



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 09:43 AM BST

PDB ID : 6WK1
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

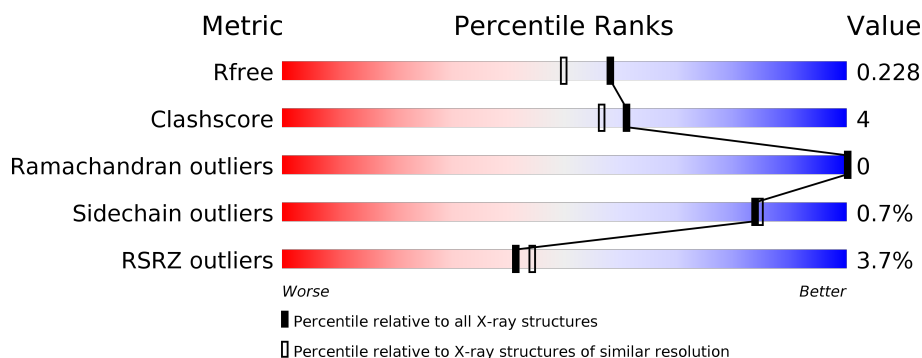
1 Overall quality at a glance

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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 on 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	<div> <div>13%</div> <div>57%</div> <div>26%</div> <div>17%</div> </div>
1	Z	23	<div> <div>13%</div> <div>78%</div> <div>17%</div> </div>
2	A	594	<div> <div>2%</div> <div>73%</div> <div>9%</div> <div>19%</div> </div>
2	B	594	<div> <div>3%</div> <div>75%</div> <div>6%</div> <div>19%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	A	605	-	-	-	X

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 (three-letter code: 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 (three-letter code: EDO) (formula: C₂H₆O₂).



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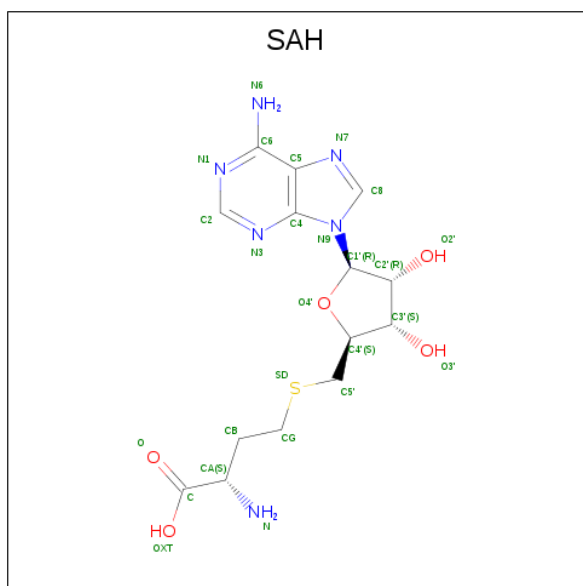
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total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

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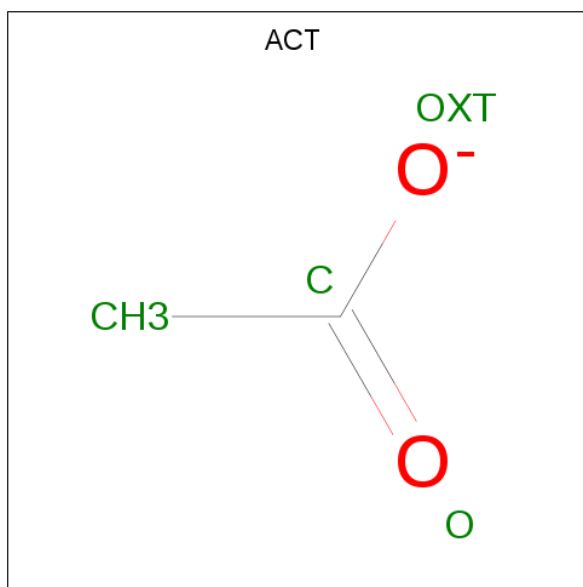
[illegible]

- Molecule 5 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $\text{C}_{14}\text{H}_{20}\text{N}_6\text{O}_5\text{S}$).



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 (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

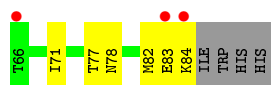
- Molecule 7 is water.

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		

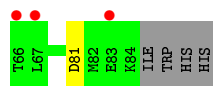
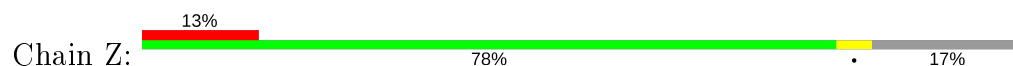
3 Residue-property plots [i](#)

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.

