



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:45 PM UTC

PDB ID : 5KJI / pdb_00005kji
Title : Crystal structure of an active polycomb repressive complex 2 in the basal state
Authors : Jiao, L.; Liu, X.
Deposited on : 2016-06-20
Resolution : 2.71 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

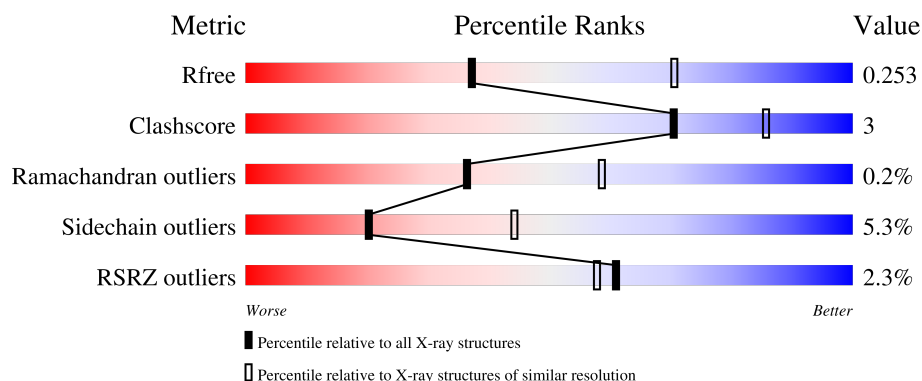
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	
2	B	937	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10028 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	479	Total	C	N	O	S	0	0	0
			3762	2403	645	694	20			

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	761	Total	C	N	O	S	0	0	0
			6121	3858	1107	1114	42			

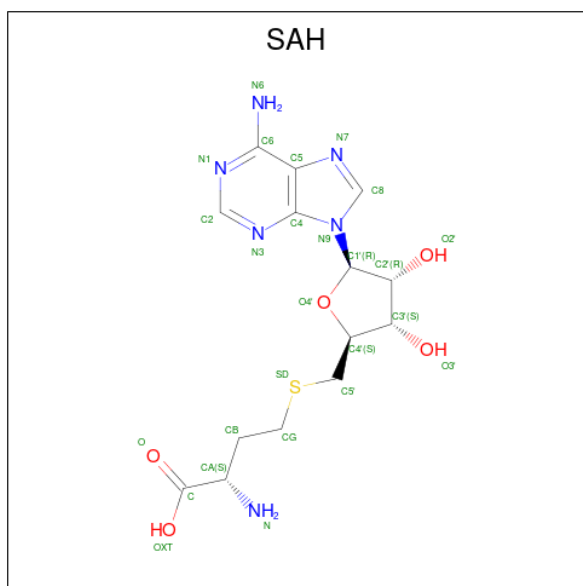
There are 15 discrepancies between the modelled and reference sequences:

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

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

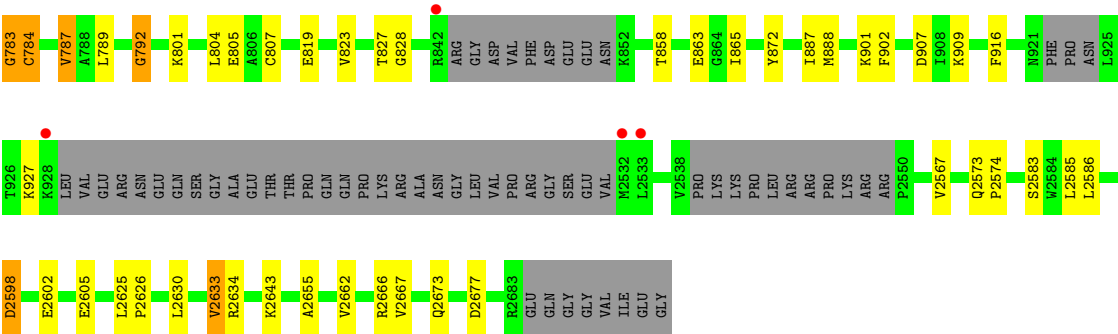
- Molecule 4 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	48	Total	O	0	0
			48	48		
5	B	63	Total	O	0	0
			63	63		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.33Å 74.62Å 127.03Å 90.00° 105.63° 90.00°	Depositor
Resolution (Å)	47.31 – 2.71 47.31 – 2.71	Depositor EDS
% Data completeness (in resolution range)	91.2 (47.31-2.71) 91.2 (47.31-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 2.69Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.179 , 0.249 0.181 , 0.253	Depositor DCC
R_{free} test set	1827 reflections (4.48%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 60.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10028	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.85	1/3873 (0.0%)	1.18	5/5276 (0.1%)
2	B	0.88	1/6251 (0.0%)	1.38	49/8430 (0.6%)
All	All	0.87	2/10124 (0.0%)	1.31	54/13706 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	PRO	CA-C	6.35	1.55	1.51
1	A	329	MET	SD-CE	-5.38	1.66	1.79

