



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2025 – 02:36 PM EDT

PDB ID : 5KJH  
Title : Crystal structure of an active polycomb repressive complex 2 in the stimulated state  
Authors : Jiao, L.; Liu, X.  
Deposited on : 2016-06-20  
Resolution : 2.27 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

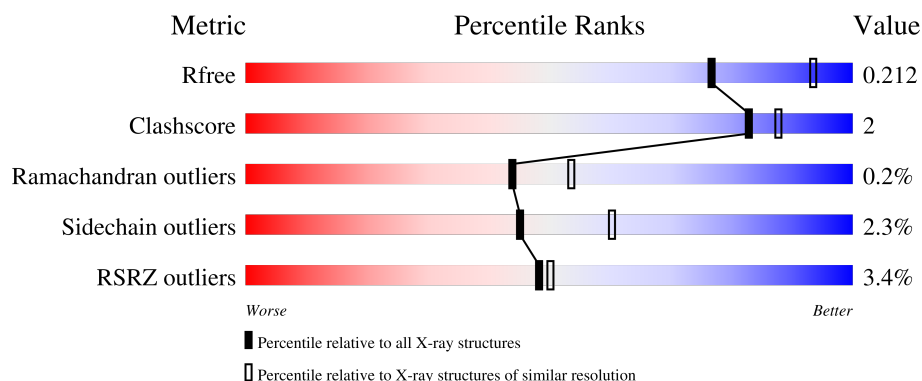
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.27 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))
$R_{free}$	164625	8487 (2.30-2.26)
Clashscore	180529	9437 (2.30-2.26)
Ramachandran outliers	177936	9341 (2.30-2.26)
Sidechain outliers	177891	9342 (2.30-2.26)
RSRZ outliers	164620	8487 (2.30-2.26)

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	605	
2	B	937	
3	D	11	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10902 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 putative polycomb protein Eed.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	0	0
			3782	2417	647	699	19			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-39	MET	-	expression tag	UNP G0S8H7
A	-38	ALA	-	expression tag	UNP G0S8H7
A	-37	SER	-	expression tag	UNP G0S8H7
A	-36	ALA	-	expression tag	UNP G0S8H7
A	-35	TRP	-	expression tag	UNP G0S8H7
A	-34	SER	-	expression tag	UNP G0S8H7
A	-33	HIS	-	expression tag	UNP G0S8H7
A	-32	PRO	-	expression tag	UNP G0S8H7
A	-31	GLN	-	expression tag	UNP G0S8H7
A	-30	PHE	-	expression tag	UNP G0S8H7
A	-29	GLU	-	expression tag	UNP G0S8H7
A	-28	LYS	-	expression tag	UNP G0S8H7
A	-27	GLY	-	expression tag	UNP G0S8H7
A	-26	GLY	-	expression tag	UNP G0S8H7
A	-25	GLY	-	expression tag	UNP G0S8H7
A	-24	SER	-	expression tag	UNP G0S8H7
A	-23	GLY	-	expression tag	UNP G0S8H7
A	-22	GLY	-	expression tag	UNP G0S8H7
A	-21	GLY	-	expression tag	UNP G0S8H7
A	-20	SER	-	expression tag	UNP G0S8H7
A	-19	GLY	-	expression tag	UNP G0S8H7
A	-18	GLY	-	expression tag	UNP G0S8H7
A	-17	SER	-	expression tag	UNP G0S8H7
A	-16	ALA	-	expression tag	UNP G0S8H7
A	-15	TRP	-	expression tag	UNP G0S8H7
A	-14	SER	-	expression tag	UNP G0S8H7
A	-13	HIS	-	expression tag	UNP G0S8H7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	PRO	-	expression tag	UNP G0S8H7
A	-11	GLN	-	expression tag	UNP G0S8H7
A	-10	PHE	-	expression tag	UNP G0S8H7
A	-9	GLU	-	expression tag	UNP G0S8H7
A	-8	LYS	-	expression tag	UNP G0S8H7
A	-7	LEU	-	expression tag	UNP G0S8H7
A	-6	GLU	-	expression tag	UNP G0S8H7
A	-5	VAL	-	expression tag	UNP G0S8H7
A	-4	LEU	-	expression tag	UNP G0S8H7
A	-3	PHE	-	expression tag	UNP G0S8H7
A	-2	GLN	-	expression tag	UNP G0S8H7
A	-1	GLY	-	expression tag	UNP G0S8H7
A	0	PRO	-	expression tag	UNP G0S8H7

