



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 03:46 AM UTC

PDB ID : 6OX3 / pdb_00006ox3
Title : SETD3 in Complex with an Actin Peptide with His73 Replaced with Lysine
Authors : Horton, J.R.; Dai, S.; Cheng, X.
Deposited on : 2019-05-13
Resolution : 1.78 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

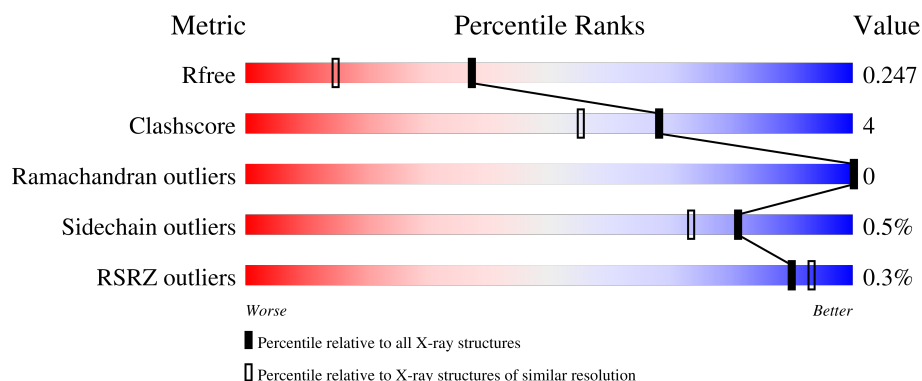
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	19	5% 84% 16%
1	Z	19	5% 95% 5%
2	A	599	74% 7% 19%
2	B	599	74% 7% 19%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8954 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 Peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Y	19	Total	C	N	O	S	0	0	0
			153	100	24	28	1			
1	Z	19	Total	C	N	O	S	0	0	0
			149	97	23	28	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	73	LYS	HIS	engineered mutation	UNP C9JUM1
Z	73	LYS	HIS	engineered mutation	UNP C9JUM1

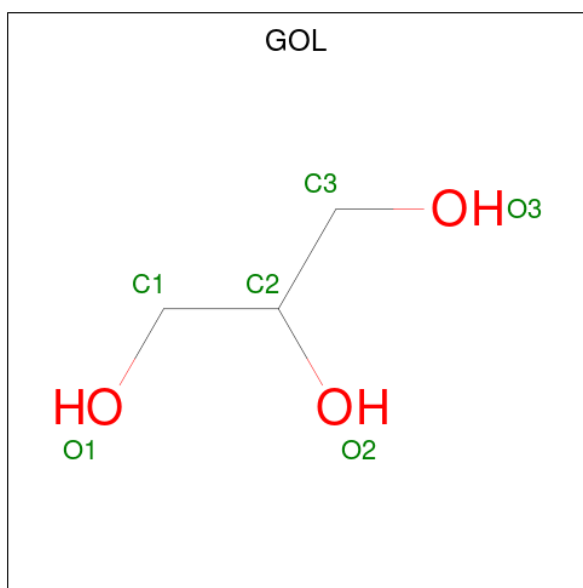
- Molecule 2 is a protein called Histone-lysine N-methyltransferase setd3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	483	Total	C	N	O	S	0	14	0
			3930	2514	664	733	19			
2	B	483	Total	C	N	O	S	0	7	0
			3896	2492	655	730	19			

There are 10 discrepancies between the modelled and reference sequences:

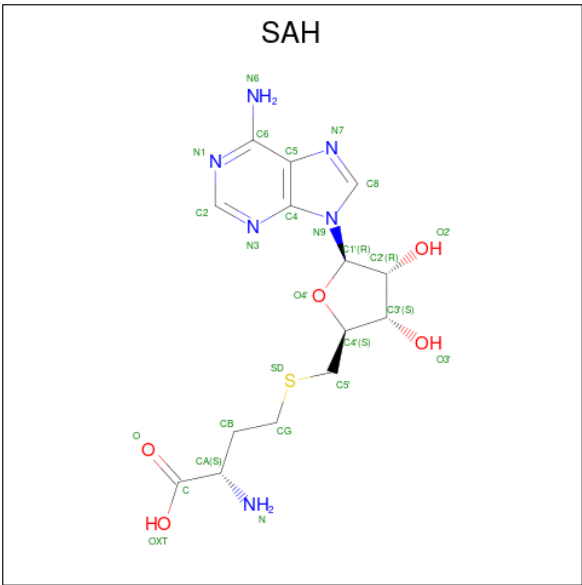
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q86TU7
A	-4	PRO	-	expression tag	UNP Q86TU7
A	-3	LEU	-	expression tag	UNP Q86TU7
A	-2	GLY	-	expression tag	UNP Q86TU7
A	-1	SER	-	expression tag	UNP Q86TU7
B	-5	GLY	-	expression tag	UNP Q86TU7
B	-4	PRO	-	expression tag	UNP Q86TU7
B	-3	LEU	-	expression tag	UNP Q86TU7
B	-2	GLY	-	expression tag	UNP Q86TU7
B	-1	SER	-	expression tag	UNP Q86TU7