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	784	CYS	CA-C-N	8.26	136.57	121.70
2	B	784	CYS	C-N-CA	8.26	136.57	121.70
2	B	737	LEU	CA-C-N	7.54	135.27	121.70
2	B	737	LEU	C-N-CA	7.54	135.27	121.70
2	B	792	GLY	CA-C-N	7.44	135.09	121.70
2	B	792	GLY	C-N-CA	7.44	135.09	121.70
2	B	2633	VAL	N-CA-CB	6.96	118.70	110.55
2	B	454	LEU	CA-C-N	6.47	133.35	121.70
2	B	454	LEU	C-N-CA	6.47	133.35	121.70
2	B	524	ASP	N-CA-C	-6.27	102.08	110.55
2	B	627	ASP	CA-CB-CG	6.16	118.76	112.60
2	B	728	ALA	CA-C-N	5.97	130.88	121.56
2	B	728	ALA	C-N-CA	5.97	130.88	121.56
2	B	221	VAL	N-CA-CB	5.93	117.09	110.51
2	B	433	ALA	CA-C-N	5.90	132.31	121.70
2	B	433	ALA	C-N-CA	5.90	132.31	121.70
2	B	787	VAL	N-CA-CB	-5.87	101.55	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2605	GLU	CB-CG-CD	5.72	122.32	112.60
2	B	2677	ASP	CA-CB-CG	5.64	118.24	112.60
2	B	776	ASP	CA-CB-CG	5.61	118.21	112.60
1	A	150	ASN	CA-CB-CG	5.60	118.20	112.60
2	B	543	ARG	CA-C-N	5.60	127.78	120.28
2	B	543	ARG	C-N-CA	5.60	127.78	120.28
2	B	436	ASN	CA-CB-CG	5.54	118.14	112.60
2	B	916	PHE	CA-CB-CG	5.52	119.32	113.80
1	A	18	PHE	CA-CB-CG	5.49	119.28	113.80
2	B	823	VAL	CA-C-N	5.46	128.23	122.11
2	B	823	VAL	C-N-CA	5.46	128.23	122.11
2	B	534	GLU	CA-C-N	5.40	131.68	121.97
2	B	534	GLU	C-N-CA	5.40	131.68	121.97
2	B	535	ILE	N-CA-CB	-5.36	102.39	111.23
2	B	2602	GLU	CA-C-N	5.33	127.88	120.63
2	B	2602	GLU	C-N-CA	5.33	127.88	120.63
2	B	728	ALA	N-CA-C	-5.29	105.96	112.90
2	B	907	ASP	CA-CB-CG	5.29	117.89	112.60
2	B	363	GLN	CA-C-N	5.27	127.66	120.54
2	B	363	GLN	C-N-CA	5.27	127.66	120.54
2	B	2598	ASP	CA-CB-CG	5.26	117.86	112.60
2	B	538	LEU	N-CA-C	5.26	116.71	110.97
2	B	749	VAL	CA-C-N	5.20	127.25	120.28
2	B	749	VAL	C-N-CA	5.20	127.25	120.28
1	A	206	GLY	CA-C-N	5.14	128.12	120.31
1	A	206	GLY	C-N-CA	5.14	128.12	120.31
2	B	364	LYS	CA-C-N	5.13	127.03	120.56
2	B	364	LYS	C-N-CA	5.13	127.03	120.56
1	A	89	ASP	CA-CB-CG	5.10	117.70	112.60
2	B	461	ASP	CA-CB-CG	5.10	117.70	112.60
2	B	537	GLY	CA-C-N	5.10	127.38	120.65
2	B	537	GLY	C-N-CA	5.10	127.38	120.65
2	B	726	GLY	CA-C-N	5.07	129.59	122.09
2	B	726	GLY	C-N-CA	5.07	129.59	122.09
2	B	450	ASP	CA-CB-CG	5.05	117.65	112.60
2	B	370	GLN	CA-C-N	5.04	126.99	120.44
2	B	370	GLN	C-N-CA	5.04	126.99	120.44

