



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2023 – 08:39 PM EDT

PDB ID : 1XQH  
Title : Crystal structure of a ternary complex of the methyltransferase SET9 (also known as SET7/9) with a P53 peptide and SAH  
Authors : Chuikov, S.; Kurash, J.K.; Wilson, J.R.; Xiao, B.; Justin, N.; Ivanov, G.S.; McKinney, K.; Tempst, P.; Prives, C.; Gamblin, S.J.; Barlev, N.A.; Reinberg, D.  
Deposited on : 2004-10-12  
Resolution : 1.75 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](mailto: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>.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

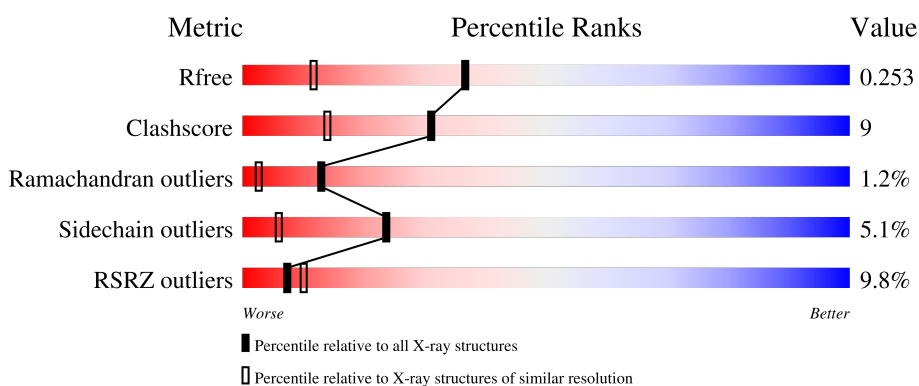
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	264	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">9%</div> <div style="flex-grow: 1; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 10px; background-color: red;"></div> <div style="position: absolute; top: 10px; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 20px; left: 0; width: 100%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 30px; left: 0; width: 100%; height: 10px; background-color: orange;"></div> <div style="position: absolute; top: 40px; left: 0; width: 100%; height: 10px; background-color: grey;"></div> </div> <div style="text-align: left;">79%</div> <div style="text-align: right;">13% • 5%</div> </div>
1	E	264	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">8%</div> <div style="flex-grow: 1; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 10px; background-color: red;"></div> <div style="position: absolute; top: 10px; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 20px; left: 0; width: 100%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 30px; left: 0; width: 100%; height: 10px; background-color: orange;"></div> <div style="position: absolute; top: 40px; left: 0; width: 100%; height: 10px; background-color: grey;"></div> </div> <div style="text-align: left;">78%</div> <div style="text-align: right;">12% • • 5%</div> </div>
2	B	10	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">20%</div> <div style="flex-grow: 1; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 10px; background-color: red;"></div> <div style="position: absolute; top: 10px; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 20px; left: 0; width: 100%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 30px; left: 0; width: 100%; height: 10px; background-color: orange;"></div> <div style="position: absolute; top: 40px; left: 0; width: 100%; height: 10px; background-color: grey;"></div> </div> <div style="text-align: left;">30%</div> <div style="text-align: right;">20% 10% 40%</div> </div>
2	F	10	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: right;">30%</div> <div style="flex-grow: 1; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 10px; background-color: red;"></div> <div style="position: absolute; top: 10px; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; top: 20px; left: 0; width: 100%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; top: 30px; left: 0; width: 100%; height: 10px; background-color: grey;"></div> </div> <div style="text-align: left;">50%</div> <div style="text-align: right;">10% 40%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SAH	A	1501	X	-	-	-
3	SAH	E	2501	X	-	-	-

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 4771 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Histone-lysine N-methyltransferase, H3 lysine-4 specific.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	250	1955	1236	319	388	12	0	1	0
1	E	250	1955	1236	319	388	12	0	1	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	103	GLY	-	cloning artifact	UNP Q8WTS6
A	104	PRO	-	cloning artifact	UNP Q8WTS6
A	105	LEU	-	cloning artifact	UNP Q8WTS6
A	106	GLY	-	cloning artifact	UNP Q8WTS6
A	107	SER	-	cloning artifact	UNP Q8WTS6
E	103	GLY	-	cloning artifact	UNP Q8WTS6
E	104	PRO	-	cloning artifact	UNP Q8WTS6
E	105	LEU	-	cloning artifact	UNP Q8WTS6
E	106	GLY	-	cloning artifact	UNP Q8WTS6
E	107	SER	-	cloning artifact	UNP Q8WTS6

- Molecule 2 is a protein called 9-mer peptide from tumor protein p53.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	6	46	30	9	7	0	0	0
2	F	6	46	30	9	7	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	372	MLZ	LYS	modified residue	UNP P04637
B	378	TYR	-	cloning artifact	UNP P04637