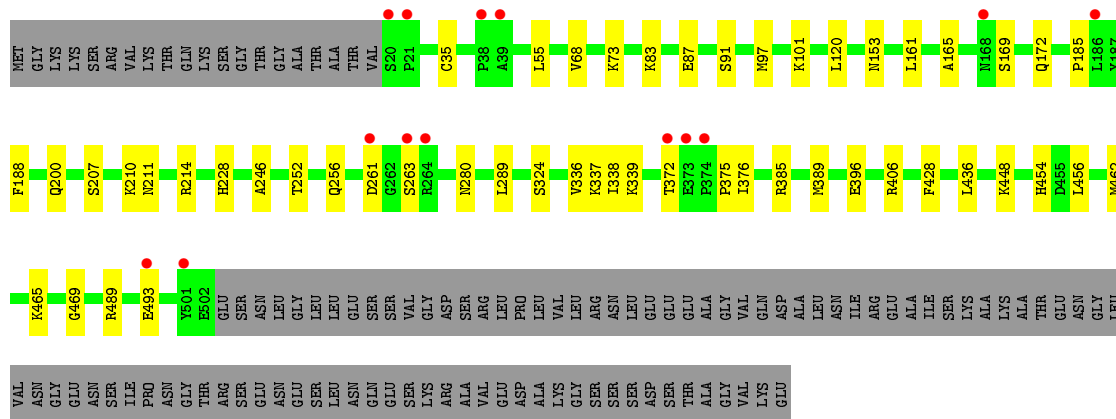
- Molecule 1: Actin, cytoplasmic 2



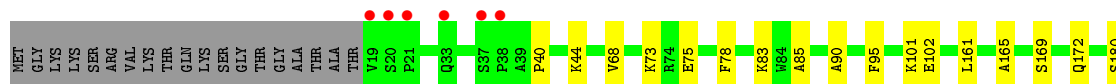
- Molecule 1: Actin, cytoplasmic 2

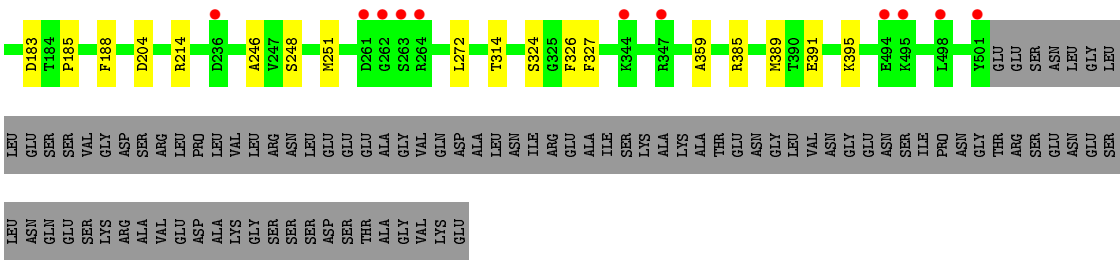


- Molecule 2: Actin-histidine N-methyltransferase



- Molecule 2: Actin-histidine N-methyltransferase





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 0.195 , 0.228	Depositor DCC
R_{free} test set	2001 reflections (1.96%)	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)	0.34 , 49.8	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	0.95	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: GOL, SAH, EDO, ACT

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	0.28	0/159	0.49	0/214
1	Z	0.28	0/155	0.44	0/210
2	A	0.31	0/3991	0.49	0/5411
2	B	0.30	0/3980	0.49	0/5397
All	All	0.31	0/8285	0.49	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	4	0
1	Z	152	0	138	1	0
2	A	3885	0	3784	40	0
2	B	3882	0	3776	28	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	15	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	74	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 4.

All (74) 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:338:ILE:HG13	3:A:603:GOL:H12	1.69	0.72
2:A:289:LEU:H	3:A:604:GOL:H12	1.53	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
2:A:261:ASP:OD2	2:A:263:SER:OG	2.12	0.63
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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:Y:101:GOL:O2	4:A:629:EDO:O1	2.29	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: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:95:PHE:CE1	2:B:272:LEU:HD21	2.53	0.43
2:B:75:GLU:HA	2:B:78:PHE:CD2	2.53	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:91:SER:OG	2:A:120:LEU:HA	2.20	0.41
2:B:385:ARG:O	2:B:389:MET:HG3	2.19	0.41
2:A:153:ASN:N	2:A:153:ASN:OD1	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:183:ASP:OD1	4:B:1004:EDO:H11	2.21	0.40
2:B:180:SER:H	4:B:1010:EDO:C1	2.34	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

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	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
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%)	413 (99%)	3 (1%)	84	84
2	B	416/518 (80%)	415 (100%)	1 (0%)	93	94
All	All	865/1080 (80%)	859 (99%)	6 (1%)	84	84

