



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:44 AM UTC

PDB ID : 6WK1 / pdb_00006wk1
Title : SETD3 in Complex with an Actin Peptide with His73 Replaced with Methionine
Authors : Dai, S.; Horton, J.R.; Cheng, X.
Deposited on : 2020-04-15
Resolution : 1.89 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

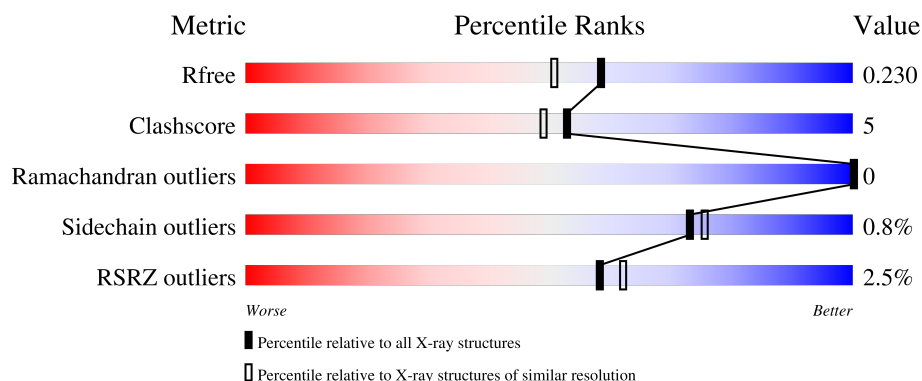
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	Y	23	13% 52% 30% 17%
1	Z	23	9% 74% 9% 17%
2	A	594	2% 72% 10% 19%
2	B	594	% 75% 6% 19%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8952 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 Actin, cytoplasmic 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Y	19	Total	C	N	O	S	0	0	0
			156	101	23	30	2			
1	Z	19	Total	C	N	O	S	0	0	0
			152	98	22	30	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	73	MET	HIS	engineered mutation	UNP P63261
Z	73	MET	HIS	engineered mutation	UNP P63261

- Molecule 2 is a protein called Actin-histidine N-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	483	Total	C	N	O	S	0	7	0
			3885	2485	654	729	17			
2	B	483	Total	C	N	O	S	0	3	0
			3882	2484	651	729	18			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

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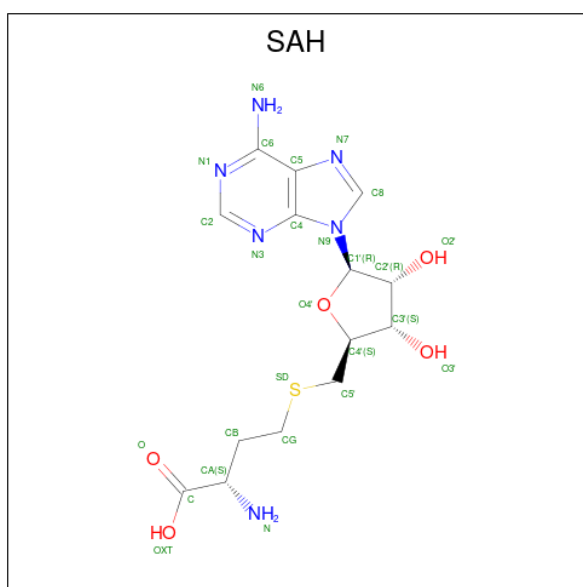
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0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

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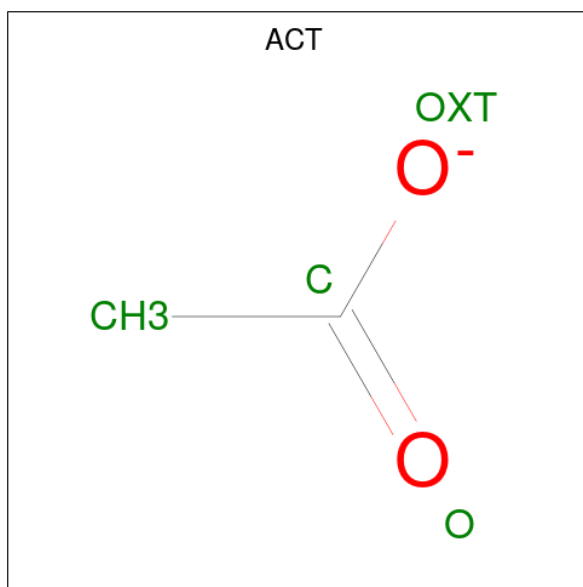
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total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

- Molecule 5 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



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

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	Y	10	Total	O	0	0
			10	10		
7	A	305	Total	O	0	0
			305	305		
7	Z	12	Total	O	0	0
			12	12		
7	B	274	Total	O	0	0
			274	274		

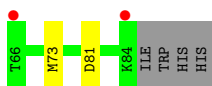
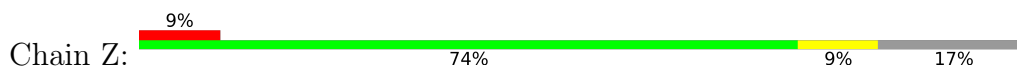
3 Residue-property plots [i](#)

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.