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



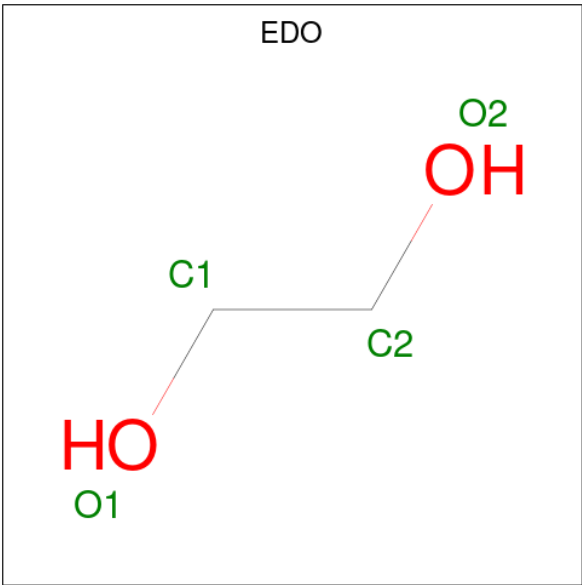
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	Y	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



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

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

Continued on next page...

Continued from previous page...

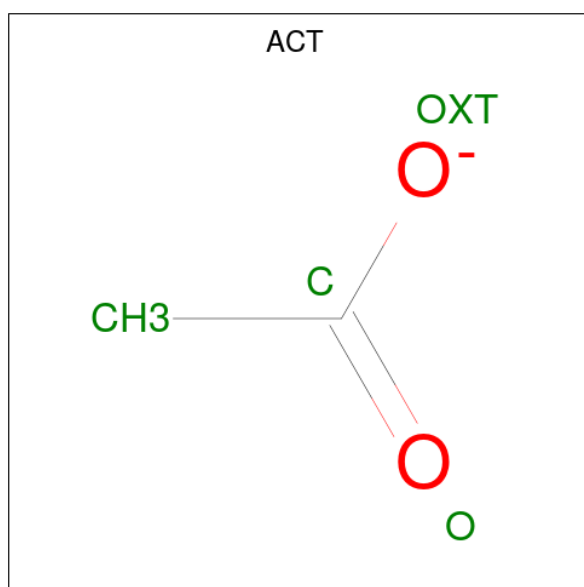
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total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

Continued on next page...

Continued from previous page...

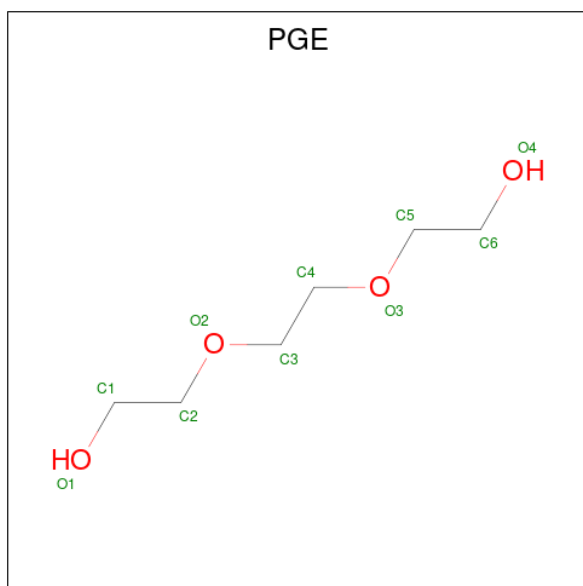
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is ACETATE ION (CCD ID: ACT) (formula: $\text{C}_2\text{H}_3\text{O}_2$).