All (6) 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	B	73	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	26	ASN
2	B	379	GLN
2	B	490	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 monosaccharides 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
6	ACT	A	624	-	1,3,3	7.00	1 (100%)	0,3,3	0.00	-
4	EDO	A	608	-	3,3,3	0.46	0	2,2,2	0.44	0
4	EDO	B	1010	-	3,3,3	0.41	0	2,2,2	0.41	0
4	EDO	A	621	-	3,3,3	0.48	0	2,2,2	0.24	0
4	EDO	A	625	-	3,3,3	0.48	0	2,2,2	0.39	0
4	EDO	A	617	-	3,3,3	0.43	0	2,2,2	0.41	0
4	EDO	B	1019	-	3,3,3	0.46	0	2,2,2	0.51	0
3	GOL	A	603	-	5,5,5	0.89	0	5,5,5	0.99	0
4	EDO	B	1014	-	3,3,3	0.35	0	2,2,2	0.50	0
3	GOL	A	632	-	5,5,5	0.86	0	5,5,5	1.01	0
4	EDO	A	627	-	3,3,3	0.49	0	2,2,2	0.44	0
4	EDO	A	620	-	3,3,3	0.49	0	2,2,2	0.26	0
4	EDO	A	623	-	3,3,3	0.64	0	2,2,2	0.12	0
4	EDO	B	1018	-	3,3,3	0.46	0	2,2,2	0.26	0
4	EDO	A	631	-	3,3,3	0.45	0	2,2,2	0.25	0
4	EDO	A	616	-	3,3,3	0.48	0	2,2,2	0.42	0
4	EDO	A	626	-	3,3,3	0.46	0	2,2,2	0.30	0
4	EDO	B	1004	-	3,3,3	0.48	0	2,2,2	0.36	0
4	EDO	A	619	-	3,3,3	0.41	0	2,2,2	0.70	0
4	EDO	A	629	-	3,3,3	0.45	0	2,2,2	0.42	0
4	EDO	A	611	-	3,3,3	0.48	0	2,2,2	0.35	0
4	EDO	A	614	-	3,3,3	0.44	0	2,2,2	0.31	0
4	EDO	A	630	-	3,3,3	0.41	0	2,2,2	0.58	0
5	SAH	B	1001	-	21,28,28	1.13	1 (4%)	20,40,40	1.68	3 (15%)
4	EDO	B	1006	-	3,3,3	0.47	0	2,2,2	0.26	0
4	EDO	B	1020	-	3,3,3	0.49	0	2,2,2	0.21	0
4	EDO	Y	102	-	3,3,3	0.48	0	2,2,2	0.31	0
4	EDO	B	1015	-	3,3,3	0.41	0	2,2,2	0.57	0
5	SAH	A	601	-	21,28,28	1.10	2 (9%)	20,40,40	1.51	3 (15%)
4	EDO	B	1005	-	3,3,3	0.47	0	2,2,2	0.31	0
4	EDO	B	1011	-	3,3,3	0.43	0	2,2,2	0.40	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	B	1009	-	3,3,3	0.46	0	2,2,2	0.34	0
4	EDO	B	1003	-	3,3,3	0.52	0	2,2,2	0.23	0
4	EDO	B	1016	-	3,3,3	0.50	0	2,2,2	0.13	0
4	EDO	A	607	-	3,3,3	0.49	0	2,2,2	0.32	0
4	EDO	B	1013	-	3,3,3	0.45	0	2,2,2	0.42	0
3	GOL	A	602	-	5,5,5	0.92	0	5,5,5	0.99	0
4	EDO	A	612	-	3,3,3	0.41	0	2,2,2	0.62	0
3	GOL	A	633	-	5,5,5	0.83	0	5,5,5	1.06	0
4	EDO	A	622	-	3,3,3	0.44	0	2,2,2	0.40	0
4	EDO	A	609	-	3,3,3	0.47	0	2,2,2	0.36	0
4	EDO	B	1007	-	3,3,3	0.52	0	2,2,2	0.25	0
4	EDO	B	1012	-	3,3,3	0.49	0	2,2,2	0.41	0
4	EDO	A	613	-	3,3,3	0.40	0	2,2,2	0.38	0
4	EDO	A	606	-	3,3,3	0.42	0	2,2,2	0.78	0
4	EDO	A	618	-	3,3,3	0.46	0	2,2,2	0.22	0
4	EDO	B	1017	-	3,3,3	0.54	0	2,2,2	0.26	0
3	GOL	Y	101	-	5,5,5	0.93	0	5,5,5	0.99	0
4	EDO	A	610	-	3,3,3	0.47	0	2,2,2	0.30	0
4	EDO	B	1002	-	3,3,3	0.47	0	2,2,2	0.30	0
3	GOL	A	604	-	5,5,5	0.91	0	5,5,5	1.04	0
4	EDO	A	628	-	3,3,3	0.45	0	2,2,2	0.38	0
4	EDO	B	1008	-	3,3,3	0.51	0	2,2,2	0.29	0
4	EDO	A	605	-	3,3,3	0.49	0	2,2,2	0.32	0
4	EDO	A	615	-	3,3,3	0.50	0	2,2,2	0.25	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
4	EDO	A	608	-	-	1/1/1/1	-
4	EDO	B	1010	-	-	1/1/1/1	-
4	EDO	A	607	-	-	1/1/1/1	-
4	EDO	A	625	-	-	0/1/1/1	-
4	EDO	A	617	-	-	0/1/1/1	-
4	EDO	B	1019	-	-	0/1/1/1	-
3	GOL	A	603	-	-	2/4/4/4	-
4	EDO	B	1014	-	-	1/1/1/1	-
3	GOL	A	632	-	-	2/4/4/4	-
4	EDO	A	627	-	-	1/1/1/1	-
4	EDO	A	620	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	623	-	-	1/1/1/1	-
4	EDO	B	1018	-	-	0/1/1/1	-
4	EDO	A	631	-	-	1/1/1/1	-
4	EDO	A	616	-	-	1/1/1/1	-
4	EDO	A	626	-	-	0/1/1/1	-
4	EDO	B	1004	-	-	1/1/1/1	-
4	EDO	A	619	-	-	1/1/1/1	-
4	EDO	A	629	-	-	0/1/1/1	-
4	EDO	A	611	-	-	0/1/1/1	-
4	EDO	A	614	-	-	0/1/1/1	-
4	EDO	A	630	-	-	1/1/1/1	-
5	SAH	B	1001	-	-	3/7/31/31	0/3/3/3
4	EDO	B	1006	-	-	1/1/1/1	-
4	EDO	B	1020	-	-	0/1/1/1	-
4	EDO	Y	102	-	-	0/1/1/1	-
4	EDO	B	1015	-	-	1/1/1/1	-
5	SAH	A	601	-	-	2/7/31/31	0/3/3/3
4	EDO	B	1005	-	-	0/1/1/1	-
4	EDO	B	1011	-	-	0/1/1/1	-
4	EDO	B	1009	-	-	0/1/1/1	-
4	EDO	B	1003	-	-	1/1/1/1	-
4	EDO	B	1016	-	-	1/1/1/1	-
4	EDO	A	621	-	-	1/1/1/1	-
4	EDO	B	1013	-	-	0/1/1/1	-
3	GOL	A	602	-	-	0/4/4/4	-
4	EDO	A	612	-	-	0/1/1/1	-
3	GOL	A	633	-	-	2/4/4/4	-
4	EDO	A	622	-	-	0/1/1/1	-
4	EDO	A	609	-	-	1/1/1/1	-
4	EDO	B	1007	-	-	0/1/1/1	-
4	EDO	B	1012	-	-	0/1/1/1	-
4	EDO	A	613	-	-	1/1/1/1	-
4	EDO	A	606	-	-	1/1/1/1	-
4	EDO	A	618	-	-	0/1/1/1	-
4	EDO	B	1017	-	-	0/1/1/1	-
3	GOL	Y	101	-	-	4/4/4/4	-
4	EDO	A	610	-	-	0/1/1/1	-
4	EDO	B	1002	-	-	0/1/1/1	-
3	GOL	A	604	-	-	0/4/4/4	-
4	EDO	A	628	-	-	1/1/1/1	-
4	EDO	B	1008	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	605	-	-	0/1/1/1	-
4	EDO	A	615	-	-	0/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	624	ACT	CH3-C	7.00	1.57	1.48
5	B	1001	SAH	C2-N3	3.75	1.38	1.32
5	A	601	SAH	C2-N3	3.56	1.37	1.32
5	A	601	SAH	C2-N1	2.22	1.38	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1001	SAH	N3-C2-N1	-5.56	119.98	128.68
5	A	601	SAH	N3-C2-N1	-4.87	121.06	128.68
5	B	1001	SAH	C5'-SD-CG	-3.07	93.07	102.27
5	A	601	SAH	CB-CG-SD	-2.60	107.48	113.31
5	A	601	SAH	C5'-SD-CG	-2.10	95.97	102.27
5	B	1001	SAH	C4-C5-N7	-2.08	107.23	109.40