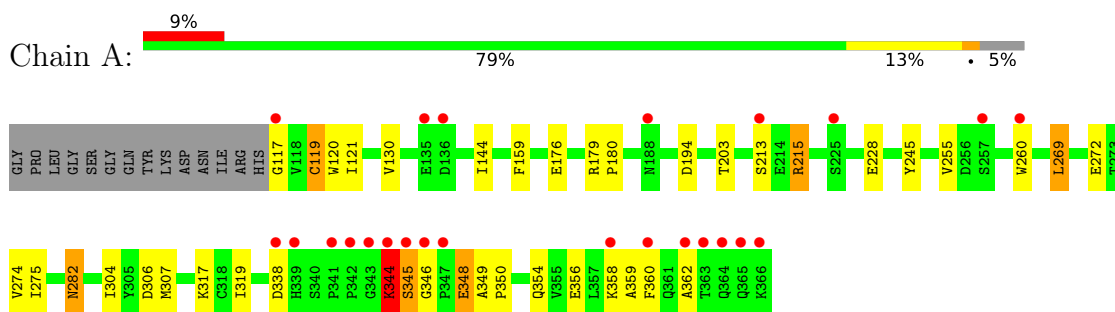
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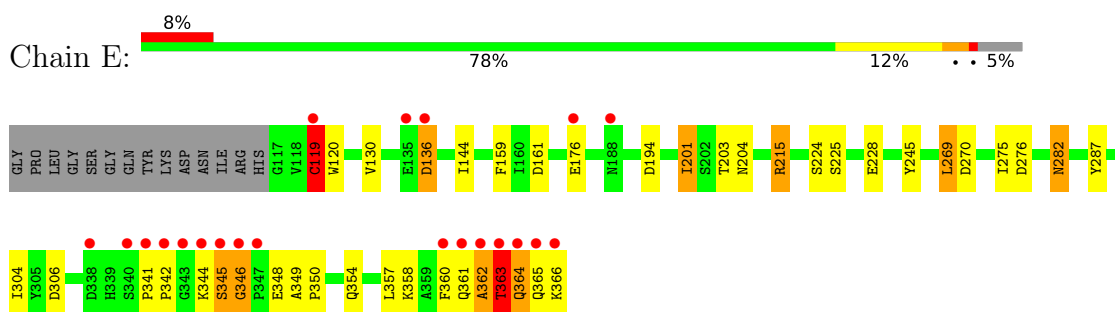
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

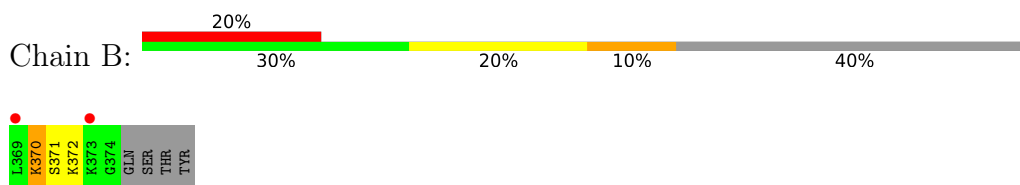
- Molecule 1: Histone-lysine N-methyltransferase, H3 lysine-4 specific



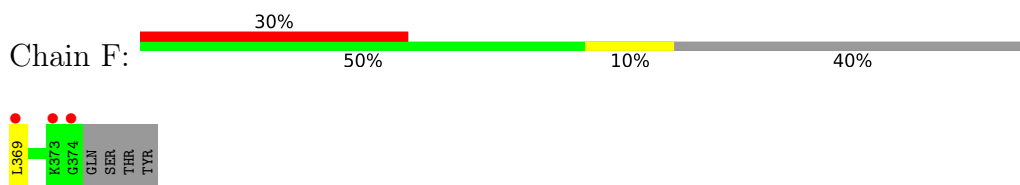
- Molecule 1: Histone-lysine N-methyltransferase, H3 lysine-4 specific



- Molecule 2: 9-mer peptide from tumor protein p53



- Molecule 2: 9-mer peptide from tumor protein p53



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	40.37Å 103.12Å 67.17Å 90.00° 90.04° 90.00°	Depositor
Resolution (Å)	20.00 – 1.75 19.81 – 1.75	Depositor EDS
% Data completeness (in resolution range)	94.7 (20.00-1.75) 94.6 (19.81-1.75)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 1.76Å)	Xtrriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.184 , 0.223 0.227 , 0.253	Depositor DCC
$R_{free}$ test set	2798 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.2	Xtrriage
Anisotropy	0.694	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 21.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.479 for h,-k,-l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4771	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	10.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.14% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MLZ, 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	A	0.48	0/2013	0.82	8/2738 (0.3%)
1	E	0.47	0/2013	0.83	11/2738 (0.4%)
2	B	0.57	0/34	0.86	0/40
2	F	0.71	0/34	1.29	0/40
All	All	0.48	0/4094	0.83	19/5556 (0.3%)