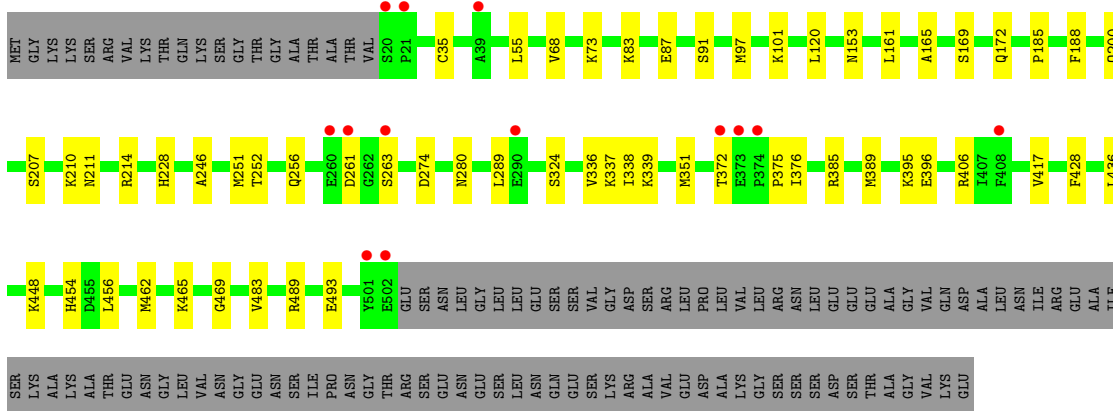
- Molecule 1: Actin, cytoplasmic 2



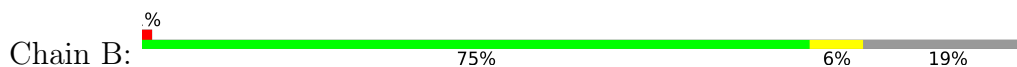
- Molecule 1: Actin, cytoplasmic 2



- Molecule 2: Actin-histidine N-methyltransferase



- Molecule 2: Actin-histidine N-methyltransferase



R214		PRO
A246		LEU
V247		VAL
S248		GLY
M251		SER
		SER
		ASN
R264		LEU
		GLU
L272		GLU
W273		ALA
D274		GLY
		VAL
		GLN
T314		ASP
		ALA
S324		LEU
G325		ASN
F326		ILE
F327		ARG
		GLU
R347		ALA
		ILE
M351		SER
		LYS
A359		ALA
G360		LYS
		ALA
R385		THR
		GLU
M389		ASN
T390		GLY
E391		LEU
		VAL
K395		ASN
		GLY
F415		GLU
P416		ASN
V417		SER
		ILE
L498		PRO
		ASN
Y501		GLY
		THR
		ARG
		SER
		GLU
		ASN
		GLY
		SER
		LEU
		LEU
		ASN
		GLN
		GLU
		SER
		VAL
		SER
		LYS
		ARG
		ASP
		GLY
		ALA
		SER
		VAL
		ARG
		LEU
		GLU

ASP
ALA
LYS
GLY
SER
SER
SER
ASP
SER
THR
ALA
GLY
VAL
LYS
GLU

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.39Å 175.53Å 66.65Å 90.00° 92.36° 90.00°	Depositor
Resolution (Å)	36.00 – 1.89 36.00 – 1.89	Depositor EDS
% Data completeness (in resolution range)	93.2 (36.00-1.89) 93.2 (36.00-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.195 , 0.228 0.196 , 0.230	Depositor DCC
R_{free} test set	2001 reflections (1.83%)	wwPDB-VP
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.571	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.059 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8952	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, GOL, ACT, 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	Y	0.20	0/159	0.41	0/214
1	Z	0.20	0/155	0.35	0/210
2	A	0.22	0/3991	0.43	0/5411
2	B	0.22	0/3980	0.42	0/5397
All	All	0.22	0/8285	0.42	0/11232

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	Y	156	0	149	5	0
1	Z	152	0	138	2	0
2	A	3885	0	3784	44	0
2	B	3882	0	3776	32	0
3	A	30	0	40	5	0
3	Y	6	0	8	2	0
4	A	104	0	156	17	0
4	B	76	0	114	16	0
4	Y	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	26	0	19	0	0
5	B	26	0	19	1	0
6	A	4	0	3	0	0
7	A	305	0	0	4	1
7	B	274	0	0	2	1
7	Y	10	0	0	0	0
7	Z	12	0	0	0	0
All	All	8952	0	8212	82	1

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 5.