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	603	GOL	C1-C2-C3-O3
3	A	632	GOL	C1-C2-C3-O3
3	Y	101	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	B	1010	EDO	O1-C1-C2-O2
4	A	623	EDO	O1-C1-C2-O2
4	A	631	EDO	O1-C1-C2-O2
4	A	616	EDO	O1-C1-C2-O2
3	A	603	GOL	O2-C2-C3-O3
4	A	607	EDO	O1-C1-C2-O2
4	A	621	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

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Mol	Chain	Res	Type	Atoms
5	B	1001	SAH	CB-CG-SD-C5'
5	A	601	SAH	CB-CG-SD-C5'
4	B	1016	EDO	O1-C1-C2-O2
4	B	1015	EDO	O1-C1-C2-O2
4	B	1004	EDO	O1-C1-C2-O2
4	B	1003	EDO	O1-C1-C2-O2
4	A	606	EDO	O1-C1-C2-O2
4	A	628	EDO	O1-C1-C2-O2
3	Y	101	GOL	O1-C1-C2-O2
4	B	1014	EDO	O1-C1-C2-O2
4	B	1006	EDO	O1-C1-C2-O2
4	A	608	EDO	O1-C1-C2-O2
4	A	613	EDO	O1-C1-C2-O2
5	A	601	SAH	C3'-C4'-C5'-SD
3	A	633	GOL	O1-C1-C2-C3
5	B	1001	SAH	C-CA-CB-CG
4	A	627	EDO	O1-C1-C2-O2
4	A	619	EDO	O1-C1-C2-O2
4	A	630	EDO	O1-C1-C2-O2

There are no ring outliers.

