



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:46 PM UTC

PDB ID : 5KJH / pdb_00005kjh
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

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

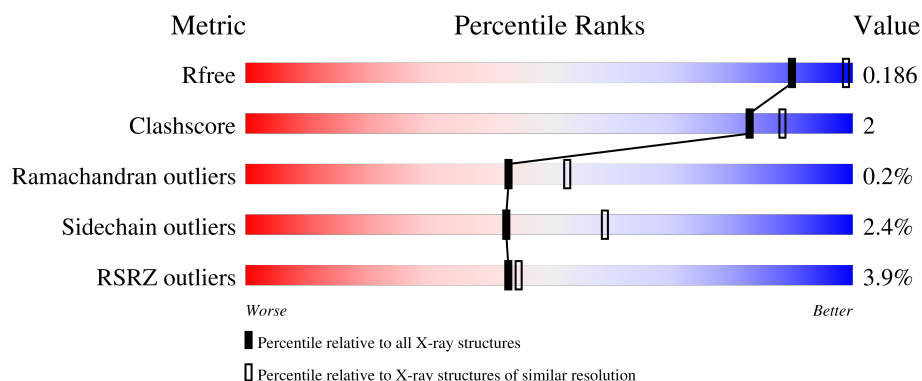
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (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 ≥ 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	0% 73% 6% 20%
2	B	937	5% 77% 8% 14%
3	D	11	9% 73% 27%

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

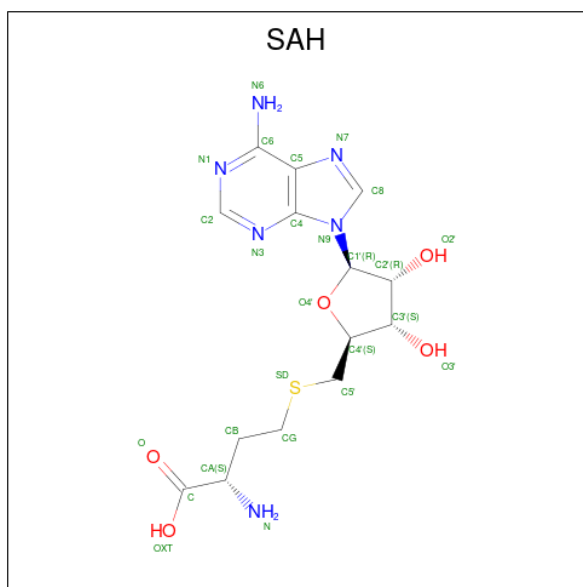
- Molecule 3 is a protein called Peptide H3K27me3.

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 (CCD ID: ZN) (formula: Zn).

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

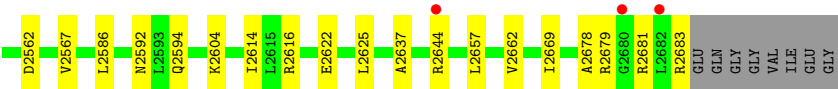
- Molecule 5 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: C₁₄H₂₀N₆O₅S).



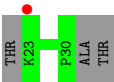
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- 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		



● Molecule 3: Peptide H3K27me3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.27Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.168 , 0.213 (Not available) , 0.186	Depositor DCC
R_{free} test set	3148 reflections (4.61%)	wwPDB-VP
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 59.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

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: M3L, SAH, ZN

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	0.87	1/3894 (0.0%)	1.14	7/5306 (0.1%)
2	B	0.83	0/6643	1.27	16/8968 (0.2%)
3	D	0.78	0/48	0.88	0/63
All	All	0.84	1/10585 (0.0%)	1.22	23/14337 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	255	ILE	CG1-CD1	-5.45	1.30	1.51

