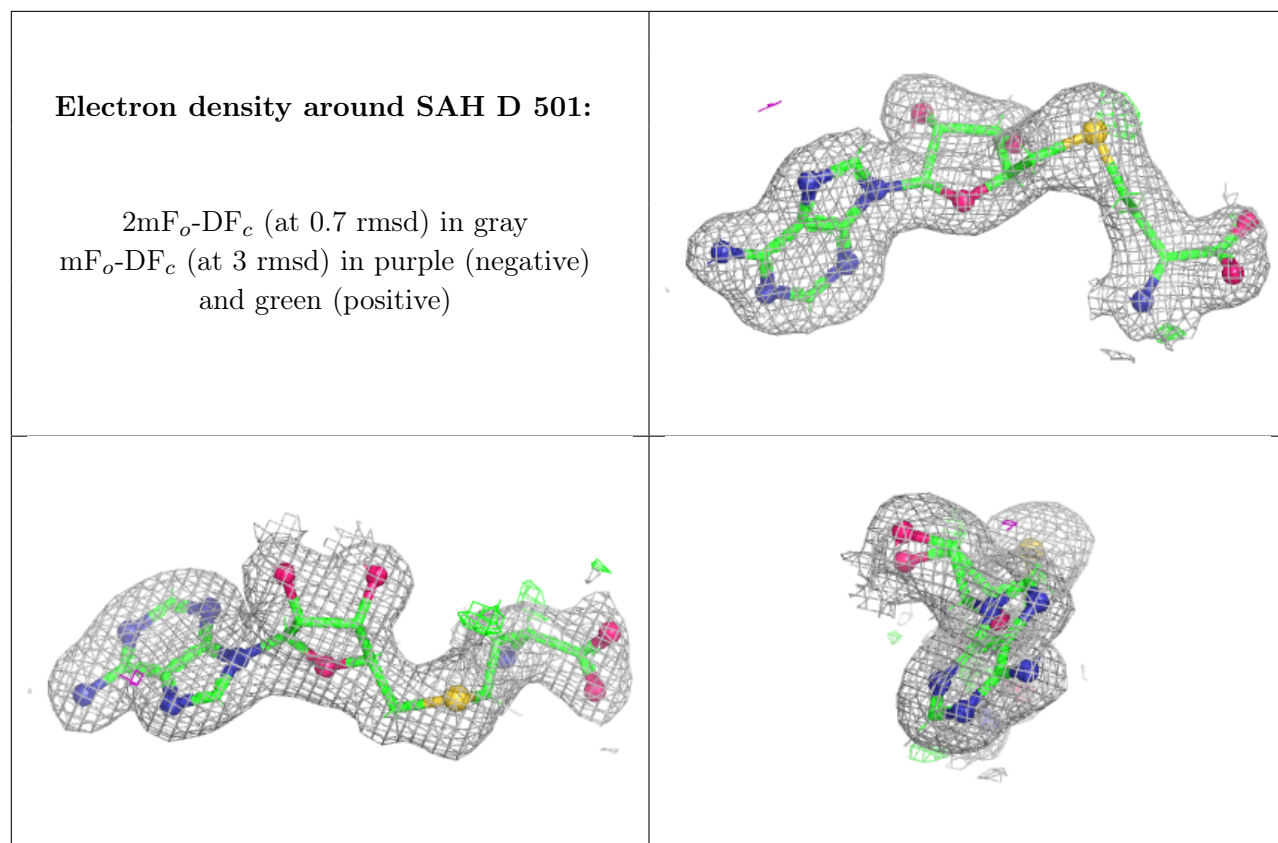
Electron density around SAH C 403:

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

**Electron density around SAH B 402:**

$2mF_o-DF_c$ (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.