- Molecule 2 is a protein called Putative uncharacterized protein,Zinc finger domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	807	Total	C	N	O	S	0	0	0
			6498	4104	1168	1185	41			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	182	SER	-	expression tag	UNP G0SDW4
B	183	ASN	-	expression tag	UNP G0SDW4
B	184	HIS	-	expression tag	UNP G0SDW4
B	185	HIS	-	expression tag	UNP G0SDW4
B	186	HIS	-	expression tag	UNP G0SDW4
B	187	HIS	-	expression tag	UNP G0SDW4
B	188	HIS	-	expression tag	UNP G0SDW4
B	189	HIS	-	expression tag	UNP G0SDW4
B	190	ALA	-	expression tag	UNP G0SDW4
B	2524	LEU	ALA	linker	UNP G0SDW4
B	2525	VAL	ALA	linker	UNP G0SDW4
B	2526	PRO	-	linker	UNP G0SDW4
B	2527	ARG	-	linker	UNP G0SDW4
B	2528	GLY	-	linker	UNP G0SDW4
B	2529	SER	-	linker	UNP G0SDW4

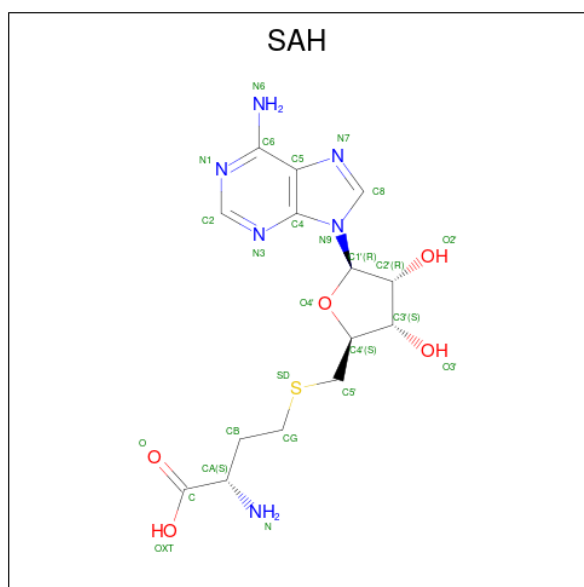
- Molecule 3 is a protein called Peptide H3K27me3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	8	Total	C	N	O	0	0	0
			60	38	13	9			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	8	Total	Zn	0	0
			8	8		

- Molecule 5 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C<sub>14</sub>H<sub>20</sub>N<sub>6</sub>O<sub>5</sub>S).



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

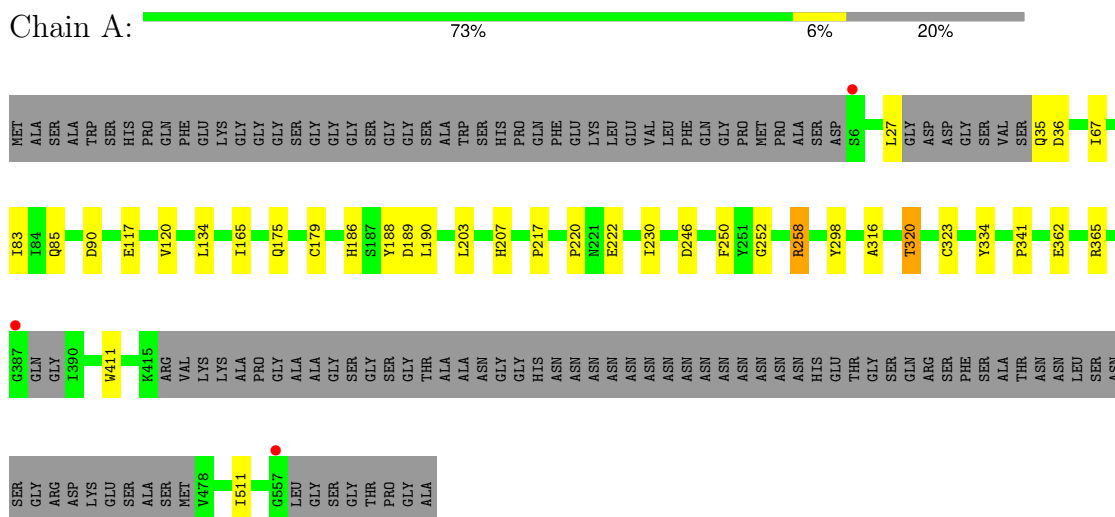
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	246	Total	O	0	0
			246	246		
6	B	278	Total	O	0	0
			278	278		
6	D	4	Total	O	0	0
			4	4		