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	B	0	1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	346	GLY	N-CA-C	-9.36	89.69	113.10
1	A	215	ARG	NE-CZ-NH2	-9.18	115.71	120.30
1	E	215	ARG	NE-CZ-NH2	-9.17	115.71	120.30
1	E	363	THR	N-CA-C	-8.16	88.97	111.00
1	A	215	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	E	215	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	E	161	ASP	CB-CG-OD2	5.93	123.64	118.30
1	E	119[A]	CYS	CA-CB-SG	5.77	124.38	114.00
1	E	119[B]	CYS	CA-CB-SG	5.77	124.38	114.00
1	A	306	ASP	CB-CG-OD2	5.61	123.35	118.30
1	E	136	ASP	CB-CG-OD2	5.53	123.28	118.30
1	A	119[A]	CYS	CA-CB-SG	5.48	123.86	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119[B]	CYS	CA-CB-SG	5.48	123.86	114.00
1	E	194	ASP	CB-CG-OD2	5.38	123.14	118.30
1	E	270	ASP	CB-CG-OD2	5.30	123.07	118.30
1	E	306	ASP	CB-CG-OD2	5.24	123.02	118.30
1	A	338	ASP	CB-CG-OD2	5.23	123.00	118.30
1	E	276	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	194	ASP	CB-CG-OD2	5.12	122.91	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	371	SER	Mainchain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1955	0	1845	33	0
1	E	1955	0	1845	38	1
2	B	46	0	58	1	0
2	F	46	0	58	1	0
3	A	26	0	15	5	0
3	E	26	0	15	2	0
4	A	351	0	0	6	1
4	B	7	0	0	0	0
4	E	352	0	0	7	0
4	F	7	0	0	0	0
All	All	4771	0	3836	72	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 9.