26 monomers are involved in 38 short contacts:

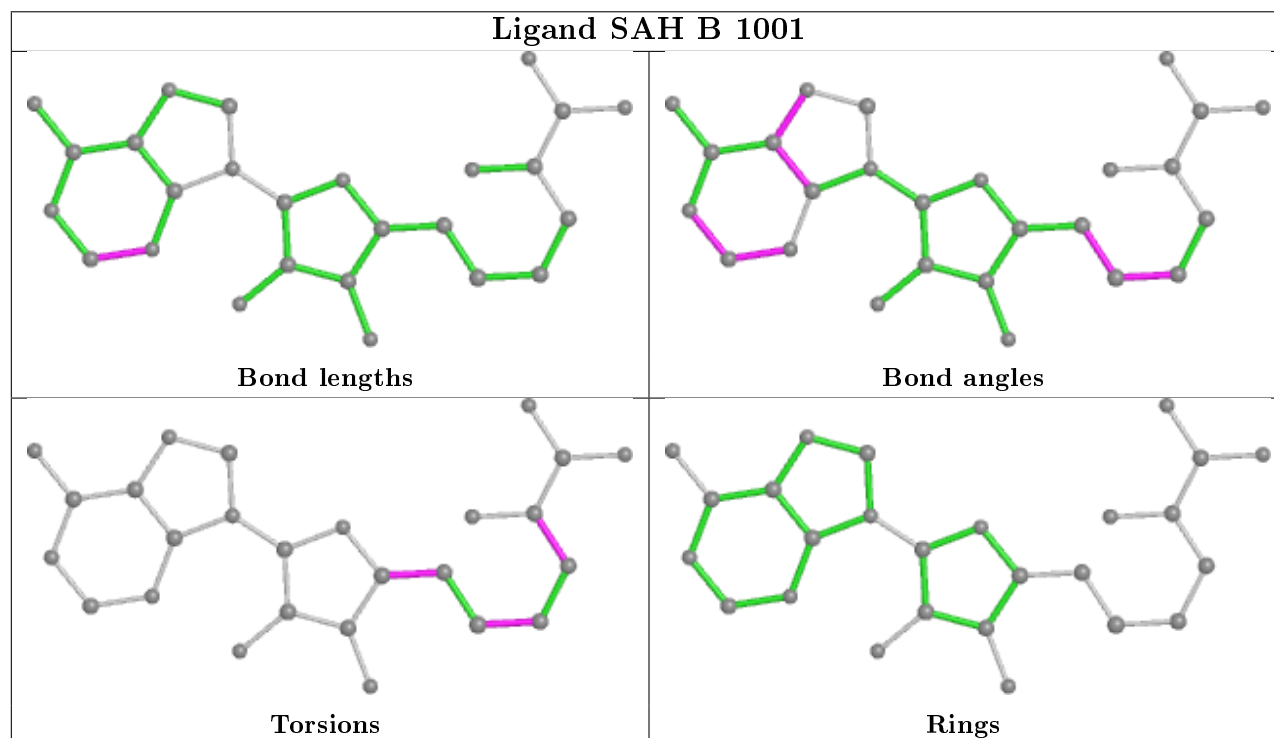
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	608	EDO	2	0
4	B	1010	EDO	1	0
4	B	1019	EDO	1	0
3	A	603	GOL	3	0
4	B	1014	EDO	2	0
4	A	623	EDO	1	0
4	A	631	EDO	2	0
4	A	616	EDO	2	0
4	B	1004	EDO	1	0
4	A	619	EDO	1	0
4	A	629	EDO	1	0
4	A	630	EDO	1	0
5	B	1001	SAH	1	0
4	B	1020	EDO	1	0
4	B	1015	EDO	3	0
4	B	1005	EDO	2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