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	3762	0	3619	24	1
2	B	6121	0	6031	47	2
3	B	8	0	0	0	0
4	B	26	0	19	1	0
5	A	48	0	0	0	0
5	B	63	0	0	0	0
All	All	10028	0	9669	67	2

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 3.

All (67) 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:452:SER:H	2:B:454:LEU:HD22	1.42	0.83
1:A:326:GLN:HB2	1:A:329:MET:HE2	1.65	0.78
2:B:452:SER:HB3	2:B:454:LEU:HD13	1.67	0.75
1:A:160:ASP:O	1:A:161:THR:HB	1.86	0.75
2:B:460:ARG:O	2:B:464:MET:HG2	1.87	0.75
2:B:454:LEU:HD23	2:B:456:ARG:HH21	1.52	0.74
2:B:763:CYS:HB3	2:B:765:ALA:H	1.55	0.71
2:B:2630:LEU:O	2:B:2634:ARG:HG3	1.94	0.68
1:A:326:GLN:CB	1:A:329:MET:HE2	2.29	0.62
2:B:2625:LEU:HD23	2:B:2662:VAL:CG1	2.29	0.62
2:B:768:ARG:HH21	2:B:782:THR:HB	1.66	0.61
1:A:316:ALA:HB1	1:A:511:ILE:HD11	1.82	0.61
2:B:2625:LEU:HD23	2:B:2662:VAL:HG12	1.83	0.61
2:B:887:ILE:HD12	2:B:902:PHE:CD1	2.38	0.59
2:B:735:THR:H	2:B:783:GLY:HA2	1.70	0.56
2:B:314:ILE:HG21	2:B:2585:LEU:HD21	1.87	0.56
1:A:66:VAL:HG22	1:A:86:LEU:HD13	1.87	0.56
1:A:384:VAL:HG13	1:A:407:MET:SD	2.46	0.55
2:B:454:LEU:N	2:B:455:ARG:HA	2.21	0.55
1:A:67:ILE:HB	1:A:85:GLN:HB3	1.88	0.55
2:B:452:SER:N	2:B:454:LEU:HD22	2.18	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:HIS:CG	1:A:190:LEU:HD21	2.43	0.54
2:B:768:ARG:HD3	2:B:784:CYS:O	2.07	0.54
2:B:2583:SER:HA	2:B:2586:LEU:HD12	1.90	0.53
2:B:763:CYS:HB3	2:B:765:ALA:N	2.23	0.52
2:B:281:ASN:CG	2:B:282:SER:H	2.19	0.51
1:A:326:GLN:HB2	1:A:329:MET:CE	2.38	0.51
1:A:90:ASP:HB3	2:B:294:LYS:HG3	1.94	0.50
2:B:789:LEU:HD21	2:B:901:LYS:HB3	1.94	0.50
2:B:372:GLU:O	2:B:376:THR:HG23	2.11	0.50
2:B:612:ARG:HE	2:B:613:PRO:HD2	1.77	0.49
2:B:604:THR:HG21	2:B:2655:ALA:HB1	1.95	0.49
2:B:2573:GLN:HG2	2:B:2574:PRO:HD2	1.95	0.48
2:B:313:ASN:OD1	2:B:827:THR:HA	2.13	0.48
2:B:828:GLY:HA2	2:B:872:TYR:O	2.14	0.48
2:B:317:LEU:HD22	2:B:525:ASN:HB3	1.96	0.47
1:A:217:PRO:HG3	1:A:228:ILE:HG21	1.97	0.47
2:B:614:GLU:HA	2:B:628:VAL:CG2	2.45	0.46
1:A:300:THR:HB	1:A:311:MET:HG2	1.97	0.46
2:B:197:TRP:CE2	2:B:390:ILE:HG12	2.51	0.45
2:B:594:GLU:HG2	2:B:621:LEU:HD22	1.99	0.45
2:B:403:ALA:HB2	2:B:420:LEU:HD23	1.98	0.45
2:B:314:ILE:CG2	2:B:2585:LEU:HD21	2.47	0.45
1:A:83:ILE:HB	2:B:288:TYR:CE2	2.52	0.45
1:A:300:THR:HA	1:A:301:PRO:HD3	1.90	0.44
2:B:2626:PRO:HB3	2:B:2667:VAL:HG21	2.00	0.44
2:B:686:HIS:HA	2:B:714:LEU:HD12	1.99	0.43
2:B:499:ALA:HB1	2:B:600:TRP:CE3	2.54	0.42
2:B:612:ARG:NE	2:B:613:PRO:HD2	2.34	0.42
1:A:175:GLN:HG2	2:B:2567:VAL:HG21	2.00	0.42
2:B:535:ILE:HD11	2:B:684:PRO:HB2	2.00	0.42
1:A:531:SER:HB3	1:A:536:TRP:HB2	2.00	0.42
1:A:163:ILE:HB	1:A:181:LEU:HB2	2.01	0.41
1:A:307:SER:HB2	2:B:467:LYS:HA	2.02	0.41
2:B:629:HIS:O	2:B:633:GLN:HG2	2.20	0.41
1:A:103:ASP:CG	1:A:106:THR:HG22	2.46	0.41
1:A:196:HIS:HB2	1:A:201:TYR:HB2	2.02	0.41
2:B:509:LEU:HB3	2:B:712:PHE:CE1	2.56	0.41
2:B:715:CYS:O	2:B:723:LYS:HE3	2.20	0.41
1:A:106:THR:HG23	1:A:108:GLN:HB2	2.03	0.41
1:A:383:VAL:CG1	1:A:408:LYS:HB2	2.51	0.41
2:B:268:LYS:HB2	2:B:285:ARG:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:591:SER:O	2:B:595:VAL:HG13	2.22	0.40
1:A:46:TYR:CE1	1:A:109:PRO:HB3	2.56	0.40
2:B:863:GLU:HG3	2:B:865:ILE:HD12	2.02	0.40
1:A:319:HIS:HB2	1:A:510:LEU:HB3	2.02	0.40
2:B:927:LYS:HG3	4:B:8009:SAH:H2	2.03	0.40