All (82) 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:Y:78:ASN:HD22	1:Y:84:LYS:HD3	1.49	0.77
1:Y:71:ILE:HA	4:A:631:EDO:H21	1.69	0.75
2:A:289:LEU:H	3:A:604:GOL:H12	1.53	0.72
2:A:338:ILE:HG13	3:A:603:GOL:H12	1.69	0.72
4:B:1005:EDO:H22	4:B:1014:EDO:H12	1.77	0.66
2:A:448:LYS:HD3	4:A:605:EDO:H22	1.79	0.65
2:B:327:PHE:H	4:B:1015:EDO:H11	1.62	0.64
1:Z:73:MET:HE1	2:B:274:ASP:HA	1.79	0.64
2:A:261:ASP:OD2	2:A:263:SER:OG	2.12	0.63
2:B:389:MET:HE2	2:B:417:VAL:HG21	1.82	0.62
2:A:101:LYS:HE2	4:B:1005:EDO:H12	1.82	0.61
2:B:83:LYS:HA	4:B:1007:EDO:H12	1.83	0.61
2:B:324:SER:OG	7:B:1101:HOH:O	2.05	0.57
2:B:169:SER:HB3	2:B:172:GLN:HG2	1.87	0.56
2:B:314:THR:HG23	4:B:1002:EDO:H21	1.87	0.56
2:A:68:VAL:HG21	2:A:165:ALA:HA	1.89	0.55
1:Y:73:MET:HE1	2:A:274:ASP:HA	1.88	0.55
2:B:327:PHE:H	4:B:1015:EDO:C1	2.19	0.54
2:A:462:MET:SD	4:A:623:EDO:H12	2.48	0.54
2:B:101:LYS:NZ	4:B:1019:EDO:O1	2.41	0.54
1:Y:77:THR:HB	3:Y:101:GOL:H12	1.90	0.53
2:B:351:MET:HE1	2:B:391:GLU:HG3	1.88	0.53
2:A:454:HIS:O	4:A:613:EDO:H12	2.07	0.53
2:A:465:LYS:NZ	4:A:619:EDO:H11	2.24	0.53
2:B:314:THR:H	4:B:1002:EDO:H21	1.74	0.53
2:A:351:MET:HE1	2:A:395:LYS:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:375:PRO:HG2	2:A:376:ILE:HG23	1.91	0.52
2:A:428:PHE:CE1	4:A:628:EDO:H12	2.45	0.52
5:B:1001:SAH:N3	4:B:1014:EDO:H11	2.24	0.52
2:A:83:LYS:NZ	2:A:87:GLU:OE2	2.39	0.52
2:B:359:ALA:HB1	4:B:1003:EDO:H11	1.92	0.51
2:A:489:ARG:O	2:A:493:GLU:HG2	2.11	0.51
2:B:95:PHE:CZ	2:B:272:LEU:HD21	2.45	0.51
2:A:396:GLU:O	2:A:406:ARG:HD2	2.11	0.51
3:Y:101:GOL:O2	4:A:629:EDO:O1	2.29	0.50
2:A:211:ASN:OD1	7:A:702:HOH:O	2.19	0.50
2:B:102:GLU:HG2	7:B:1266:HOH:O	2.10	0.50
1:Y:78:ASN:ND2	1:Y:84:LYS:HD3	2.21	0.50
2:A:200:GLN:OE1	4:A:608:EDO:H22	2.13	0.49
2:A:207:SER:HA	4:A:616:EDO:H11	1.95	0.49
2:A:97:MET:SD	4:A:630:EDO:H12	2.54	0.48
2:A:436:LEU:HD21	3:A:603:GOL:H11	1.96	0.48
2:B:68:VAL:HG21	2:B:165:ALA:HA	1.95	0.48
1:Z:81:ASP:OD2	2:B:214:ARG:NH2	2.36	0.47
2:A:289:LEU:N	3:A:604:GOL:H12	2.27	0.47
2:A:169:SER:HB3	2:A:172:GLN:HG2	1.97	0.46
2:A:210:LYS:HD3	4:A:616:EDO:H12	1.98	0.46
2:A:456:LEU:HD12	4:A:613:EDO:H11	1.97	0.46
2:B:391:GLU:O	2:B:395:LYS:HG2	2.15	0.46
2:A:35:CYS:HB3	2:A:214:ARG:HB2	1.97	0.45
2:B:326:PHE:HA	4:B:1015:EDO:H11	1.98	0.45
2:A:339:LYS:HB3	3:A:603:GOL:H2	1.98	0.45
2:A:428:PHE:HE1	4:A:628:EDO:H12	1.81	0.45
2:B:85:ALA:HB1	2:B:90:ALA:HB3	1.99	0.44
2:A:389:MET:HE2	2:A:417:VAL:HG21	1.99	0.44
2:B:248:SER:HA	2:B:251:MET:HG2	2.00	0.44
2:A:337:LYS:HG3	4:A:612:EDO:H21	1.99	0.43
2:B:75:GLU:HA	2:B:78:PHE:CD2	2.53	0.43
2:B:95:PHE:CE1	2:B:272:LEU:HD21	2.53	0.43
2:B:102:GLU:O	4:B:1005:EDO:O1	2.31	0.43
2:B:40:PRO:HB2	2:B:44:LYS:HB2	2.01	0.43
2:A:200:GLN:HB2	4:A:608:EDO:H11	2.00	0.43
2:A:469:GLY:HA3	7:A:850:HOH:O	2.19	0.43
2:A:385:ARG:O	2:A:389:MET:HG3	2.18	0.42
2:B:161:LEU:HG	2:B:246:ALA:HB2	2.01	0.42
2:A:256:GLN:HB3	4:A:631:EDO:H22	2.01	0.42
2:A:336:VAL:HG12	4:A:606:EDO:O1	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:ASP:OD1	4:B:1020:EDO:H12	2.19	0.42
2:A:252:THR:HG22	2:A:324[B]:SER:HA	2.02	0.42
2:B:185:PRO:HA	2:B:188:PHE:CD1	2.54	0.42
2:A:185:PRO:HA	2:A:188:PHE:CD1	2.54	0.42
2:A:101:LYS:NZ	2:B:101:LYS:HE2	2.35	0.42
2:A:372:THR:HB	7:A:772:HOH:O	2.19	0.41
2:B:314:THR:H	4:B:1002:EDO:C2	2.32	0.41
2:A:91:SER:OG	2:A:120:LEU:HA	2.20	0.41
2:A:251:MET:HE2	2:A:251:MET:HB3	1.93	0.41
2:B:385:ARG:O	2:B:389:MET:HG3	2.19	0.41
2:A:153:ASN:OD1	2:A:153:ASN:N	2.53	0.41
2:A:161:LEU:HG	2:A:246:ALA:HB2	2.03	0.41
2:A:73:LYS:NZ	7:A:703:HOH:O	2.28	0.40
2:B:180:SER:H	4:B:1010:EDO:C1	2.34	0.40
2:B:183:ASP:OD1	4:B:1004:EDO:H11	2.21	0.40

All (1) 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)
7:A:912:HOH:O	7:B:1218:HOH:O[1_455]	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	Y	17/23 (74%)	17 (100%)	0	0	100	100
1	Z	17/23 (74%)	17 (100%)	0	0	100	100
2	A	488/594 (82%)	481 (99%)	7 (1%)	0	100	100
2	B	484/594 (82%)	479 (99%)	5 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1006/1234 (82%)	994 (99%)	12 (1%)	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	Y	17/22 (77%)	15 (88%)	2 (12%)	5	2
1	Z	16/22 (73%)	16 (100%)	0	100	100
2	A	416/518 (80%)	412 (99%)	4 (1%)	68	70
2	B	416/518 (80%)	415 (100%)	1 (0%)	87	90
All	All	865/1080 (80%)	858 (99%)	7 (1%)	73	75

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Y	82	MET
1	Y	83	GLU
2	A	55	LEU
2	A	228	HIS
2	A	280	ASN
2	A	483	VAL
2	B	101	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	135	ASN
2	A	149	GLN
2	A	256	GLN
2	B	26	ASN
2	B	168	ASN

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Mol	Chain	Res	Type
2	B	379	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