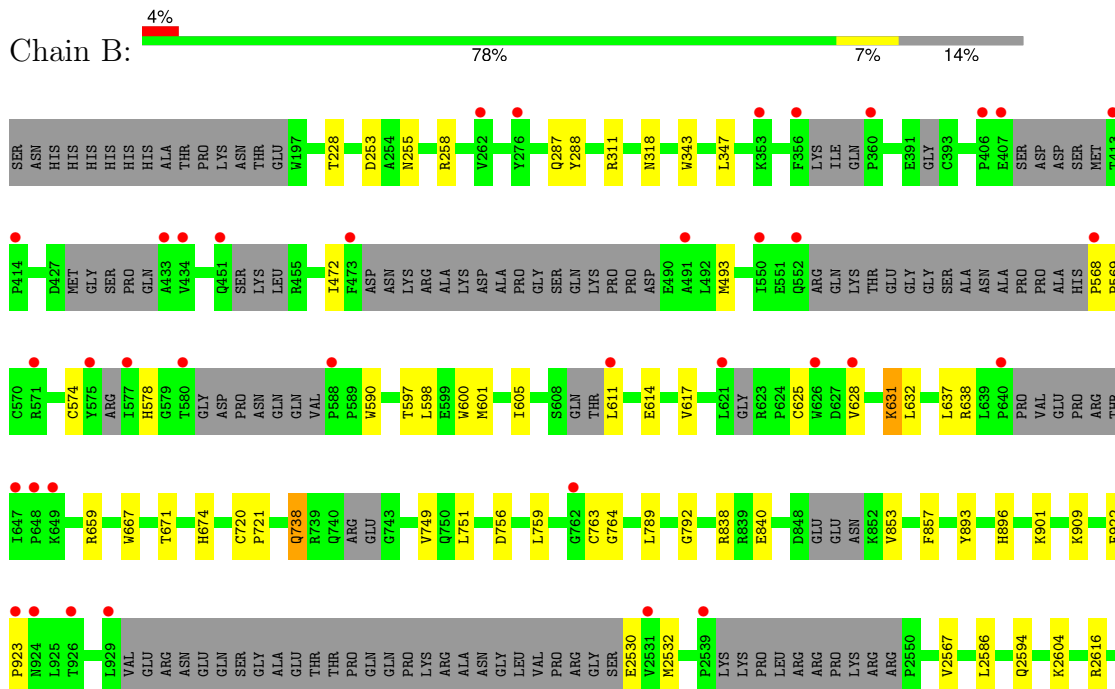
### 3 Residue-property plots

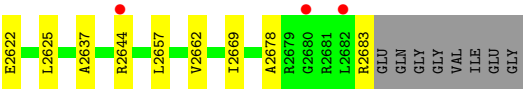
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

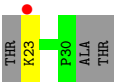


- Molecule 2: Putative uncharacterized protein,Zinc finger domain-containing protein





● Molecule 3: Peptide H3K27me3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.55Å 74.61Å 128.51Å 90.00° 107.70° 90.00°	Depositor
Resolution (Å)	45.84 – 2.27 45.84 – 2.27	Depositor EDS
% Data completeness (in resolution range)	90.7 (45.84-2.27) 90.7 (45.84-2.27)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.04	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.24 (at 2.27Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, $R_{free}$	0.168 , 0.213 0.169 , 0.212	Depositor DCC
$R_{free}$ test set	3148 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.9	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 59.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	10902	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SAH, ZN, M3L

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	0.53	0/3894	0.68	0/5306
2	B	0.49	0/6643	0.65	0/8968
3	D	0.53	0/48	0.62	0/63
All	All	0.51	0/10585	0.66	0/14337

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

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	3782	0	3634	19	0
2	B	6498	0	6380	31	1
3	D	60	0	70	0	0
4	B	8	0	0	0	0
5	B	26	0	19	1	0
6	A	246	0	0	0	0
6	B	278	0	0	0	0
6	D	4	0	0	0	0
All	All	10902	0	10103	48	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 2.