All (72) 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:E:228:GLU:O	3:E:2501:SAH:HA	1.75	0.87
1:E:201:ILE:HD13	1:E:201:ILE:O	1.75	0.86
1:A:228:GLU:O	3:A:1501:SAH:HA	1.76	0.85
1:E:120:TRP:CE3	1:E:130:VAL:HG21	2.12	0.84
1:E:357:LEU:O	1:E:361:GLN:HB2	1.77	0.83
1:E:282:ASN:HD22	1:E:282:ASN:H	1.27	0.81
1:A:282:ASN:HD22	1:A:282:ASN:H	1.31	0.79
1:A:228:GLU:HB2	3:A:1501:SAH:O	1.83	0.78
1:A:120:TRP:CE3	1:A:130:VAL:HG21	2.23	0.73
1:E:120:TRP:CE3	1:E:130:VAL:CG2	2.74	0.71
1:A:120:TRP:CE3	1:A:130:VAL:CG2	2.75	0.69
1:E:361:GLN:O	1:E:362:ALA:HB3	1.92	0.69
1:E:120:TRP:CZ3	1:E:130:VAL:HG21	2.28	0.69
1:E:341:PRO:CD	1:E:346:GLY:O	2.41	0.68
1:A:120:TRP:CZ3	1:A:130:VAL:HG21	2.28	0.67
1:A:215:ARG:NH2	4:A:1512:HOH:O	2.24	0.66
1:E:341:PRO:CG	1:E:346:GLY:O	2.45	0.64
1:A:307:MET:SD	1:A:317:LYS:HE2	2.38	0.64
1:E:341:PRO:HG2	1:E:346:GLY:O	1.99	0.63
1:E:215:ARG:NH2	4:E:2664:HOH:O	2.33	0.62
1:E:228:GLU:HB2	3:E:2501:SAH:O	1.99	0.62
1:A:344:LYS:HE3	1:A:345:SER:H	1.66	0.61
1:E:269:LEU:HG	1:E:275:ILE:HD11	1.85	0.59
1:A:176:GLU:HG2	4:A:1622:HOH:O	2.03	0.59
1:A:356:GLU:HG3	4:A:1638:HOH:O	2.04	0.58
1:E:341:PRO:HD2	1:E:346:GLY:O	2.08	0.54
1:E:361:GLN:O	1:E:362:ALA:CB	2.54	0.54
1:E:203:THR:HG21	4:E:2843:HOH:O	2.07	0.54
1:A:356:GLU:OE1	3:A:1501:SAH:N6	2.40	0.53
1:E:282:ASN:H	1:E:282:ASN:ND2	2.03	0.53
1:A:319:ILE:HD12	1:A:319:ILE:N	2.24	0.53
1:A:120:TRP:CE3	1:A:130:VAL:HG22	2.44	0.53
1:A:344:LYS:HA	1:A:344:LYS:CE	2.34	0.52
1:E:201:ILE:HD13	1:E:201:ILE:C	2.30	0.52
1:E:341:PRO:HD2	1:E:346:GLY:C	2.29	0.52
1:A:228:GLU:CB	3:A:1501:SAH:O	2.56	0.50
1:E:357:LEU:O	1:E:361:GLN:CB	2.53	0.50
4:E:2816:HOH:O	2:F:369:LEU:CD2	2.60	0.49
1:E:269:LEU:HG	1:E:275:ILE:CD1	2.43	0.48
1:A:360:PHE:O	1:A:362:ALA:O	2.32	0.48
1:E:201:ILE:HD12	1:E:287:TYR:CE1	2.48	0.47
1:A:282:ASN:H	1:A:282:ASN:ND2	2.06	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:ILE:HG13	4:A:1524:HOH:O	2.14	0.47
1:E:204:ASN:HB3	4:E:2639:HOH:O	2.15	0.46
1:E:224:SER:HB3	4:E:2848:HOH:O	2.15	0.46
1:A:344:LYS:HE3	1:A:344:LYS:HA	1.98	0.45
1:A:359:ALA:O	1:A:362:ALA:O	2.35	0.45
1:A:349:ALA:HB1	1:A:350:PRO:HD2	1.99	0.45
3:A:1501:SAH:HG2	3:A:1501:SAH:O4'	2.16	0.44
1:E:364:GLN:NE2	1:E:366:LYS:HB2	2.33	0.44
1:A:144:ILE:HD12	1:A:159:PHE:HB2	2.01	0.43
1:E:341:PRO:HA	1:E:342:PRO:HD3	1.85	0.43
1:A:203:THR:HG21	4:A:1848:HOH:O	2.19	0.43
1:E:282:ASN:HD22	1:E:282:ASN:N	2.05	0.43
1:E:354:GLN:O	1:E:358:LYS:HG3	2.19	0.43
1:A:121:ILE:HG12	1:E:119[A]:CYS:SG	2.59	0.43
1:A:354:GLN:O	1:A:358:LYS:HG3	2.18	0.43
1:A:260:TRP:CH2	2:B:370:LYS:HA	2.54	0.43
1:E:360:PHE:O	1:E:362:ALA:N	2.52	0.43
1:E:357:LEU:O	1:E:361:GLN:N	2.42	0.43
1:A:344:LYS:HE3	1:A:345:SER:N	2.31	0.42
1:E:225:SER:HB2	4:E:2611:HOH:O	2.19	0.42
1:A:260:TRP:NE1	1:A:348:GLU:OE1	2.45	0.42
1:E:120:TRP:CE3	1:E:130:VAL:HG22	2.53	0.42
1:E:144:ILE:HB	1:E:159:PHE:CD1	2.54	0.42
1:E:304:ILE:HG13	4:E:2524:HOH:O	2.20	0.41
1:E:360:PHE:CZ	1:E:364:GLN:OE1	2.74	0.41
1:A:269:LEU:HG	1:A:275:ILE:HD11	2.02	0.41
1:A:179:ARG:HA	1:A:180:PRO:HD3	1.96	0.41
1:E:349:ALA:HB1	1:E:350:PRO:HD2	2.03	0.40
1:A:255:VAL:HG21	1:A:274:VAL:HG11	2.03	0.40
1:A:117:GLY:N	4:A:1766:HOH:O	2.54	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)
1:E:366:LYS:NZ	4:A:1845:HOH:O[2_555]	2.12	0.08

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	249/264 (94%)	236 (95%)	12 (5%)	1 (0%)	34	17
1	E	249/264 (94%)	234 (94%)	11 (4%)	4 (2%)	9	1
2	B	3/10 (30%)	2 (67%)	0	1 (33%)	0	0
2	F	3/10 (30%)	2 (67%)	1 (33%)	0	100	100
All	All	504/548 (92%)	474 (94%)	24 (5%)	6 (1%)	13	3

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	370	LYS
1	E	346	GLY
1	E	362	ALA
1	E	363	THR
1	A	344	LYS
1	E	345	SER

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	214/224 (96%)	204 (95%)	10 (5%)	26	7
1	E	214/224 (96%)	200 (94%)	14 (6%)	17	3
2	B	4/8 (50%)	4 (100%)	0	100	100
2	F	4/8 (50%)	4 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	436/464 (94%)	412 (94%)	24 (6%)	24 5

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119[A]	CYS
1	A	119[B]	CYS
1	A	213	SER
1	A	245	TYR
1	A	269	LEU
1	A	272	GLU
1	A	282	ASN
1	A	344	LYS
1	A	345	SER
1	A	348	GLU
1	E	119[A]	CYS
1	E	119[B]	CYS
1	E	136	ASP
1	E	176	GLU
1	E	201	ILE
1	E	245	TYR
1	E	269	LEU
1	E	282	ASN
1	E	344	LYS
1	E	345	SER
1	E	348	GLU
1	E	363	THR
1	E	364	GLN
1	E	365	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	239	ASN
1	A	282	ASN
1	E	282	ASN
1	E	364	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