55 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	$\# Z > 2$
5	SAH	B	1001	-	27,28,28	1.06	3 (11%)	36,40,40	2.02	10 (27%)
4	EDO	A	614	-	3,3,3	0.41	0	2,2,2	0.35	0
4	EDO	A	613	-	3,3,3	0.37	0	2,2,2	0.42	0
4	EDO	B	1018	-	3,3,3	0.43	0	2,2,2	0.31	0
4	EDO	A	620	-	3,3,3	0.46	0	2,2,2	0.31	0
4	EDO	A	618	-	3,3,3	0.43	0	2,2,2	0.27	0
4	EDO	A	622	-	3,3,3	0.41	0	2,2,2	0.44	0
4	EDO	A	608	-	3,3,3	0.43	0	2,2,2	0.47	0
4	EDO	A	629	-	3,3,3	0.42	0	2,2,2	0.46	0
4	EDO	A	607	-	3,3,3	0.45	0	2,2,2	0.36	0
4	EDO	A	630	-	3,3,3	0.38	0	2,2,2	0.61	0
4	EDO	B	1017	-	3,3,3	0.51	0	2,2,2	0.31	0
3	GOL	A	602	-	5,5,5	0.95	0	5,5,5	1.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	B	1019	-	3,3,3	0.43	0	2,2,2	0.55	0
4	EDO	B	1012	-	3,3,3	0.46	0	2,2,2	0.45	0
4	EDO	B	1016	-	3,3,3	0.47	0	2,2,2	0.17	0
3	GOL	A	603	-	5,5,5	0.92	0	5,5,5	1.07	0
4	EDO	A	616	-	3,3,3	0.45	0	2,2,2	0.45	0
4	EDO	A	605	-	3,3,3	0.46	0	2,2,2	0.36	0
4	EDO	B	1002	-	3,3,3	0.44	0	2,2,2	0.35	0
4	EDO	A	610	-	3,3,3	0.44	0	2,2,2	0.35	0
4	EDO	A	631	-	3,3,3	0.43	0	2,2,2	0.29	0
4	EDO	B	1009	-	3,3,3	0.43	0	2,2,2	0.38	0
4	EDO	A	619	-	3,3,3	0.38	0	2,2,2	0.73	0
4	EDO	B	1005	-	3,3,3	0.44	0	2,2,2	0.35	0
4	EDO	B	1013	-	3,3,3	0.42	0	2,2,2	0.46	0
4	EDO	B	1006	-	3,3,3	0.44	0	2,2,2	0.31	0
3	GOL	Y	101	-	5,5,5	0.95	0	5,5,5	1.07	0
5	SAH	A	601	-	27,28,28	1.04	4 (14%)	36,40,40	1.86	10 (27%)
4	EDO	A	612	-	3,3,3	0.38	0	2,2,2	0.65	0
4	EDO	B	1007	-	3,3,3	0.49	0	2,2,2	0.30	0
3	GOL	A	633	-	5,5,5	0.85	0	5,5,5	1.14	1 (20%)
4	EDO	B	1020	-	3,3,3	0.46	0	2,2,2	0.26	0
4	EDO	B	1004	-	3,3,3	0.45	0	2,2,2	0.40	0
4	EDO	A	609	-	3,3,3	0.44	0	2,2,2	0.40	0
4	EDO	A	621	-	3,3,3	0.45	0	2,2,2	0.28	0
4	EDO	A	627	-	3,3,3	0.46	0	2,2,2	0.48	0
4	EDO	A	615	-	3,3,3	0.47	0	2,2,2	0.30	0
4	EDO	A	623	-	3,3,3	0.60	0	2,2,2	0.13	0
3	GOL	A	604	-	5,5,5	0.94	0	5,5,5	1.12	0
4	EDO	Y	102	-	3,3,3	0.45	0	2,2,2	0.36	0
4	EDO	B	1010	-	3,3,3	0.39	0	2,2,2	0.43	0
4	EDO	B	1014	-	3,3,3	0.32	0	2,2,2	0.54	0
4	EDO	A	606	-	3,3,3	0.40	0	2,2,2	0.80	0
4	EDO	B	1011	-	3,3,3	0.40	0	2,2,2	0.44	0
6	ACT	A	624	-	3,3,3	1.50	1 (33%)	3,3,3	1.46	0
4	EDO	A	611	-	3,3,3	0.45	0	2,2,2	0.40	0
4	EDO	A	628	-	3,3,3	0.42	0	2,2,2	0.42	0
4	EDO	B	1003	-	3,3,3	0.49	0	2,2,2	0.28	0
4	EDO	B	1008	-	3,3,3	0.48	0	2,2,2	0.34	0
3	GOL	A	632	-	5,5,5	0.89	0	5,5,5	1.09	0
4	EDO	A	617	-	3,3,3	0.40	0	2,2,2	0.45	0
4	EDO	B	1015	-	3,3,3	0.39	0	2,2,2	0.60	0
4	EDO	A	625	-	3,3,3	0.45	0	2,2,2	0.43	0
4	EDO	A	626	-	3,3,3	0.43	0	2,2,2	0.35	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SAH	B	1001	-	-	2/15/31/31	0/3/3/3
4	EDO	A	614	-	-	0/1/1/1	-
4	EDO	A	613	-	-	1/1/1/1	-
4	EDO	B	1018	-	-	0/1/1/1	-
4	EDO	A	620	-	-	0/1/1/1	-
4	EDO	A	618	-	-	0/1/1/1	-
4	EDO	A	622	-	-	0/1/1/1	-
4	EDO	A	608	-	-	1/1/1/1	-
4	EDO	A	629	-	-	0/1/1/1	-
4	EDO	A	607	-	-	1/1/1/1	-
4	EDO	A	630	-	-	1/1/1/1	-
4	EDO	B	1017	-	-	0/1/1/1	-
3	GOL	A	602	-	-	0/4/4/4	-
4	EDO	B	1019	-	-	0/1/1/1	-
4	EDO	B	1012	-	-	0/1/1/1	-
4	EDO	B	1016	-	-	1/1/1/1	-
3	GOL	A	603	-	-	2/4/4/4	-
4	EDO	A	616	-	-	1/1/1/1	-
4	EDO	A	605	-	-	0/1/1/1	-
4	EDO	B	1002	-	-	0/1/1/1	-
4	EDO	A	610	-	-	0/1/1/1	-
4	EDO	A	631	-	-	1/1/1/1	-
4	EDO	B	1009	-	-	0/1/1/1	-
4	EDO	A	619	-	-	1/1/1/1	-
4	EDO	B	1005	-	-	0/1/1/1	-
4	EDO	B	1013	-	-	0/1/1/1	-
4	EDO	B	1006	-	-	1/1/1/1	-
3	GOL	Y	101	-	-	4/4/4/4	-
5	SAH	A	601	-	-	2/15/31/31	0/3/3/3
4	EDO	A	612	-	-	0/1/1/1	-
4	EDO	B	1007	-	-	0/1/1/1	-
3	GOL	A	633	-	-	1/4/4/4	-
4	EDO	B	1020	-	-	0/1/1/1	-
4	EDO	B	1004	-	-	1/1/1/1	-
4	EDO	A	609	-	-	1/1/1/1	-
4	EDO	A	621	-	-	1/1/1/1	-
4	EDO	A	627	-	-	1/1/1/1	-
4	EDO	A	615	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	623	-	-	1/1/1/1	-
3	GOL	A	604	-	-	0/4/4/4	-
4	EDO	Y	102	-	-	0/1/1/1	-
4	EDO	B	1010	-	-	1/1/1/1	-
4	EDO	B	1014	-	-	1/1/1/1	-
4	EDO	A	606	-	-	1/1/1/1	-
4	EDO	B	1011	-	-	0/1/1/1	-
4	EDO	A	611	-	-	0/1/1/1	-
4	EDO	A	628	-	-	1/1/1/1	-
4	EDO	B	1003	-	-	1/1/1/1	-
4	EDO	B	1008	-	-	0/1/1/1	-
3	GOL	A	632	-	-	2/4/4/4	-
4	EDO	A	617	-	-	0/1/1/1	-
4	EDO	B	1015	-	-	1/1/1/1	-
4	EDO	A	625	-	-	0/1/1/1	-
4	EDO	A	626	-	-	0/1/1/1	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1001	SAH	C8-N7	2.51	1.36	1.31
5	B	1001	SAH	C2-N3	2.37	1.38	1.33
5	A	601	SAH	C8-N7	2.33	1.36	1.31
5	A	601	SAH	C2-N1	2.31	1.38	1.33
5	A	601	SAH	OXT-C	-2.23	1.23	1.30
5	A	601	SAH	C2-N3	2.19	1.37	1.33
6	A	624	ACT	CH3-C	2.17	1.57	1.49
5	B	1001	SAH	OXT-C	-2.02	1.24	1.30