All (48) 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:A:246:ASP:OD1	1:A:258:ARG:HD3	1.80	0.80
2:B:2622:GLU:HB2	2:B:2662:VAL:HG13	1.73	0.69
2:B:318:ASN:HB3	2:B:838:ARG:HH12	1.64	0.63
2:B:738:GLN:HA	2:B:749:VAL:HG11	1.81	0.62
1:A:189:ASP:HB2	1:A:207:HIS:HD2	1.67	0.60
2:B:253:ASP:HB3	2:B:255:ASN:OD1	2.04	0.57
2:B:574:CYS:HA	2:B:625:CYS:HB3	1.85	0.57
2:B:763:CYS:H	2:B:764:GLY:HA2	1.72	0.53
2:B:763:CYS:N	2:B:764:GLY:HA2	2.24	0.53
1:A:186:HIS:CG	1:A:190:LEU:HD21	2.44	0.52
1:A:120:VAL:HB	1:A:134:LEU:HB2	1.93	0.50
2:B:611:LEU:HD13	2:B:2669:ILE:HG13	1.93	0.50
1:A:217:PRO:HD3	1:A:230:ILE:HD11	1.94	0.49
2:B:601:MET:O	2:B:605:ILE:HG12	2.12	0.49
2:B:789:LEU:HD11	2:B:901:LYS:HB3	1.95	0.47
1:A:203:LEU:HG	1:A:250:PHE:CE2	2.50	0.47
1:A:320:THR:CG2	1:A:320:THR:O	2.62	0.47
2:B:597:THR:HA	2:B:600:TRP:CE2	2.51	0.46
2:B:632:LEU:HD12	2:B:637:LEU:HD12	1.98	0.46
2:B:311:ARG:HH22	2:B:792:GLY:HA3	1.81	0.46
1:A:186:HIS:CD2	1:A:190:LEU:HD21	2.51	0.46
2:B:2625:LEU:HD21	2:B:2657:LEU:HD13	1.98	0.46
1:A:316:ALA:HB1	1:A:511:ILE:HD11	1.99	0.45
2:B:756:ASP:HB3	2:B:759:LEU:HB2	1.99	0.44
2:B:893:TYR:CE2	2:B:896:HIS:HA	2.53	0.44
1:A:67:ILE:HB	1:A:85:GLN:HB3	1.98	0.44
1:A:189:ASP:HB2	1:A:207:HIS:CD2	2.50	0.44
2:B:2637:ALA:HB1	2:B:2678:ALA:HB2	2.01	0.43
1:A:320:THR:HG23	1:A:323:CYS:SG	2.59	0.42
2:B:614:GLU:HB3	2:B:625:CYS:SG	2.60	0.42
2:B:343:TRP:O	2:B:347:LEU:HG	2.20	0.42
2:B:720:CYS:HA	2:B:721:PRO:HD3	1.93	0.42
2:B:667:TRP:O	2:B:671:THR:HG22	2.19	0.42
2:B:2586:LEU:HD11	2:B:2616:ARG:HD3	2.01	0.41
1:A:165:ILE:HB	1:A:179:CYS:HB3	2.03	0.41
1:A:362:GLU:HB2	1:A:411:TRP:HZ2	1.86	0.41
2:B:258:ARG:HG2	2:B:287:GLN:OE1	2.20	0.41
2:B:853:VAL:HG13	5:B:8009:SAH:H4'	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:TYR:O	1:A:341:PRO:HA	2.21	0.41
2:B:590:TRP:CG	2:B:631:LYS:HD3	2.56	0.41
1:A:220:PRO:HB2	1:A:222:GLU:HG2	2.02	0.41
2:B:568:PRO:HA	2:B:569:PRO:HD3	1.96	0.41
2:B:2594:GLN:HA	2:B:2604:LYS:HD3	2.01	0.41
1:A:83:ILE:HB	2:B:288:TYR:CE2	2.55	0.41
1:A:320:THR:O	1:A:320:THR:HG22	2.21	0.41
1:A:252:GLY:HA3	2:B:228:THR:HG23	2.01	0.40
2:B:674:HIS:HB3	2:B:751:LEU:HA	2.03	0.40
2:B:598:LEU:HA	2:B:617:VAL:HG21	2.02	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)
2:B:909:LYS:CE	2:B:2532:MET:CE[2_9510]	2.19	0.01