2 non-standard protein/DNA/RNA residues 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
2	MLZ	F	372	2	8,9,10	0.63	0	4,9,11	1.36	0
2	MLZ	B	372	2	8,9,10	0.60	0	4,9,11	1.30	1 (25%)

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
2	MLZ	F	372	2	-	0/7/8/10	-
2	MLZ	B	372	2	-	1/7/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	372	MLZ	CM-NZ-CE	2.03	117.80	111.95

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	372	MLZ	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SAH	E	2501	-	24,28,28	4.73	11 (45%)	25,40,40	2.61	10 (40%)
3	SAH	A	1501	-	24,28,28	4.81	12 (50%)	25,40,40	2.55	10 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SAH	E	2501	-	3/3/6/6	8/11/31/31	0/3/3/3
3	SAH	A	1501	-	2/2/6/6	7/11/31/31	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1501	SAH	C2'-C1'	-14.36	1.32	1.53
3	E	2501	SAH	C2'-C1'	-14.03	1.32	1.53
3	A	1501	SAH	O2'-C2'	-8.66	1.22	1.43
3	E	2501	SAH	O2'-C2'	-8.50	1.23	1.43
3	A	1501	SAH	O3'-C3'	-7.80	1.24	1.43
3	E	2501	SAH	O3'-C3'	-7.55	1.25	1.43
3	A	1501	SAH	C2'-C3'	-7.15	1.33	1.53
3	E	2501	SAH	C2'-C3'	-7.09	1.33	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2501	SAH	C3'-C4'	-6.81	1.35	1.53
3	A	1501	SAH	C3'-C4'	-6.72	1.35	1.53
3	A	1501	SAH	O-C	6.58	1.42	1.22
3	E	2501	SAH	O-C	6.30	1.41	1.22
3	E	2501	SAH	OXT-C	4.31	1.44	1.30
3	A	1501	SAH	OXT-C	4.11	1.44	1.30
3	E	2501	SAH	C5'-C4'	-4.01	1.36	1.52
3	A	1501	SAH	C5'-C4'	-3.98	1.36	1.52
3	A	1501	SAH	C5'-SD	-3.84	1.65	1.80
3	E	2501	SAH	C5'-SD	-3.81	1.65	1.80
3	E	2501	SAH	O4'-C1'	2.94	1.45	1.41
3	A	1501	SAH	O4'-C1'	2.71	1.44	1.41
3	A	1501	SAH	C5-C4	2.66	1.48	1.40
3	E	2501	SAH	C5-C4	2.48	1.47	1.40
3	A	1501	SAH	C2-N3	2.15	1.35	1.32

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	2501	SAH	O3'-C3'-C4'	6.11	128.73	111.05
3	A	1501	SAH	O3'-C3'-C4'	5.91	128.13	111.05
3	E	2501	SAH	C5'-C4'-C3'	5.85	129.68	115.06
3	A	1501	SAH	C5'-C4'-C3'	5.49	128.77	115.06
3	A	1501	SAH	O4'-C4'-C5'	4.47	120.35	108.83
3	E	2501	SAH	O4'-C4'-C5'	4.01	119.15	108.83
3	E	2501	SAH	C3'-C2'-C1'	3.49	106.23	100.98
3	E	2501	SAH	C4'-C5'-SD	3.42	126.07	113.78
3	E	2501	SAH	N3-C2-N1	-3.34	123.45	128.68
3	A	1501	SAH	C3'-C2'-C1'	3.17	105.75	100.98
3	A	1501	SAH	N3-C2-N1	-3.15	123.76	128.68
3	A	1501	SAH	C4'-C5'-SD	3.09	124.89	113.78
3	E	2501	SAH	O2'-C2'-C1'	2.92	121.63	110.85
3	A	1501	SAH	O3'-C3'-C2'	2.91	121.25	111.82
3	E	2501	SAH	C2'-C3'-C4'	2.71	107.91	102.64
3	A	1501	SAH	C2'-C3'-C4'	2.63	107.76	102.64
3	E	2501	SAH	O3'-C3'-C2'	2.61	120.27	111.82
3	A	1501	SAH	O2'-C2'-C1'	2.42	119.78	110.85
3	A	1501	SAH	CB-CG-SD	-2.29	108.17	113.31
3	E	2501	SAH	CB-CG-SD	-2.05	108.71	113.31

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1501	SAH	C3'
3	A	1501	SAH	CA
3	E	2501	SAH	C3'
3	E	2501	SAH	CA
3	E	2501	SAH	C4'