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1001	SAH	N3-C2-N1	-5.68	119.98	128.58
5	A	601	SAH	N3-C2-N1	-4.97	121.06	128.58
5	B	1001	SAH	C5-C4-N3	-4.82	120.08	126.72
5	A	601	SAH	C5-C4-N3	-4.13	121.03	126.72
5	A	601	SAH	N9-C8-N7	-3.86	108.46	113.94
5	B	1001	SAH	C2-N3-C4	3.85	121.23	111.83
5	B	1001	SAH	N9-C8-N7	-3.54	108.91	113.94
5	B	1001	SAH	C5-N7-C8	3.24	108.54	103.45
5	A	601	SAH	C5-N7-C8	3.22	108.52	103.45
5	B	1001	SAH	C5'-SD-CG	-3.10	93.07	102.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	SAH	C2-N3-C4	3.00	119.17	111.83
5	B	1001	SAH	C4-C5-N7	-2.93	107.23	110.58
5	A	601	SAH	CB-CG-SD	-2.68	107.48	113.45
5	A	601	SAH	OXT-C-O	-2.65	118.07	124.08
5	B	1001	SAH	C5-C4-N9	2.60	108.64	105.81
5	A	601	SAH	N3-C4-N9	2.55	131.50	127.17
5	B	1001	SAH	OXT-C-O	-2.47	118.47	124.08
5	B	1001	SAH	N3-C4-N9	2.41	131.26	127.17
5	A	601	SAH	C4-C5-N7	-2.35	107.90	110.58
5	A	601	SAH	C5'-SD-CG	-2.12	95.97	102.26
3	A	633	GOL	C3-C2-C1	-2.03	104.37	111.80

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Y	101	GOL	C1-C2-C3-O3
3	A	603	GOL	C1-C2-C3-O3
3	A	632	GOL	C1-C2-C3-O3
3	A	632	GOL	O2-C2-C3-O3
3	Y	101	GOL	O1-C1-C2-C3
3	Y	101	GOL	O2-C2-C3-O3
4	A	616	EDO	O1-C1-C2-O2
4	A	623	EDO	O1-C1-C2-O2
4	A	631	EDO	O1-C1-C2-O2
3	A	603	GOL	O2-C2-C3-O3
4	B	1010	EDO	O1-C1-C2-O2
4	A	607	EDO	O1-C1-C2-O2
3	A	633	GOL	O1-C1-C2-O2
5	B	1001	SAH	C3'-C4'-C5'-SD
4	A	609	EDO	O1-C1-C2-O2
5	A	601	SAH	CB-CG-SD-C5'
5	B	1001	SAH	CB-CG-SD-C5'
4	A	606	EDO	O1-C1-C2-O2
4	A	621	EDO	O1-C1-C2-O2
4	B	1015	EDO	O1-C1-C2-O2
4	B	1003	EDO	O1-C1-C2-O2
3	Y	101	GOL	O1-C1-C2-O2
4	A	608	EDO	O1-C1-C2-O2
4	A	613	EDO	O1-C1-C2-O2
4	A	628	EDO	O1-C1-C2-O2
4	B	1004	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	B	1014	EDO	O1-C1-C2-O2
4	B	1016	EDO	O1-C1-C2-O2
4	A	627	EDO	O1-C1-C2-O2
4	A	630	EDO	O1-C1-C2-O2
5	A	601	SAH	C3'-C4'-C5'-SD
4	B	1006	EDO	O1-C1-C2-O2
4	A	619	EDO	O1-C1-C2-O2