## 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	A	473/605 (78%)	464 (98%)	9 (2%)	0	100	100
2	B	773/937 (82%)	741 (96%)	30 (4%)	2 (0%)	37	45
3	D	5/11 (46%)	5 (100%)	0	0	100	100
All	All	1251/1553 (81%)	1210 (97%)	39 (3%)	2 (0%)	44	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	923	PRO
2	B	472	ILE

### 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	A	406/495 (82%)	395 (97%)	11 (3%)	40	54
2	B	707/816 (87%)	693 (98%)	14 (2%)	50	65
3	D	4/6 (67%)	3 (75%)	1 (25%)	0	0
All	All	1117/1317 (85%)	1091 (98%)	26 (2%)	45	60

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	35	GLN
1	A	36	ASP
1	A	90	ASP
1	A	117	GLU
1	A	175	GLN
1	A	188	TYR
1	A	258	ARG
1	A	298	TYR
1	A	320	THR
1	A	365	ARG
2	B	493	MET
2	B	578	HIS
2	B	628	VAL
2	B	631	LYS
2	B	638	ARG
2	B	659	ARG
2	B	738	GLN
2	B	840	GLU
2	B	857	PHE
2	B	922	PHE
2	B	2530	GLU
2	B	2567	VAL
2	B	2644	ARG
2	B	2683	ARG
3	D	23	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	M3L	D	27	3	10,11,12	0.47	0	9,14,16	0.29	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
3	M3L	D	27	3	-	0/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 8 are monoatomic - leaving 1 for Mogul analysis.

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	8009	-	23,28,28	0.72	0	22,40,40	1.00	2 (9%)

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	8009	-	-	5/11/31/31	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	8009	SAH	CB-CA-N	2.60	116.89	110.12
5	B	8009	SAH	C5-C6-N6	2.16	123.59	120.31

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	8009	SAH	C3'-C4'-C5'-SD
5	B	8009	SAH	O-C-CA-CB
5	B	8009	SAH	OXT-C-CA-CB
5	B	8009	SAH	O-C-CA-N