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

- Molecule 7 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	Y	14	Total	O	0	0
			14	14		
8	A	303	Total	O	0	0
			303	303		
8	Z	13	Total	O	0	0
			13	13		
8	B	264	Total	O	0	0
			264	264		

3 Residue-property plots [i](#)

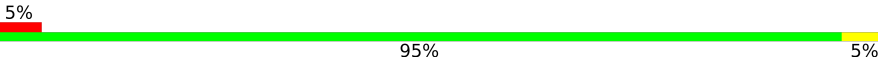
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

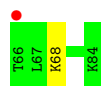
- Molecule 1: Actin Peptide

Chain Y:  84% 16%



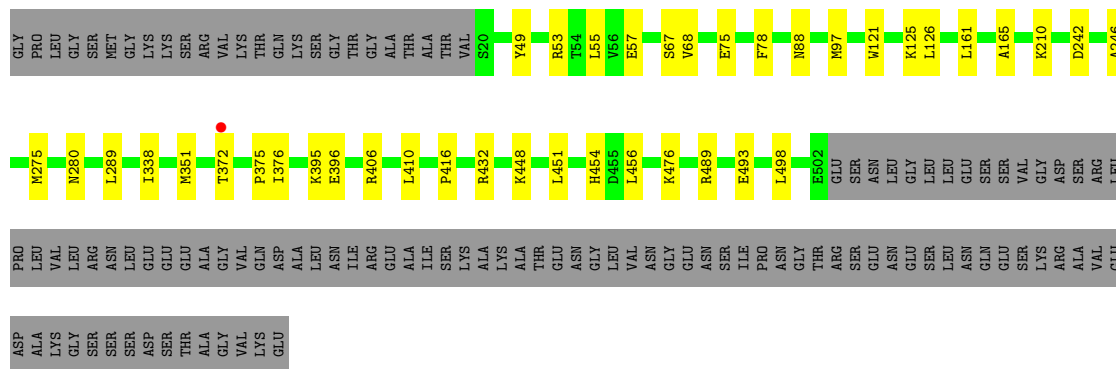
- Molecule 1: Actin Peptide

Chain Z:  5% 95% 5%



- Molecule 2: Histone-lysine N-methyltransferase setd3

Chain A:  74% 7% 19%



- Molecule 2: Histone-lysine N-methyltransferase setd3

Chain B:  74% 7% 19%



L196	SER
I202	ARG
R214	LEU
E241	PRO
R244	LEU
W245	VAL
A246	LEU
L272	ARG
M275	ASN
T314	LEU
F327	GLU
K344	GLU
L348	ALA
M351	LEU
A359	ALA
F371	ILE
M389	SER
T390	LYS
E391	LYS
K395	ALA
E396	THR
R406	GLU
V417	ASN
M462	GLY
L473	ASN
Y501	PRO
GLU	ASN
GLU	GLY
SER	THR
SER	ARG
ASN	SER
LEU	GLU
GLY	ASN
LEU	GLU
LEU	SER
GLU	LEU
SER	ASN
SER	GLN
VAL	GLU
GLY	SER
ASP	LYS
	ARG

ALA
VAL
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	60.23Å 175.75Å 66.47Å 90.00° 92.39° 90.00°	Depositor
Resolution (Å)	36.64 – 1.78 36.64 – 1.78	Depositor EDS
% Data completeness (in resolution range)	97.8 (36.64-1.78) 97.7 (36.64-1.78)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 1.78Å)	Xtriage
Refinement program	PHENIX (1.14_3260)	Depositor
R, R_{free}	0.208 , 0.246 0.210 , 0.247	Depositor DCC
R_{free} test set	1992 reflections (1.53%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 31.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.076 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8954	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.80% 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: PGE, SAH, EDO, GOL, 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	0.18	0/156	0.34	0/210
1	Z	0.17	0/152	0.31	0/206
2	A	0.21	0/4044	0.42	0/5482
2	B	0.20	0/3997	0.40	0/5419
All	All	0.20	0/8349	0.41	0/11317

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
2	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	372[B]	THR	Peptide

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	153	0	149	2	0
1	Z	149	0	138	1	0
2	A	3930	0	3842	27	0
2	B	3896	0	3795	29	0
3	A	24	0	32	3	0
3	Y	6	0	8	1	0
4	A	26	0	19	0	0
4	B	26	0	19	0	0
5	A	88	0	132	6	0
5	B	48	0	72	5	0
6	A	4	0	3	0	0
7	B	10	0	14	2	0
8	A	303	0	0	3	0
8	B	264	0	0	1	0
8	Y	14	0	0	0	0
8	Z	13	0	0	0	0
All	All	8954	0	8223	60	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 60 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)
2:B:97[A]:MET:HE1	2:B:275:MET:HE2	1.58	0.85
2:B:351:MET:HE1	2:B:391:GLU:HG3	1.63	0.80
2:A:289:LEU:H	3:A:605:GOL:H12	1.53	0.73
2:A:338:ILE:HG13	3:A:604:GOL:H12	1.76	0.65
2:A:97[B]:MET:HE1	2:A:275:MET:HE2	1.79	0.64

There are no symmetry-related clashes.