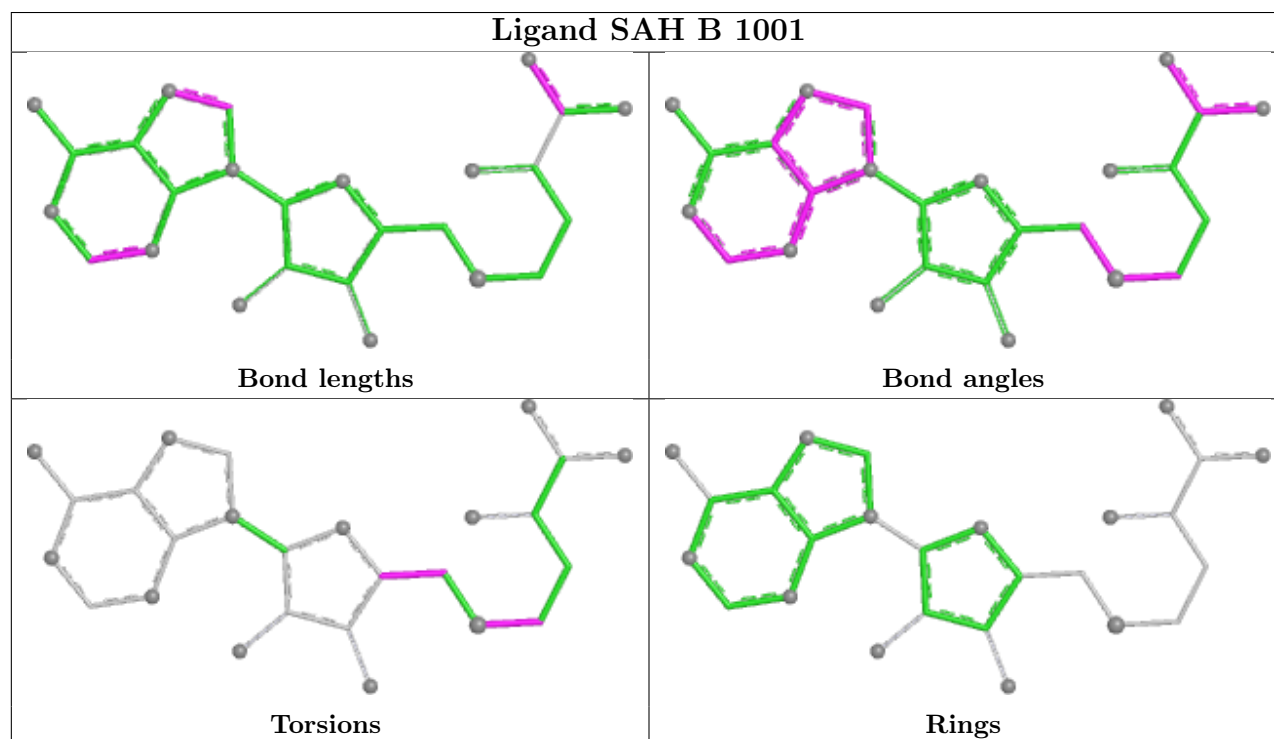
There are no ring outliers.

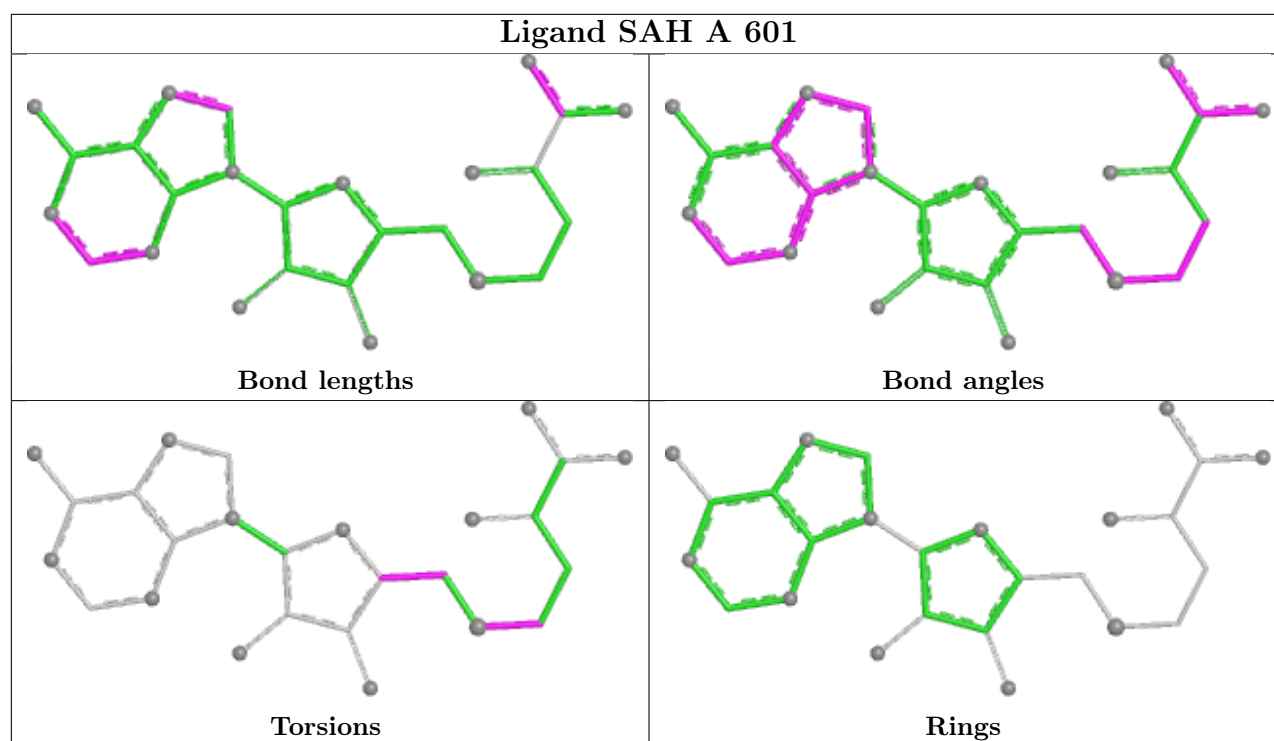
26 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1001	SAH	1	0
4	A	613	EDO	2	0
4	A	608	EDO	2	0
4	A	629	EDO	1	0
4	A	630	EDO	1	0
4	B	1019	EDO	1	0
3	A	603	GOL	3	0
4	A	616	EDO	2	0
4	A	605	EDO	1	0
4	B	1002	EDO	3	0
4	A	631	EDO	2	0
4	A	619	EDO	1	0
4	B	1005	EDO	3	0
3	Y	101	GOL	2	0
4	A	612	EDO	1	0
4	B	1007	EDO	1	0
4	B	1020	EDO	1	0
4	B	1004	EDO	1	0
4	A	623	EDO	1	0
3	A	604	GOL	2	0
4	B	1010	EDO	1	0
4	B	1014	EDO	2	0
4	A	606	EDO	1	0
4	A	628	EDO	2	0
4	B	1003	EDO	1	0
4	B	1015	EDO	3	0