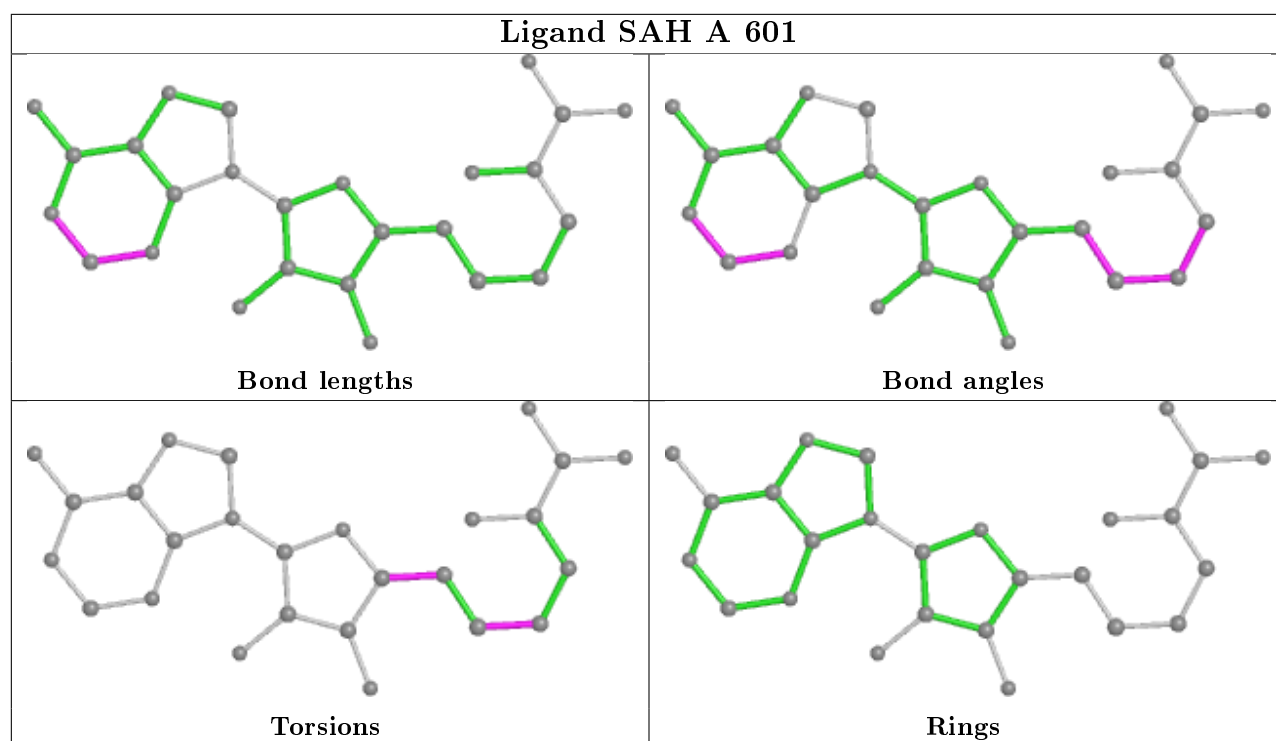
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1007	EDO	1	0
4	A	613	EDO	2	0
4	A	606	EDO	1	0
3	Y	101	GOL	2	0
4	B	1002	EDO	3	0
3	A	604	GOL	2	0
4	A	628	EDO	2	0
4	A	605	EDO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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%)	0.82	3 (15%) 2 2	17, 25, 56, 59	0
1	Z	19/23 (82%)	0.80	3 (15%) 2 2	17, 28, 57, 61	0
2	A	483/594 (81%)	0.17	14 (2%) 51 54	13, 25, 42, 63	0
2	B	483/594 (81%)	0.22	17 (3%) 44 47	14, 26, 45, 64	0
All	All	1004/1234 (81%)	0.22	37 (3%) 41 44	13, 25, 44, 64	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	19	VAL	7.0
1	Z	66	THR	6.5
1	Y	66	THR	6.4
2	B	261	ASP	4.2
2	B	21	PRO	4.2
1	Y	84	LYS	4.1
2	B	501	TYR	3.9
2	A	263	SER	3.8
2	B	37	SER	3.7
2	B	347	ARG	3.4
2	A	20	SER	3.3
2	A	21	PRO	3.1
2	B	38	PRO	3.0
2	A	264	ARG	2.8
2	B	494	GLU	2.8
2	A	374	PRO	2.8
2	B	498	LEU	2.8
2	A	38	PRO	2.7
2	A	168	ASN	2.7
2	B	495	LYS	2.7
2	B	262	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	236	ASP	2.6
2	B	263	SER	2.6
1	Z	83	GLU	2.6
2	B	20	SER	2.5
2	B	344	LYS	2.5
2	A	39	ALA	2.4
2	A	501	TYR	2.4
1	Y	83	GLU	2.4
2	A	186	LEU	2.3
2	A	493	GLU	2.3
2	A	373	GLU	2.2
2	B	264	ARG	2.2
2	A	261	ASP	2.2
2	B	33	GLN	2.2
2	A	372	THR	2.1
1	Z	67	LEU	2.1

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 monosaccharides 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(\AA^2)	Q<0.9
3	GOL	A	604	6/6	0.66	0.23	50,58,58,60	0
4	EDO	A	605	4/4	0.66	0.45	58,60,63,63	0
4	EDO	A	615	4/4	0.66	0.28	42,46,56,56	0
3	GOL	A	632	6/6	0.67	0.26	49,53,56,57	0
3	GOL	A	633	6/6	0.73	0.31	44,46,49,53	0
4	EDO	B	1009	4/4	0.76	0.28	32,43,44,45	0
4	EDO	B	1017	4/4	0.78	0.13	35,35,42,46	0