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	17/19 (90%)	16 (94%)	1 (6%)	0	100	100
1	Z	17/19 (90%)	17 (100%)	0	0	100	100
2	A	495/599 (83%)	492 (99%)	3 (1%)	0	100	100
2	B	488/599 (82%)	483 (99%)	5 (1%)	0	100	100
All	All	1017/1236 (82%)	1008 (99%)	9 (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	16/18 (89%)	16 (100%)	0	100	100
1	Z	15/18 (83%)	15 (100%)	0	100	100
2	A	422/521 (81%)	419 (99%)	3 (1%)	76	66
2	B	418/521 (80%)	417 (100%)	1 (0%)	87	83
All	All	871/1078 (81%)	867 (100%)	4 (0%)	81	73

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	55	LEU
2	A	280	ASN
2	A	410	LEU
2	B	344	LYS

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

Mol	Chain	Res	Type
2	A	135	ASN
2	A	149	GLN
2	A	280	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	149	GLN
2	B	288	ASN

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 ⓘ

43 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	EDO	A	620	-	3,3,3	0.44	0	2,2,2	0.39	0
5	EDO	A	624	-	3,3,3	0.43	0	2,2,2	0.35	0
5	EDO	A	617	-	3,3,3	0.45	0	2,2,2	0.33	0
5	EDO	A	608	-	3,3,3	0.43	0	2,2,2	0.36	0
5	EDO	A	615	-	3,3,3	0.43	0	2,2,2	0.35	0
4	SAH	A	601	-	27,28,28	1.08	2 (7%)	36,40,40	0.63	0
3	GOL	A	602	-	5,5,5	0.98	0	5,5,5	1.06	0
5	EDO	B	605	-	3,3,3	0.43	0	2,2,2	0.36	0
3	GOL	A	603	-	5,5,5	0.74	0	5,5,5	1.17	0
5	EDO	B	606	-	3,3,3	0.45	0	2,2,2	0.41	0
5	EDO	A	613	-	3,3,3	0.43	0	2,2,2	0.38	0
5	EDO	A	614	-	3,3,3	0.44	0	2,2,2	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	B	612	-	3,3,3	0.43	0	2,2,2	0.43	0
5	EDO	A	622	-	3,3,3	0.43	0	2,2,2	0.35	0
5	EDO	A	606	-	3,3,3	0.44	0	2,2,2	0.39	0
5	EDO	A	607	-	3,3,3	0.42	0	2,2,2	0.51	0
5	EDO	A	626	-	3,3,3	0.44	0	2,2,2	0.33	0
5	EDO	B	609	-	3,3,3	0.44	0	2,2,2	0.39	0
5	EDO	A	616	-	3,3,3	0.44	0	2,2,2	0.36	0
5	EDO	B	611	-	3,3,3	0.44	0	2,2,2	0.44	0
6	ACT	A	628	-	3,3,3	0.80	0	3,3,3	0.80	0
4	SAH	B	601	-	27,28,28	1.02	2 (7%)	36,40,40	0.64	0
5	EDO	A	621	-	3,3,3	0.46	0	2,2,2	0.27	0
5	EDO	A	627	-	3,3,3	0.45	0	2,2,2	0.22	0
5	EDO	A	612	-	3,3,3	0.46	0	2,2,2	0.50	0
5	EDO	B	610	-	3,3,3	0.44	0	2,2,2	0.37	0