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

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	Y	19/23 (82%)	0.61	3 (15%) 5 5	17, 25, 56, 59	0
1	Z	19/23 (82%)	0.62	2 (10%) 11 12	17, 28, 57, 61	0
2	A	483/594 (81%)	0.18	13 (2%) 56 60	12, 25, 42, 63	7 (1%)
2	B	483/594 (81%)	0.24	7 (1%) 73 76	12, 26, 45, 64	3 (0%)
All	All	1004/1234 (81%)	0.22	25 (2%) 58 62	12, 25, 44, 64	10 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	19	VAL	5.7
2	A	374	PRO	4.7
2	A	501	TYR	3.8
2	A	373	GLU	3.7
2	A	372	THR	3.7
2	B	501	TYR	3.3
1	Z	84	LYS	3.2
1	Z	66	THR	3.0
1	Y	84	LYS	2.9
1	Y	66	THR	2.9
2	B	264	ARG	2.7
2	A	263	SER	2.6
2	A	502	GLU	2.6
2	A	290	GLU	2.5
2	A	21	PRO	2.5
2	B	498	LEU	2.4
2	A	39	ALA	2.4
2	B	347	ARG	2.3
2	A	20	SER	2.3
2	A	408	PHE	2.3
2	A	261	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	Y	83	GLU	2.1
2	B	415	PHE	2.0
2	B	360	GLY	2.0
2	A	260	GLU	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
4	EDO	A	605	4/4	0.61	0.20	58,60,63,63	0
3	GOL	A	604	6/6	0.68	0.18	50,58,58,60	0
4	EDO	A	625	4/4	0.71	0.22	39,39,46,46	0
4	EDO	B	1013	4/4	0.76	0.17	36,44,47,54	0
3	GOL	A	633	6/6	0.79	0.16	44,46,49,53	0
4	EDO	B	1016	4/4	0.80	0.21	34,41,41,42	0
4	EDO	A	616	4/4	0.81	0.17	31,37,39,42	0
4	EDO	A	622	4/4	0.82	0.15	34,34,38,41	0
4	EDO	A	615	4/4	0.82	0.15	42,46,56,56	0
4	EDO	Y	102	4/4	0.84	0.16	35,35,38,52	0
3	GOL	A	602	6/6	0.85	0.14	41,47,48,50	0
4	EDO	A	627	4/4	0.85	0.13	39,39,45,48	0
3	GOL	A	603	6/6	0.85	0.17	27,32,33,43	0
4	EDO	A	609	4/4	0.85	0.15	36,41,42,44	0
4	EDO	B	1017	4/4	0.85	0.13	35,35,42,46	0
4	EDO	B	1020	4/4	0.85	0.18	40,43,45,52	0
4	EDO	B	1007	4/4	0.86	0.13	39,41,42,47	0
4	EDO	B	1012	4/4	0.86	0.24	37,38,39,39	0
3	GOL	A	632	6/6	0.86	0.12	49,53,56,57	0