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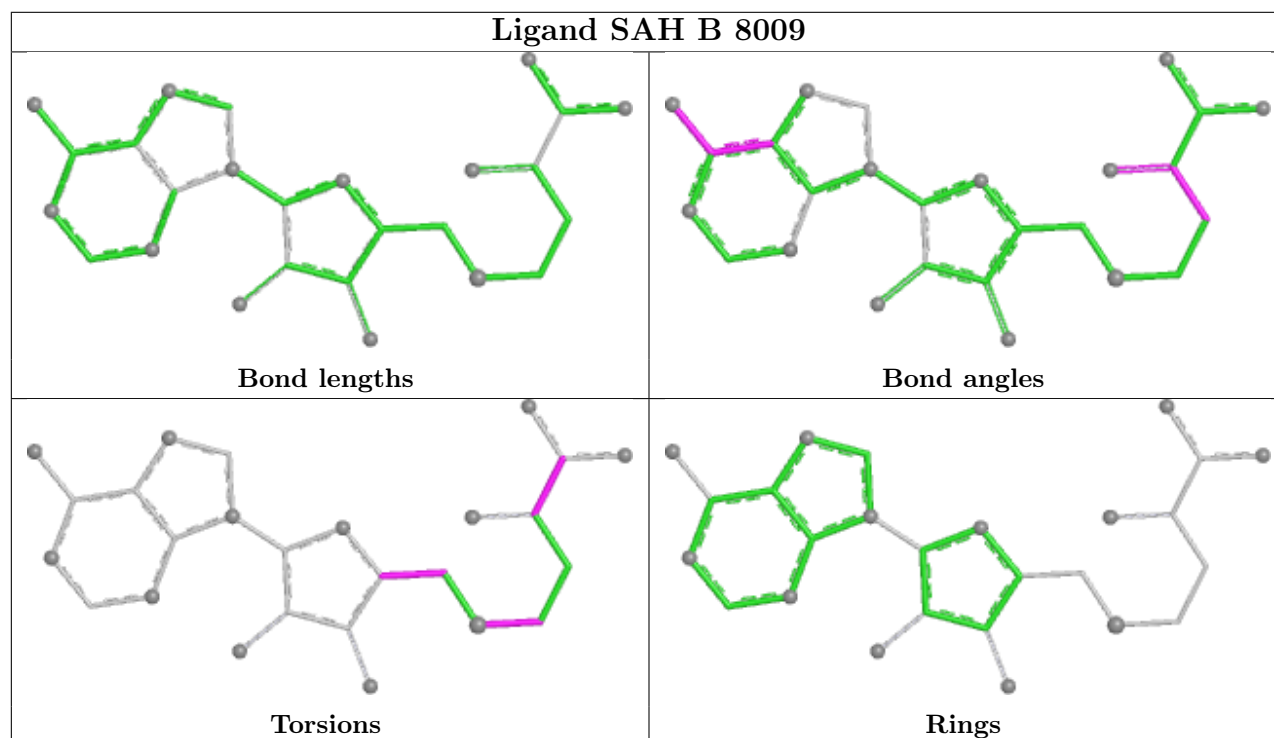
Mol	Chain	Res	Type	Atoms
5	B	8009	SAH	CB-CG-SD-C5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	8009	SAH	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, 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	481/605 (79%)	-0.58	3 (0%) 85 86	14, 28, 61, 83	0
2	B	807/937 (86%)	0.08	40 (4%) 35 36	18, 45, 85, 123	0
3	D	7/11 (63%)	0.63	1 (14%) 7 8	31, 36, 50, 76	0
All	All	1295/1553 (83%)	-0.16	44 (3%) 48 50	14, 38, 80, 123	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	473	PHE	5.2
1	A	387	GLY	5.0
2	B	434	VAL	5.0
2	B	647	ILE	4.6
2	B	929	LEU	4.3
2	B	588	PRO	4.1
2	B	433	ALA	4.0
2	B	413	THR	3.9
2	B	356	PHE	3.8
2	B	580	THR	3.8
2	B	568	PRO	3.6
2	B	648	PRO	3.6
2	B	407	GLU	3.5
2	B	276	TYR	3.3
2	B	577	ILE	3.3
2	B	628	VAL	3.3
2	B	2531	VAL	3.3
2	B	2539	PRO	3.2
2	B	621	LEU	3.1
2	B	924	ASN	3.0
2	B	491	ALA	2.7
2	B	640	PRO	2.7
1	A	557	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	626	TRP	2.7
2	B	926	THR	2.6
2	B	611	LEU	2.6
2	B	923	PRO	2.6
2	B	360	PRO	2.6
2	B	649	LYS	2.6
2	B	414	PRO	2.5
2	B	575	TYR	2.4
2	B	406	PRO	2.3
1	A	6	SER	2.3
2	B	451	GLN	2.3
2	B	353	LYS	2.2
2	B	262	VAL	2.2
2	B	762	GLY	2.2
2	B	2682	LEU	2.1
2	B	550	ILE	2.1
3	D	23	LYS	2.1
2	B	552	GLN	2.1
2	B	2644	ARG	2.1
2	B	2680	GLY	2.0
2	B	571	ARG	2.0

## 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( $\text{\AA}^2$ )	Q<0.9
3	M3L	D	27	12/13	0.96	0.07	18,22,29,29	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