5	EDO	A	611	-	3,3,3	0.44	0	2,2,2	0.33	0
5	EDO	A	609	-	3,3,3	0.43	0	2,2,2	0.39	0
5	EDO	B	604	-	3,3,3	0.44	0	2,2,2	0.38	0
3	GOL	Y	101	-	5,5,5	0.93	0	5,5,5	1.04	0
5	EDO	A	618	-	3,3,3	0.43	0	2,2,2	0.37	0
5	EDO	B	607	-	3,3,3	0.44	0	2,2,2	0.37	0
7	PGE	B	614	-	9,9,9	0.51	0	8,8,8	0.27	0
5	EDO	A	610	-	3,3,3	0.43	0	2,2,2	0.35	0
3	GOL	A	605	-	5,5,5	0.94	0	5,5,5	1.08	0
5	EDO	A	625	-	3,3,3	0.43	0	2,2,2	0.40	0
5	EDO	A	619	-	3,3,3	0.43	0	2,2,2	0.38	0
5	EDO	A	623	-	3,3,3	0.46	0	2,2,2	0.49	0
5	EDO	B	613	-	3,3,3	0.43	0	2,2,2	0.45	0
5	EDO	B	602	-	3,3,3	0.44	0	2,2,2	0.34	0
5	EDO	B	603	-	3,3,3	0.43	0	2,2,2	0.32	0
5	EDO	B	608	-	3,3,3	0.43	0	2,2,2	0.32	0
3	GOL	A	604	-	5,5,5	0.89	0	5,5,5	1.02	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	EDO	A	620	-	-	0/1/1/1	-
5	EDO	A	624	-	-	0/1/1/1	-
5	EDO	A	617	-	-	0/1/1/1	-
5	EDO	A	608	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	615	-	-	0/1/1/1	-
4	SAH	A	601	-	-	1/15/31/31	0/3/3/3
3	GOL	A	602	-	-	1/4/4/4	-
5	EDO	B	605	-	-	0/1/1/1	-
3	GOL	A	603	-	-	2/4/4/4	-
5	EDO	B	606	-	-	1/1/1/1	-
5	EDO	A	613	-	-	0/1/1/1	-
5	EDO	A	614	-	-	1/1/1/1	-
5	EDO	B	612	-	-	1/1/1/1	-
5	EDO	A	622	-	-	0/1/1/1	-
5	EDO	A	606	-	-	0/1/1/1	-
5	EDO	A	607	-	-	1/1/1/1	-
5	EDO	A	626	-	-	1/1/1/1	-
5	EDO	B	609	-	-	0/1/1/1	-
5	EDO	A	616	-	-	0/1/1/1	-
5	EDO	B	611	-	-	0/1/1/1	-
4	SAH	B	601	-	-	1/15/31/31	0/3/3/3
5	EDO	A	621	-	-	1/1/1/1	-
5	EDO	A	627	-	-	1/1/1/1	-
5	EDO	A	612	-	-	1/1/1/1	-
5	EDO	B	610	-	-	1/1/1/1	-
5	EDO	A	611	-	-	0/1/1/1	-
5	EDO	A	609	-	-	1/1/1/1	-
5	EDO	B	604	-	-	0/1/1/1	-
3	GOL	Y	101	-	-	3/4/4/4	-
5	EDO	A	618	-	-	1/1/1/1	-
5	EDO	B	607	-	-	0/1/1/1	-
7	PGE	B	614	-	-	2/7/7/7	-
5	EDO	A	610	-	-	1/1/1/1	-
3	GOL	A	605	-	-	0/4/4/4	-
5	EDO	A	625	-	-	1/1/1/1	-
5	EDO	A	619	-	-	1/1/1/1	-
5	EDO	A	623	-	-	0/1/1/1	-
5	EDO	B	613	-	-	1/1/1/1	-
5	EDO	B	602	-	-	0/1/1/1	-
5	EDO	B	603	-	-	1/1/1/1	-
5	EDO	B	608	-	-	0/1/1/1	-
3	GOL	A	604	-	-	4/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	SAH	C8-N9	3.25	1.43	1.37
4	B	601	SAH	CB-CA	2.58	1.58	1.53
4	A	601	SAH	C5-C4	2.28	1.43	1.39
4	B	601	SAH	C8-N9	2.23	1.41	1.37