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2681	ARG	N-CA-C	-7.84	102.04	111.69
1	A	36	ASP	CA-C-N	7.76	131.02	120.38
1	A	36	ASP	C-N-CA	7.76	131.02	120.38
2	B	437	ALA	N-CA-C	-6.71	104.04	111.82
2	B	437	ALA	CA-C-N	6.25	128.57	120.44
2	B	437	ALA	C-N-CA	6.25	128.57	120.44
2	B	763	CYS	CA-C-N	6.08	132.65	121.70
2	B	763	CYS	C-N-CA	6.08	132.65	121.70
2	B	627	ASP	CA-CB-CG	6.07	118.67	112.60
1	A	37	LEU	N-CA-C	6.05	118.65	111.33
2	B	2562	ASP	N-CA-C	-5.81	102.33	109.65
1	A	320	THR	CB-CA-C	5.73	119.92	110.87
2	B	2592	ASN	CA-CB-CG	5.68	118.28	112.60
2	B	776	ASP	CA-C-N	5.51	127.92	120.38
2	B	776	ASP	C-N-CA	5.51	127.92	120.38
1	A	189	ASP	CA-CB-CG	5.47	118.07	112.60
1	A	320	THR	N-CA-CB	-5.26	101.62	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	366	ALA	CA-C-N	5.12	127.09	120.44
2	B	366	ALA	C-N-CA	5.12	127.09	120.44
1	A	208	ASP	CA-CB-CG	5.12	117.72	112.60
2	B	738	GLN	CA-C-N	5.07	129.11	121.40
2	B	738	GLN	C-N-CA	5.07	129.11	121.40
2	B	2679	ARG	N-CA-C	-5.01	103.79	110.55

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	32	1
3	D	60	0	71	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	10104	49	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 (49) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:493:MET:HE3	2:B:640:PRO:HD3	1.96	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	473/605 (78%)	464 (98%)	9 (2%)	0	100	100
2	B	773/937 (82%)	741 (96%)	30 (4%)	2 (0%)	36	44
3	D	5/11 (46%)	5 (100%)	0	0	100	100
All	All	1251/1553 (81%)	1210 (97%)	39 (3%)	2 (0%)	43	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 [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	406/495 (82%)	397 (98%)	9 (2%)	45	62
2	B	707/816 (87%)	689 (98%)	18 (2%)	42	58
3	D	4/6 (67%)	4 (100%)	0	100	100
All	All	1117/1317 (85%)	1090 (98%)	27 (2%)	43	59

All (27) 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	258	ARG
1	A	320	THR
1	A	336	VAL
1	A	365	ARG
2	B	415	GLN
2	B	472	ILE
2	B	493	MET
2	B	578	HIS
2	B	620	ILE
2	B	628	VAL
2	B	631	LYS
2	B	638	ARG
2	B	659	ARG
2	B	735	THR
2	B	738	GLN
2	B	805	GLU
2	B	840	GLU
2	B	2530	GLU
2	B	2567	VAL
2	B	2614	ILE
2	B	2644	ARG
2	B	2683	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	GLN
1	A	221	ASN
1	A	223	HIS
1	A	375	GLN
1	A	397	GLN
1	A	496	GLN
2	B	222	ASN
2	B	234	GLN
2	B	405	GLN
2	B	415	GLN
2	B	416	GLN
2	B	419	ASN
2	B	552	GLN
2	B	633	GLN
2	B	650	GLN
2	B	738	GLN
2	B	740	GLN
2	B	895	ASN

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	-	27,28,28	0.35	0	36,40,40	0.64	1 (2%)

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	-	-	5/15/31/31	0/3/3/3

There are no bond length outliers.

All (1) 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

There are no chirality outliers.

All (5) torsion outliers are listed below:

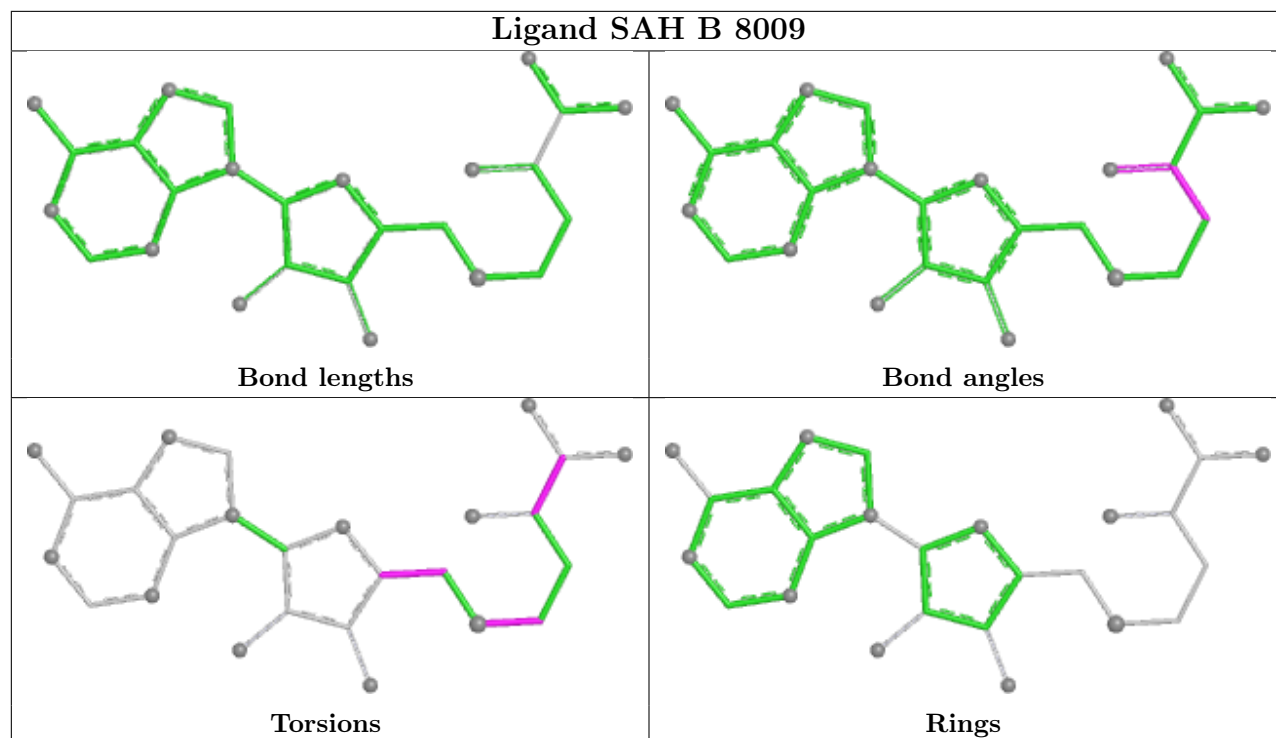
Mol	Chain	Res	Type	Atoms
5	B	8009	SAH	C3'-C4'-C5'-SD
5	B	8009	SAH	O-C-CA-CB
5	B	8009	SAH	OXT-C-CA-CB
5	B	8009	SAH	O-C-CA-N
5	B	8009	SAH	CB-CG-SD-C5'

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, 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	A	481/605 (79%)	-0.47	4 (0%) 82 84	14, 28, 61, 83	0
2	B	807/937 (86%)	0.18	45 (5%) 30 31	18, 45, 85, 123	0
3	D	7/11 (63%)	0.72	1 (14%) 6 6	31, 36, 50, 76	0
All	All	1295/1553 (83%)	-0.06	50 (3%) 43 45	14, 38, 80, 123	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	473	PHE	5.4
1	A	387	GLY	5.2
2	B	434	VAL	5.1
2	B	647	ILE	4.7
2	B	929	LEU	4.4
2	B	588	PRO	4.2
2	B	433	ALA	4.1
2	B	413	THR	4.0
2	B	356	PHE	4.0
2	B	580	THR	3.9
2	B	568	PRO	3.7
2	B	648	PRO	3.7
2	B	276	TYR	3.5
2	B	407	GLU	3.5
2	B	628	VAL	3.4
2	B	577	ILE	3.4
2	B	2531	VAL	3.4
2	B	2539	PRO	3.3
2	B	621	LEU	3.2
2	B	924	ASN	3.1
2	B	491	ALA	2.9
2	B	626	TRP	2.8
1	A	557	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	640	PRO	2.8
2	B	926	THR	2.7
2	B	611	LEU	2.7
2	B	923	PRO	2.7
2	B	360	PRO	2.7
2	B	414	PRO	2.6
2	B	649	LYS	2.6
2	B	575	TYR	2.6
2	B	406	PRO	2.4
1	A	6	SER	2.3
2	B	451	GLN	2.3
2	B	262	VAL	2.3
2	B	762	GLY	2.3
2	B	353	LYS	2.3
2	B	2682	LEU	2.2
2	B	550	ILE	2.2
2	B	552	GLN	2.2
2	B	2680	GLY	2.2
3	D	23	LYS	2.1
2	B	2644	ARG	2.1
2	B	922	PHE	2.1
2	B	571	ARG	2.1
2	B	925	LEU	2.1
2	B	743	GLY	2.1
1	A	415	LYS	2.0
2	B	630	ARG	2.0
2	B	2550	PRO	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, 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(Å ²)	Q<0.9
3	M3L	D	27	12/13	0.96	0.07	18,22,29,29	0