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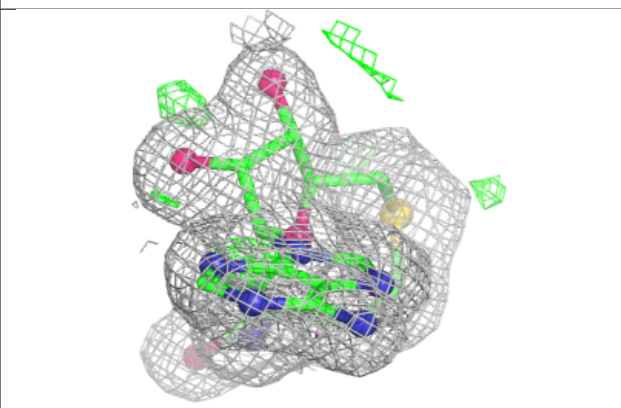
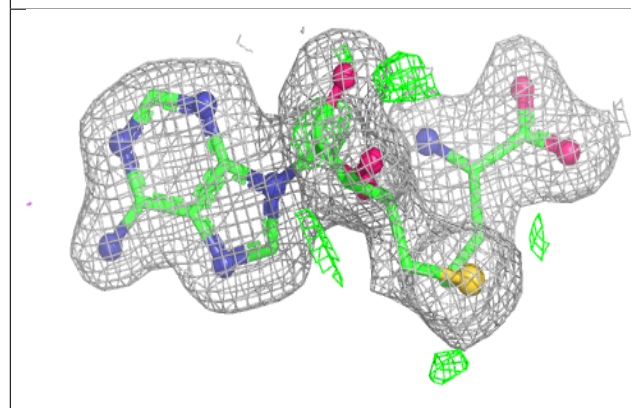
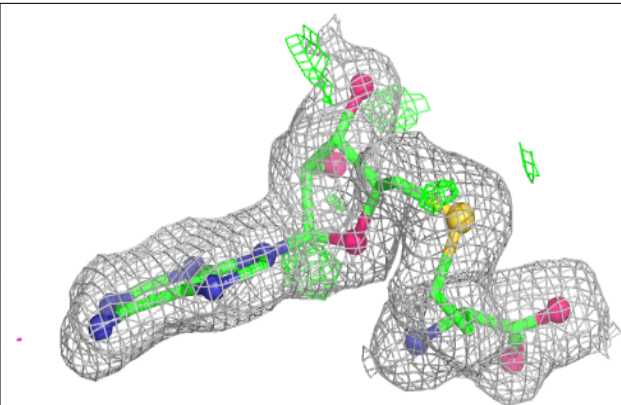
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	A	608	4/4	0.86	0.19	24,34,38,47	0
4	EDO	A	629	4/4	0.86	0.16	39,46,46,50	0
4	EDO	B	1005	4/4	0.86	0.16	38,39,39,40	0
6	ACT	A	624	4/4	0.86	0.13	31,40,43,44	0
4	EDO	A	612	4/4	0.87	0.16	36,38,39,40	0
4	EDO	B	1004	4/4	0.87	0.16	30,40,44,45	0
4	EDO	B	1009	4/4	0.87	0.12	32,43,44,45	0
4	EDO	A	623	4/4	0.88	0.13	24,31,32,36	0
4	EDO	B	1015	4/4	0.88	0.24	24,33,40,40	0
4	EDO	A	606	4/4	0.89	0.16	28,31,32,37	0
4	EDO	A	619	4/4	0.89	0.20	32,34,35,38	0
4	EDO	A	611	4/4	0.89	0.14	29,31,33,43	0
4	EDO	B	1019	4/4	0.90	0.13	31,37,37,38	0
4	EDO	B	1014	4/4	0.90	0.17	23,27,33,36	0
4	EDO	A	610	4/4	0.90	0.12	28,32,32,39	0
3	GOL	Y	101	6/6	0.91	0.15	28,34,39,46	0
4	EDO	A	613	4/4	0.91	0.17	30,32,36,37	0
4	EDO	A	628	4/4	0.91	0.10	28,32,35,48	0
4	EDO	A	617	4/4	0.91	0.11	34,37,41,43	0
4	EDO	B	1010	4/4	0.91	0.18	26,28,35,47	0
4	EDO	A	631	4/4	0.91	0.19	31,32,33,50	0
4	EDO	B	1003	4/4	0.91	0.17	31,35,43,43	0
4	EDO	B	1002	4/4	0.92	0.13	25,34,39,44	0
4	EDO	A	614	4/4	0.92	0.12	31,31,32,37	0
4	EDO	A	621	4/4	0.92	0.12	32,39,39,42	0
4	EDO	A	607	4/4	0.92	0.13	30,40,41,42	0
4	EDO	A	626	4/4	0.93	0.10	37,38,45,48	0
4	EDO	B	1008	4/4	0.93	0.11	29,33,34,36	0
4	EDO	B	1011	4/4	0.93	0.09	31,32,32,42	0
4	EDO	B	1006	4/4	0.94	0.09	28,31,35,37	0
4	EDO	A	630	4/4	0.94	0.09	25,25,26,35	0
4	EDO	B	1018	4/4	0.94	0.11	27,32,33,39	0
4	EDO	A	620	4/4	0.95	0.09	22,27,28,31	0
5	SAH	A	601	26/26	0.96	0.07	13,18,22,24	0
5	SAH	B	1001	26/26	0.96	0.07	12,18,22,24	0
4	EDO	A	618	4/4	0.96	0.10	31,31,33,34	0

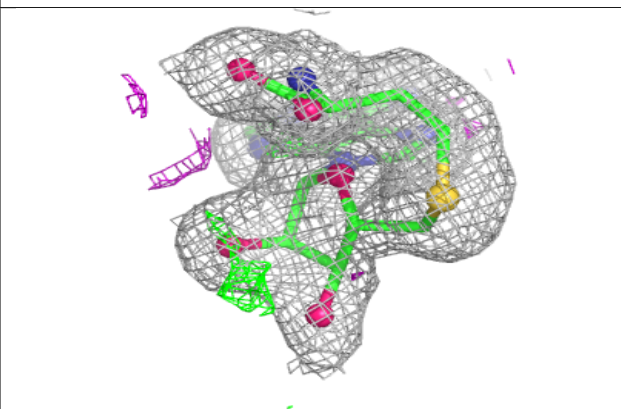
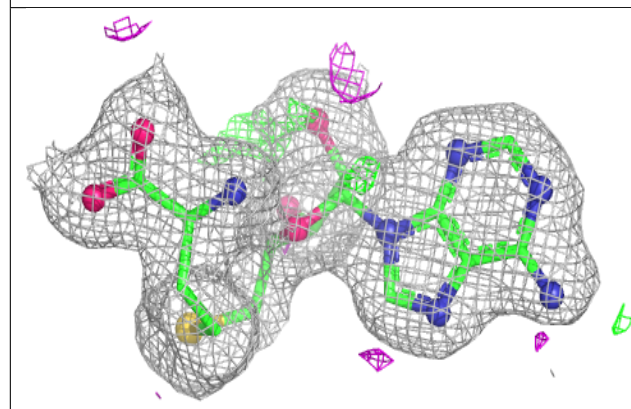
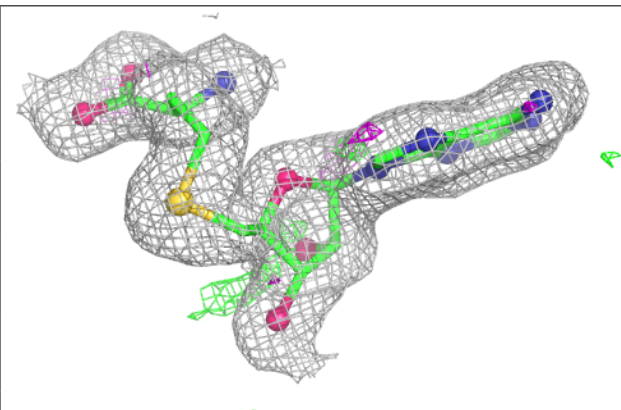
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAH A 601:

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

**Electron density around SAH B 1001:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.