There are no bond angle outliers.

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	603	GOL	O1-C1-C2-C3
3	A	604	GOL	C1-C2-C3-O3
3	Y	101	GOL	O2-C2-C3-O3
3	A	604	GOL	O2-C2-C3-O3
3	Y	101	GOL	C1-C2-C3-O3

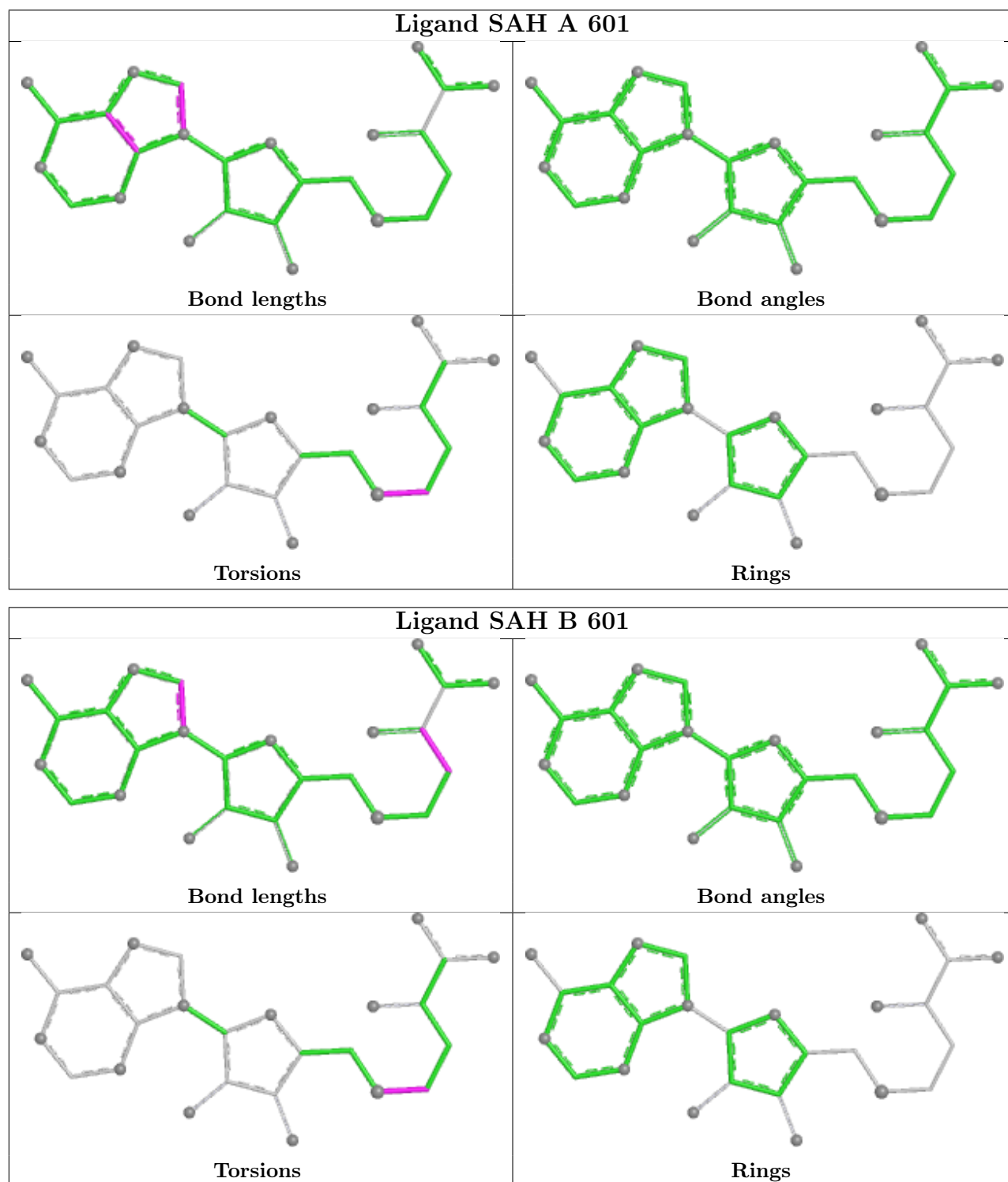
There are no ring outliers.

11 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	617	EDO	1	0
5	A	613	EDO	3	0
5	A	606	EDO	1	0
5	B	610	EDO	2	0
3	Y	101	GOL	1	0
7	B	614	PGE	2	0
3	A	605	GOL	1	0
5	A	619	EDO	1	0
5	B	602	EDO	2	0
5	B	603	EDO	1	0
3	A	604	GOL	2	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 ⓘ

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	19/19 (100%)	-0.76	0 100 100	17, 29, 67, 74	0
1	Z	19/19 (100%)	-0.63	1 (5%) 32 38	17, 32, 76, 83	0
2	A	483/599 (80%)	-1.02	1 (0%) 91 93	9, 25, 46, 69	14 (2%)
2	B	483/599 (80%)	-0.94	1 (0%) 91 93	11, 27, 49, 69	7 (1%)
All	All	1004/1236 (81%)	-0.97	3 (0%) 90 93	9, 26, 49, 83	21 (2%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Z	66	THR	2.4
2	B	19	VAL	2.3
2	A	372[A]	THR	2.2

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](#)