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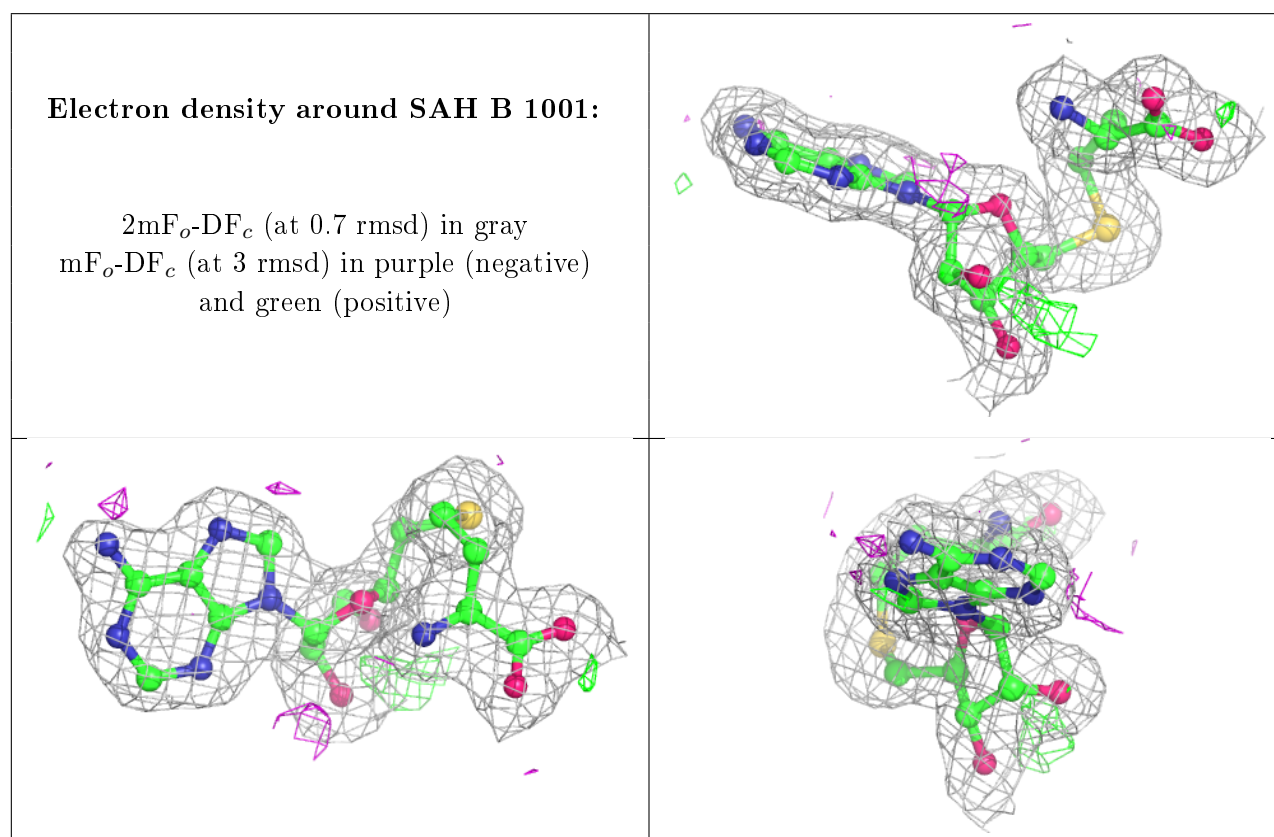
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	EDO	B	1016	4/4	0.79	0.20	34,41,41,42	0
3	GOL	A	602	6/6	0.79	0.24	41,47,48,50	0
3	GOL	A	603	6/6	0.80	0.19	27,32,33,43	0
4	EDO	A	627	4/4	0.82	0.16	39,39,45,48	0
4	EDO	B	1002	4/4	0.82	0.23	25,34,39,44	0
4	EDO	A	625	4/4	0.83	0.21	39,39,46,46	0
4	EDO	B	1015	4/4	0.83	0.29	24,33,40,40	0
4	EDO	B	1004	4/4	0.85	0.22	30,40,44,45	0
4	EDO	A	621	4/4	0.85	0.14	32,39,39,42	0
4	EDO	A	616	4/4	0.86	0.19	31,37,39,42	0
4	EDO	B	1007	4/4	0.86	0.16	39,41,42,47	0
4	EDO	B	1020	4/4	0.86	0.18	40,43,45,52	0
4	EDO	A	611	4/4	0.87	0.17	29,31,33,43	0
4	EDO	B	1012	4/4	0.87	0.22	37,38,39,39	0
4	EDO	B	1013	4/4	0.87	0.15	36,44,47,54	0
4	EDO	A	623	4/4	0.88	0.16	24,31,32,36	0
4	EDO	A	612	4/4	0.88	0.18	36,38,39,40	0
3	GOL	Y	101	6/6	0.88	0.18	28,34,39,46	0
4	EDO	A	622	4/4	0.89	0.14	34,34,38,41	0
4	EDO	B	1005	4/4	0.89	0.14	38,39,39,40	0
4	EDO	B	1003	4/4	0.90	0.26	31,35,43,43	0
4	EDO	B	1014	4/4	0.90	0.17	23,27,33,36	0
4	EDO	A	610	4/4	0.90	0.14	28,32,32,39	0
4	EDO	B	1010	4/4	0.90	0.23	26,28,35,47	0
4	EDO	A	613	4/4	0.90	0.17	30,32,36,37	0
4	EDO	A	606	4/4	0.90	0.17	28,31,32,37	0
4	EDO	A	607	4/4	0.91	0.12	30,40,41,42	0
4	EDO	A	609	4/4	0.91	0.15	36,41,42,44	0
4	EDO	A	631	4/4	0.91	0.34	31,32,33,50	0
4	EDO	A	608	4/4	0.91	0.16	24,34,38,47	0
4	EDO	A	617	4/4	0.92	0.18	34,37,41,43	0
4	EDO	B	1019	4/4	0.92	0.11	31,37,37,38	0
4	EDO	Y	102	4/4	0.92	0.21	35,35,38,52	0
6	ACT	A	624	4/4	0.92	0.12	31,40,43,44	0
4	EDO	B	1008	4/4	0.93	0.10	29,33,34,36	0
4	EDO	A	619	4/4	0.93	0.17	32,34,35,38	0
4	EDO	B	1011	4/4	0.93	0.14	31,32,32,42	0
4	EDO	A	629	4/4	0.94	0.19	39,46,46,50	0
4	EDO	B	1018	4/4	0.94	0.12	27,32,33,39	0
5	SAH	B	1001	26/26	0.94	0.13	12,18,22,24	0
4	EDO	A	630	4/4	0.94	0.15	25,25,26,35	0
4	EDO	A	620	4/4	0.94	0.10	22,27,28,31	0