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1501	SAH	N-CA-CB-CG
3	A	1501	SAH	O-C-CA-N
3	A	1501	SAH	CA-CB-CG-SD
3	E	2501	SAH	N-CA-CB-CG
3	E	2501	SAH	CA-CB-CG-SD
3	E	2501	SAH	OXT-C-CA-N
3	A	1501	SAH	OXT-C-CA-N
3	E	2501	SAH	O-C-CA-CB
3	E	2501	SAH	O-C-CA-N
3	A	1501	SAH	C3'-C4'-C5'-SD
3	E	2501	SAH	C3'-C4'-C5'-SD
3	A	1501	SAH	O-C-CA-CB
3	E	2501	SAH	OXT-C-CA-CB
3	E	2501	SAH	CB-CG-SD-C5'
3	A	1501	SAH	CB-CG-SD-C5'

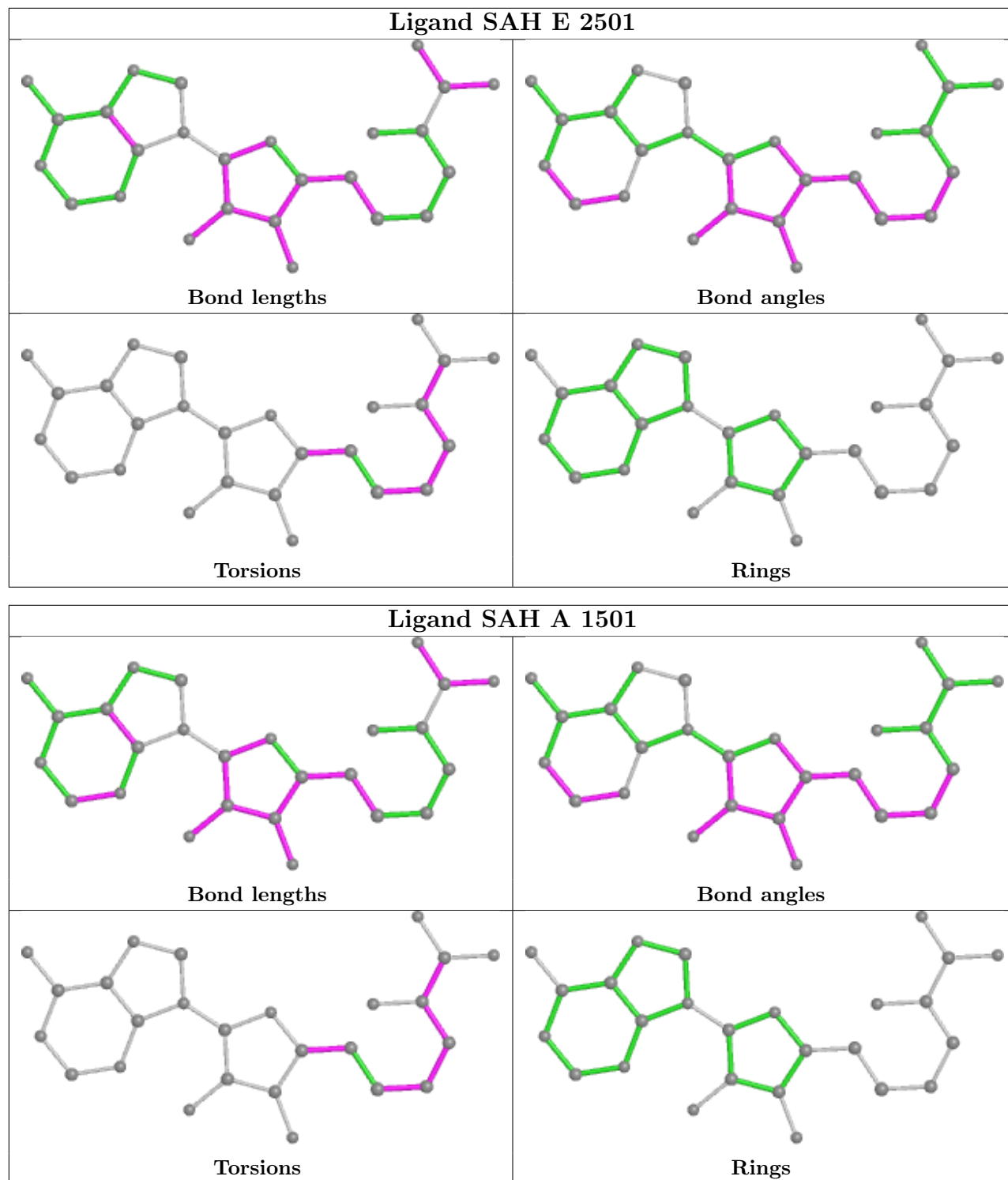
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2501	SAH	2	0
3	A	1501	SAH	5	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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	372:MLZ	C	373:LYS	N	1.63