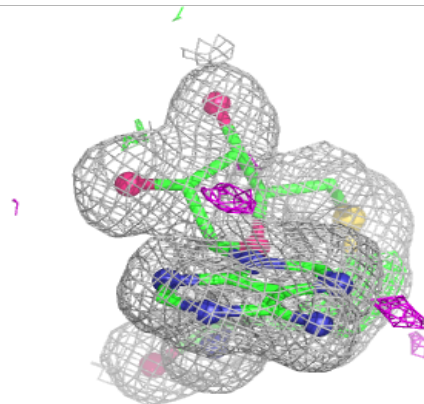
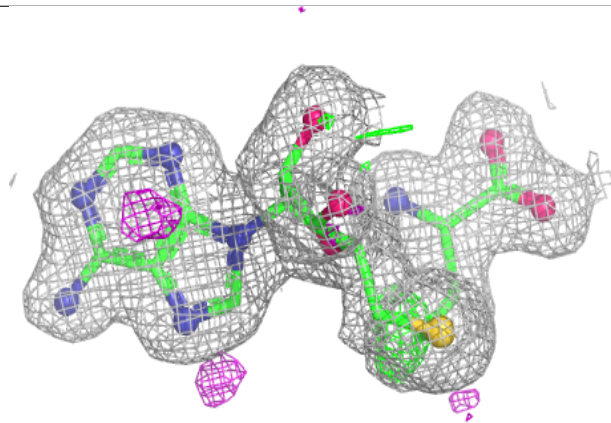
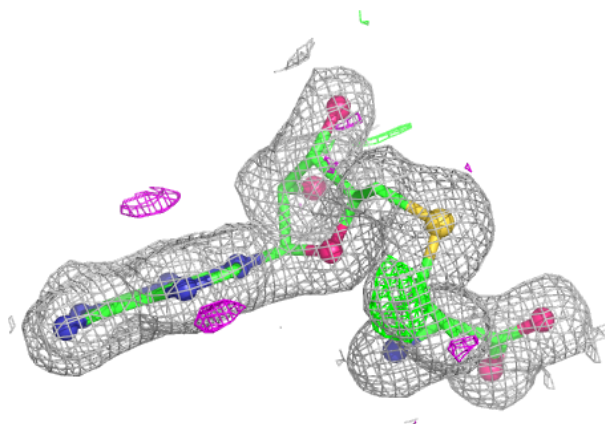
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