6.3 Carbohydrates [i](#)

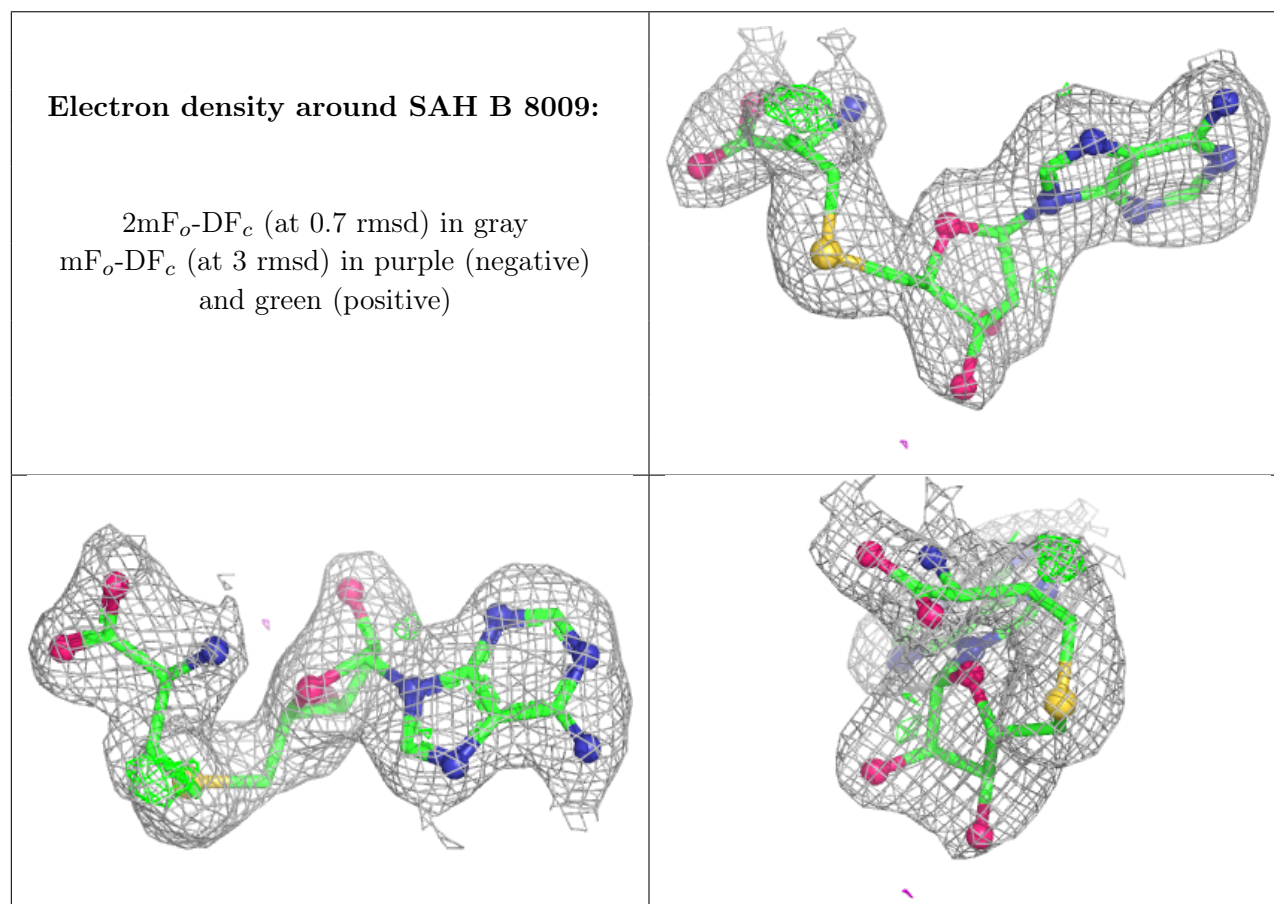
There are no oligosaccharides in this entry.

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	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.