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	250/264 (94%)	0.68	24 (9%) <b>8</b> <b>10</b>	2, 4, 21, 29	1 (0%)
1	E	250/264 (94%)	0.80	21 (8%) <b>11</b> <b>14</b>	2, 4, 22, 52	1 (0%)
2	B	5/10 (50%)	2.93	2 (40%) <b>0</b> <b>0</b>	8, 10, 26, 26	0
2	F	5/10 (50%)	2.73	3 (60%) <b>0</b> <b>0</b>	9, 11, 28, 28	0
All	All	510/548 (93%)	0.78	50 (9%) <b>7</b> <b>10</b>	2, 4, 24, 52	2 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	369	LEU	9.6
1	E	345	SER	9.3
1	E	342	PRO	7.8
1	E	344	LYS	7.4
1	E	343	GLY	7.4
1	A	343	GLY	7.1
1	E	346	GLY	6.9
2	F	369	LEU	6.8
1	E	366	LYS	6.5
1	E	363	THR	6.2
1	A	342	PRO	6.1
1	A	344	LYS	5.9
1	A	345	SER	4.8
1	E	135	GLU	4.4
1	A	363	THR	4.3
1	A	135	GLU	4.2
1	A	362	ALA	4.1
1	A	366	LYS	4.1
1	E	361	GLN	3.9
1	E	136	ASP	3.9
1	A	346	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
2	F	374	GLY	3.5
1	E	365	GLN	3.4
1	A	136	ASP	3.2
2	F	373	LYS	3.1
1	A	257	SER	3.1
1	E	341	PRO	3.1
1	E	119[A]	CYS	2.9
1	E	347	PRO	2.9
1	A	364	GLN	2.9
1	A	260	TRP	2.9
1	A	360	PHE	2.8
1	A	347	PRO	2.8
1	E	188	ASN	2.7
1	E	338	ASP	2.6
1	A	117	GLY	2.6
1	A	341	PRO	2.6
1	A	225	SER	2.5
1	E	360	PHE	2.4
1	A	339	HIS	2.4
1	A	188	ASN	2.4
1	E	340	SER	2.3
1	A	365	GLN	2.3
2	B	373	LYS	2.2
1	E	364	GLN	2.2
1	A	338	ASP	2.2
1	E	362	ALA	2.2
1	A	213	SER	2.1
1	A	358	LYS	2.1
1	E	176	GLU	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	MLZ	B	372	10/11	0.90	0.11	2,2,3,3	0
2	MLZ	F	372	10/11	0.94	0.10	2,2,2,2	0

### 6.3 Carbohydrates [i](#)

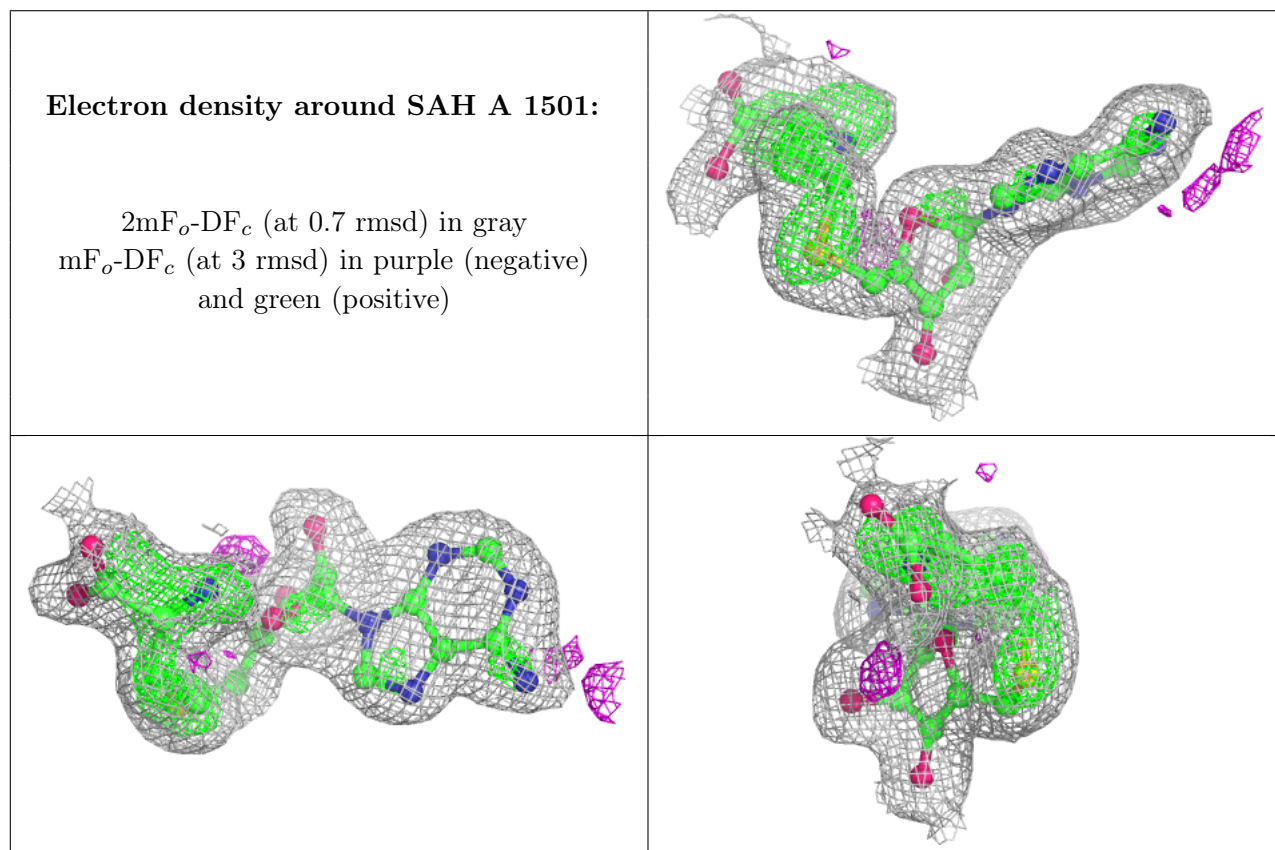
There are no monosaccharides in this entry.