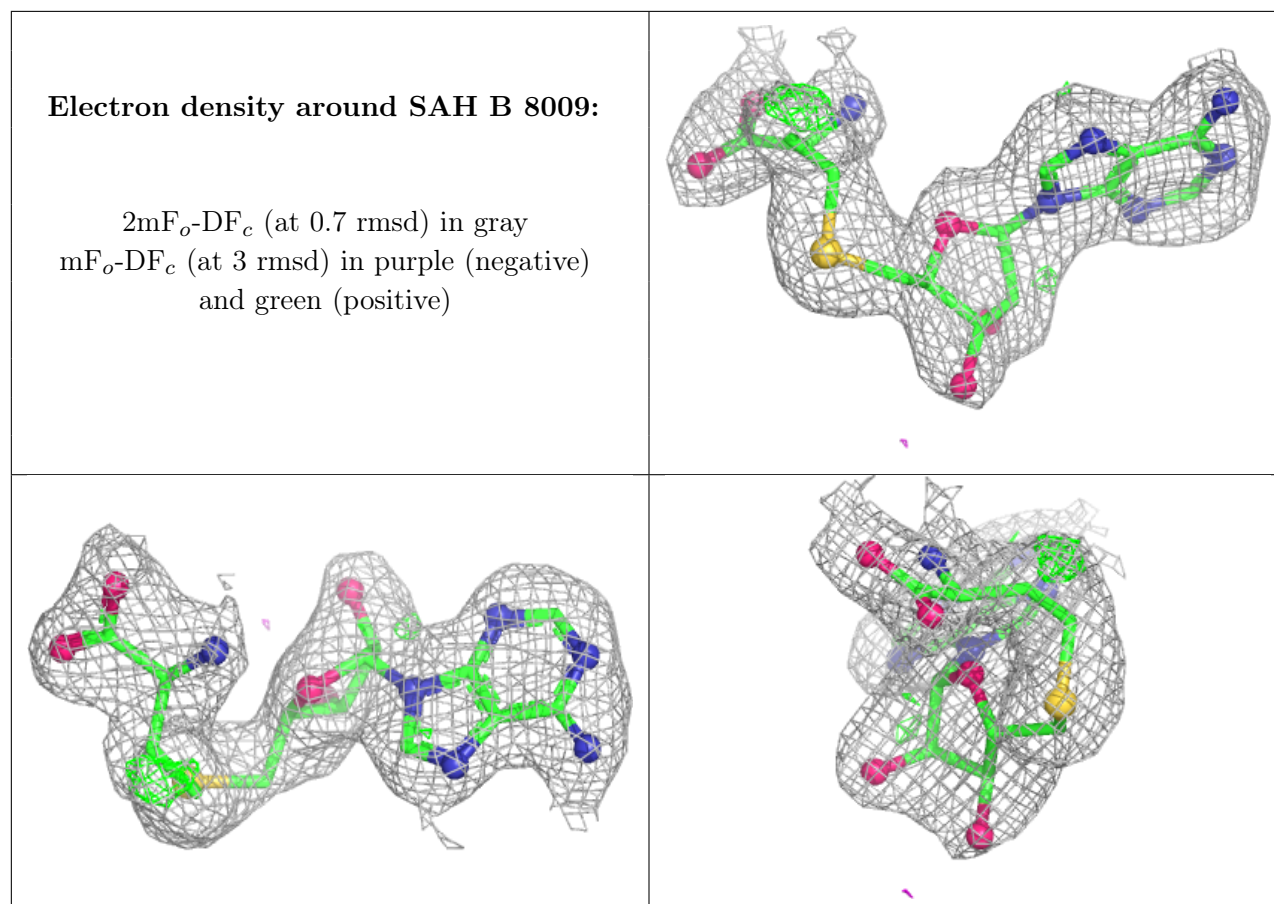
## 6.4 Ligands [i](#)

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
5	SAH	B	8009	26/26	0.93	0.09	13,25,33,38	26
4	ZN	B	8008	1/1	0.99	0.03	79,79,79,79	0
4	ZN	B	8003	1/1	1.00	0.03	36,36,36,36	0
4	ZN	B	8004	1/1	1.00	0.02	31,31,31,31	0
4	ZN	B	8005	1/1	1.00	0.01	31,31,31,31	0
4	ZN	B	8006	1/1	1.00	0.01	29,29,29,29	0
4	ZN	B	8007	1/1	1.00	0.02	26,26,26,26	0
4	ZN	B	8001	1/1	1.00	0.03	33,33,33,33	0
4	ZN	B	8002	1/1	1.00	0.04	37,37,37,37	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.