All (2) 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:A:485:ASP:OD2	2:B:394:THR:OG1[2_949]	2.12	0.08
2:B:418:SER:OG	2:B:636:ASP:OD2[2_849]	2.18	0.02

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	471/605 (78%)	453 (96%)	18 (4%)	0	100	100
2	B	729/937 (78%)	689 (94%)	37 (5%)	3 (0%)	30	52
All	All	1200/1542 (78%)	1142 (95%)	55 (5%)	3 (0%)	36	59

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	783	GLY
2	B	792	GLY
2	B	665	SER

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	404/495 (82%)	387 (96%)	17 (4%)	26	53
2	B	664/816 (81%)	624 (94%)	40 (6%)	17	39
All	All	1068/1311 (82%)	1011 (95%)	57 (5%)	20	44

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	THR
1	A	72	GLN
1	A	90	ASP
1	A	154	ILE
1	A	161	THR
1	A	171	GLU
1	A	225	GLU
1	A	226	ILE
1	A	269	ARG
1	A	330	ARG
1	A	336	VAL
1	A	349	LYS
1	A	351	LYS
1	A	384	VAL
1	A	390	ILE
1	A	492	ARG
1	A	520	ASP
2	B	196	GLU
2	B	201	LYS
2	B	265	MET
2	B	278	LYS
2	B	282	SER
2	B	285	ARG
2	B	297	ARG
2	B	376	THR
2	B	391	GLU
2	B	396	SER