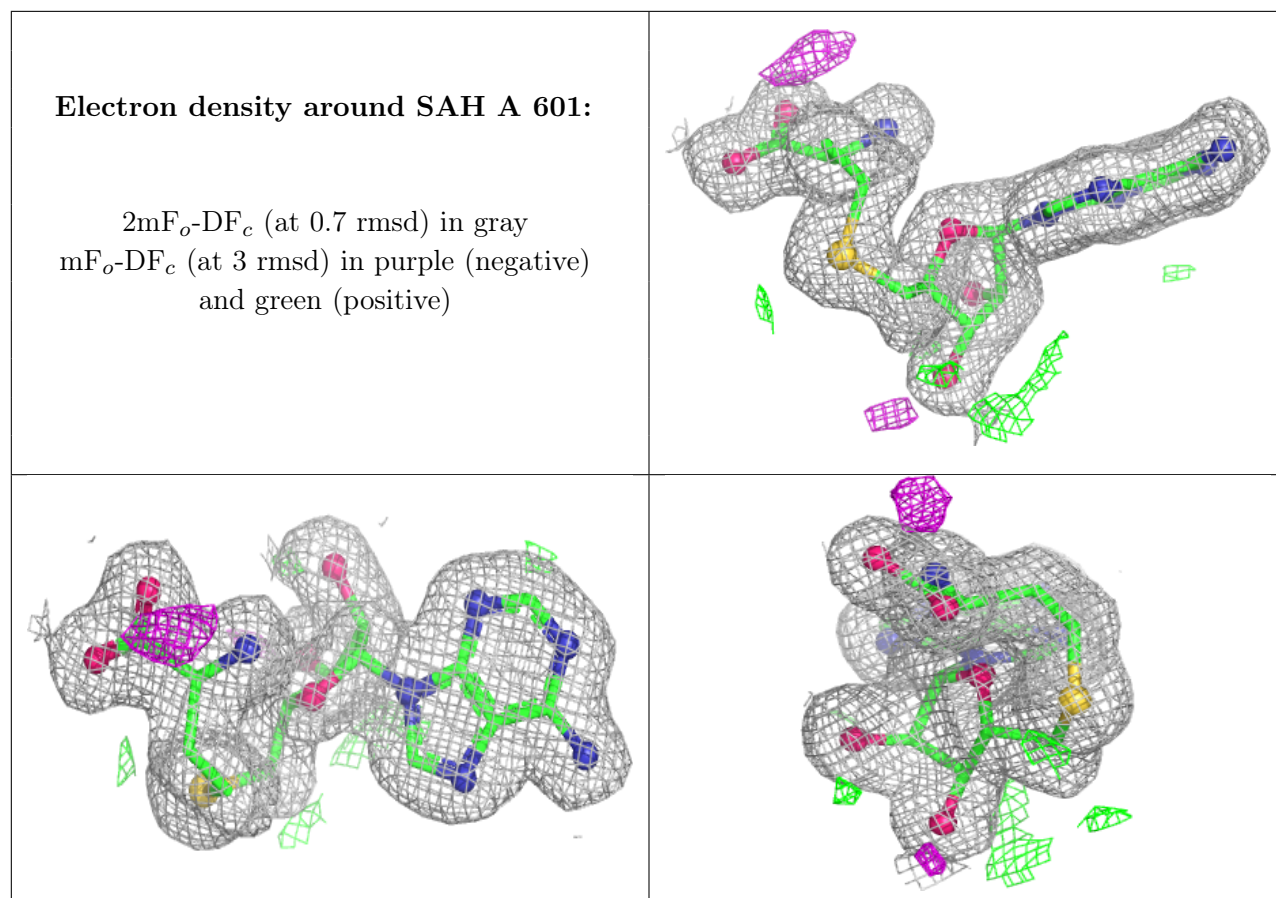
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	A	618	4/4	0.96	0.08	45,50,53,53	0
5	EDO	A	619	4/4	0.96	0.09	53,54,56,57	0
5	EDO	A	622	4/4	0.96	0.06	41,42,43,44	0
5	EDO	A	614	4/4	0.97	0.07	39,44,45,47	0
3	GOL	A	602	6/6	0.97	0.07	52,57,61,63	0
5	EDO	A	606	4/4	0.97	0.07	58,63,68,72	0
5	EDO	A	608	4/4	0.97	0.10	62,63,63,64	0
5	EDO	A	626	4/4	0.97	0.11	38,42,46,47	0
5	EDO	B	603	4/4	0.97	0.09	57,58,58,60	0
5	EDO	B	607	4/4	0.97	0.06	52,53,53,56	0
5	EDO	B	609	4/4	0.97	0.07	47,50,50,52	0
5	EDO	B	612	4/4	0.97	0.10	53,58,61,63	0
3	GOL	A	604	6/6	0.98	0.06	32,33,37,42	0
5	EDO	A	616	4/4	0.98	0.08	42,44,45,49	0
5	EDO	A	617	4/4	0.98	0.05	43,51,55,62	0
3	GOL	A	605	6/6	0.98	0.07	62,66,70,72	0
3	GOL	Y	101	6/6	0.98	0.05	37,42,48,52	0
5	EDO	A	620	4/4	0.98	0.06	45,48,48,53	0
5	EDO	A	607	4/4	0.98	0.07	32,35,44,47	0
3	GOL	A	603	6/6	0.98	0.07	31,39,42,49	0
5	EDO	A	627	4/4	0.98	0.05	23,27,31,33	0
5	EDO	B	602	4/4	0.98	0.07	56,56,57,58	0
5	EDO	A	609	4/4	0.98	0.07	46,51,52,57	0
5	EDO	B	605	4/4	0.98	0.08	47,52,57,59	0
5	EDO	B	606	4/4	0.98	0.07	27,28,37,39	0
5	EDO	A	610	4/4	0.98	0.07	50,50,50,50	0
5	EDO	B	608	4/4	0.98	0.05	36,42,43,45	0
5	EDO	A	611	4/4	0.98	0.08	58,64,66,69	0
5	EDO	B	610	4/4	0.98	0.09	33,38,43,49	0
5	EDO	B	611	4/4	0.98	0.06	34,38,40,40	0
5	EDO	A	612	4/4	0.98	0.06	48,49,51,52	0
5	EDO	B	613	4/4	0.98	0.06	49,52,53,55	0
7	PGE	B	614	10/10	0.98	0.07	20,46,55,55	0
5	EDO	A	623	4/4	0.99	0.05	33,35,39,40	0
5	EDO	A	624	4/4	0.99	0.04	25,28,30,31	0
5	EDO	A	625	4/4	0.99	0.05	40,42,43,43	0
4	SAH	B	601	26/26	0.99	0.03	9,15,20,23	0
5	EDO	A	615	4/4	0.99	0.05	37,46,50,50	0
4	SAH	A	601	26/26	0.99	0.03	8,15,22,23	0
5	EDO	A	621	4/4	0.99	0.04	36,36,39,41	0
5	EDO	B	604	4/4	0.99	0.05	38,39,40,40	0
6	ACT	A	628	4/4	0.99	0.04	32,38,39,41	0
5	EDO	A	613	4/4	0.99	0.07	31,32,36,43	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 B 601:

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 ⓘ

There are no such residues in this entry.