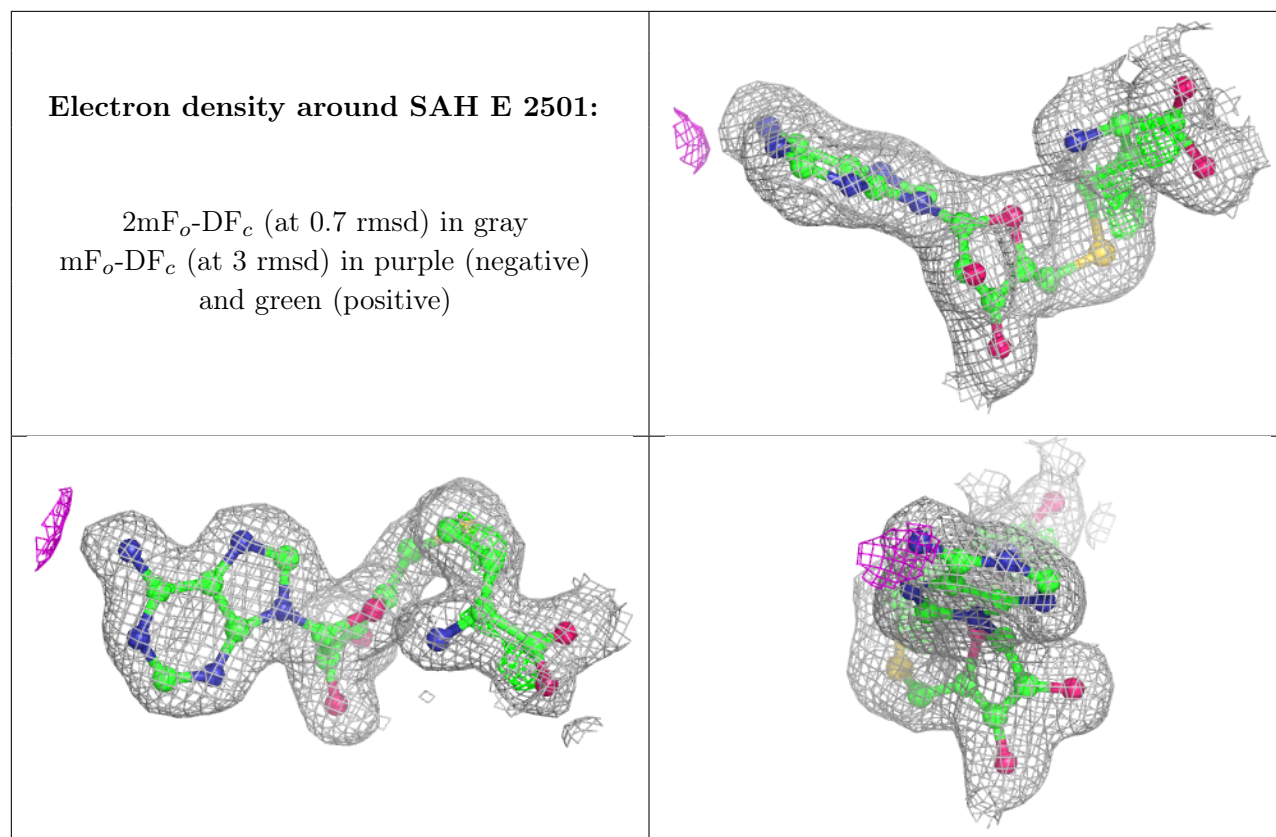
### 6.4 Ligands [i](#)

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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SAH	A	1501	26/26	0.78	0.23	35,38,41,42	0
3	SAH	E	2501	26/26	0.93	0.09	2,3,8,8	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.