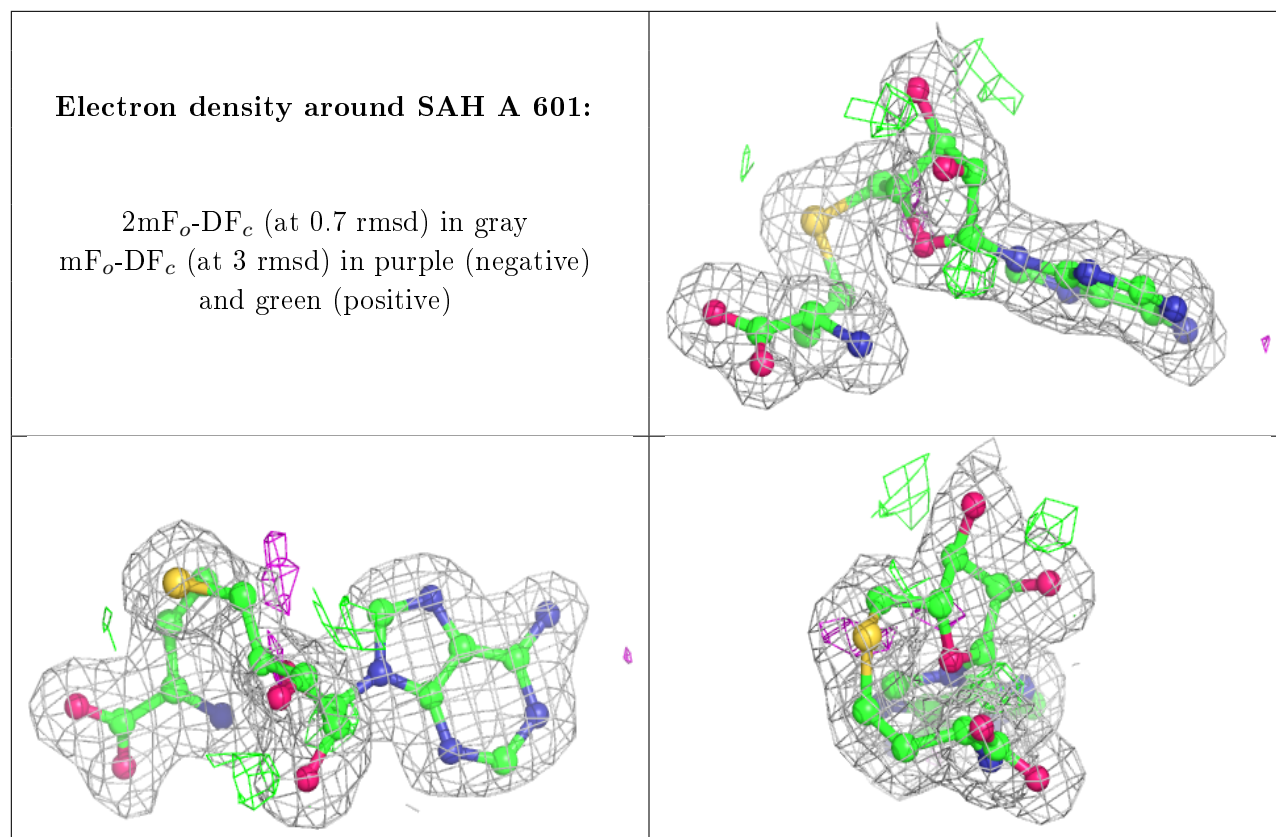
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	SAH	A	601	26/26	0.95	0.12	13,18,22,24	0
4	EDO	A	618	4/4	0.95	0.16	31,31,33,34	0
4	EDO	B	1006	4/4	0.96	0.12	28,31,35,37	0
4	EDO	A	614	4/4	0.96	0.21	31,31,32,37	0
4	EDO	A	628	4/4	0.97	0.07	28,32,35,48	0
4	EDO	A	626	4/4	0.97	0.17	37,38,45,48	0

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





6.5 Other polymers [i](#)

There are no such residues in this entry.