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Mol	Chain	Res	Type
2	B	397	ASN
2	B	435	ARG
2	B	442	GLU
2	B	457	VAL
2	B	517	GLU
2	B	535	ILE
2	B	595	VAL
2	B	628	VAL
2	B	650	GLN
2	B	664	MET
2	B	727	CYS
2	B	737	LEU
2	B	761	LYS
2	B	763	CYS
2	B	767	GLU
2	B	782	THR
2	B	787	VAL
2	B	801	LYS
2	B	804	LEU
2	B	805	GLU
2	B	807	CYS
2	B	819	GLU
2	B	858	THR
2	B	888	MET
2	B	909	LYS
2	B	2598	ASP
2	B	2633	VAL
2	B	2643	LYS
2	B	2666	ARG
2	B	2673	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	116	ASN
1	A	150	ASN
1	A	221	ASN
1	A	243	ASN
1	A	375	GLN
1	A	386	GLN
1	A	496	GLN

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Mol	Chain	Res	Type
1	A	506	ASN
2	B	222	ASN
2	B	287	GLN
2	B	494	GLN
2	B	695	ASN
2	B	740	GLN
2	B	803	GLN
2	B	2618	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

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	$\# Z > 2$
4	SAH	B	8009	-	27,28,28	0.33	0	36,40,40	0.59	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SAH	B	8009	-	-	4/15/31/31	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

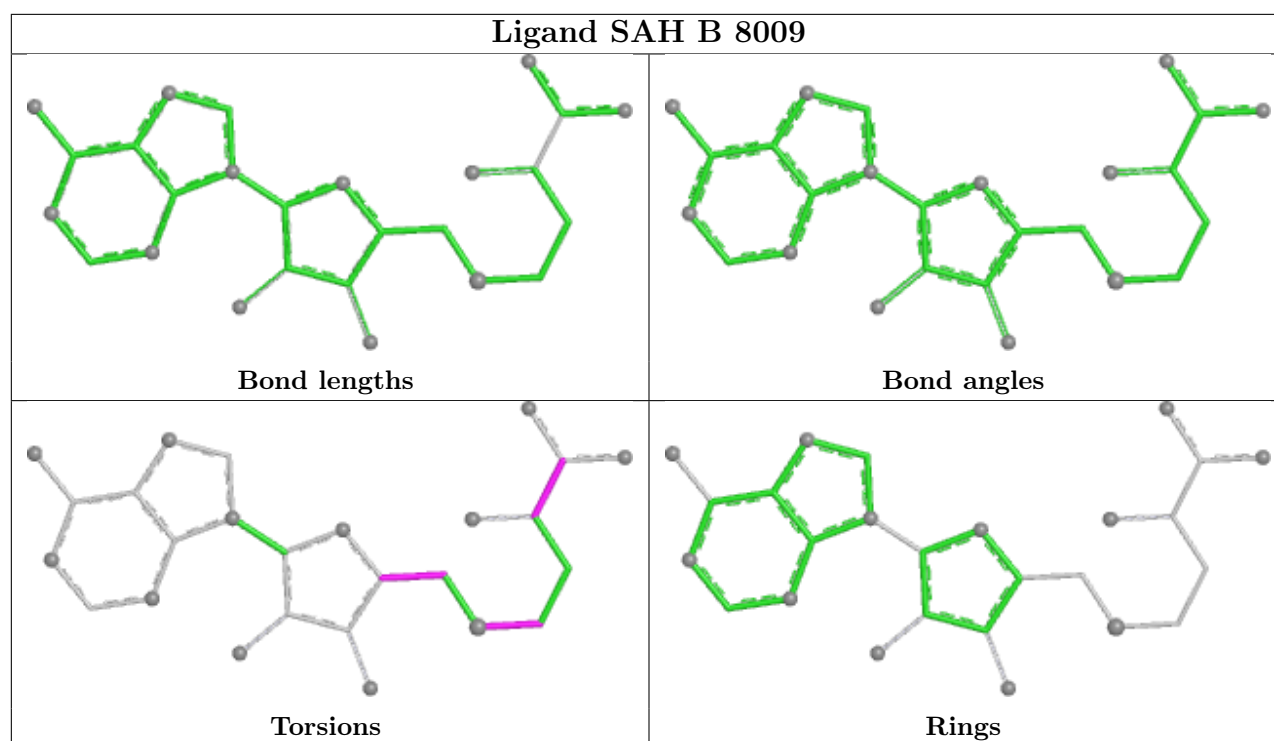
Mol	Chain	Res	Type	Atoms
4	B	8009	SAH	OXT-C-CA-CB
4	B	8009	SAH	C3'-C4'-C5'-SD
4	B	8009	SAH	O-C-CA-CB
4	B	8009	SAH	CB-CG-SD-C5'

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	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	479/605 (79%)	-0.38	5 (1%) 79 78	16, 38, 72, 96	0
2	B	761/937 (81%)	0.01	23 (3%) 52 49	17, 50, 86, 115	0
All	All	1240/1542 (80%)	-0.14	28 (2%) 61 58	16, 46, 81, 115	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	473	PHE	4.1
2	B	648	PRO	3.8
2	B	647	ILE	3.6
2	B	411	SER	3.6
2	B	738	GLN	3.2
1	A	25	LYS	3.2
1	A	303	VAL	2.8
1	A	477	MET	2.8
2	B	433	ALA	2.8
2	B	404	SER	2.7
2	B	253	ASP	2.6
2	B	609	GLN	2.5
1	A	37	LEU	2.5
2	B	428	MET	2.4
2	B	435	ARG	2.4
2	B	412	MET	2.4
2	B	2532	MET	2.4
2	B	277	GLY	2.3
2	B	276	TYR	2.3
1	A	390	ILE	2.3
2	B	2533	LEU	2.2
2	B	553	ARG	2.2
2	B	730	HIS	2.1
2	B	842	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	640	PRO	2.1
2	B	928	LYS	2.1
2	B	434	VAL	2.1
2	B	263	PRO	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

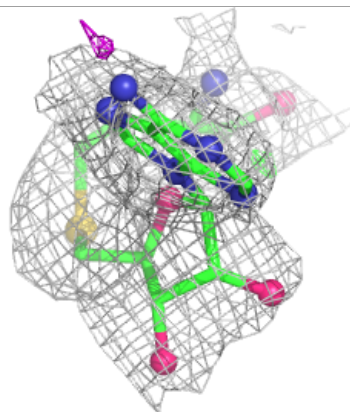
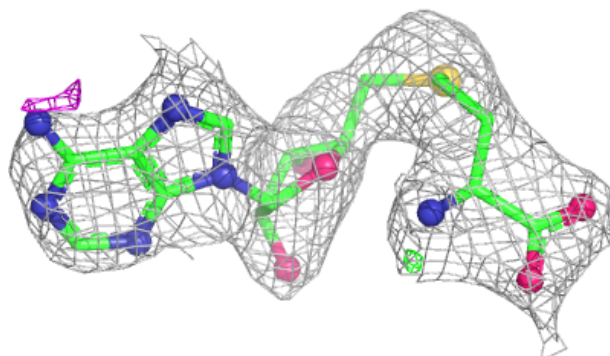
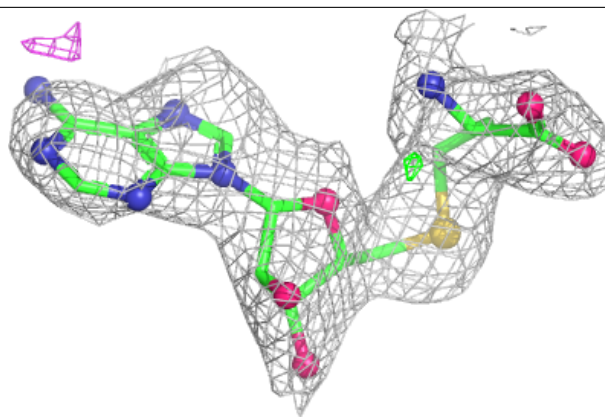
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
4	SAH	B	8009	26/26	0.93	0.08	44,57,64,67	0
3	ZN	B	8004	1/1	0.99	0.02	48,48,48,48	0
3	ZN	B	8008	1/1	0.99	0.02	52,52,52,52	0
3	ZN	B	8002	1/1	0.99	0.04	45,45,45,45	0
3	ZN	B	8005	1/1	1.00	0.03	46,46,46,46	0
3	ZN	B	8006	1/1	1.00	0.06	41,41,41,41	0
3	ZN	B	8007	1/1	1.00	0.04	31,31,31,31	0
3	ZN	B	8003	1/1	1.00	0.03	51,51,51,51	0
3	ZN	B	8001	1/1	1.00	0.03	41,41,41,41	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 8009:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.