



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 11:04 pm BST

PDB ID : 5TQR  
Title : ctPRC2 in an autoinhibited conformation bound to S-adenosylmethionine  
Authors : Bratkowski, M.A.; Liu, X.  
Deposited on : 2016-10-24  
Resolution : 2.57 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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

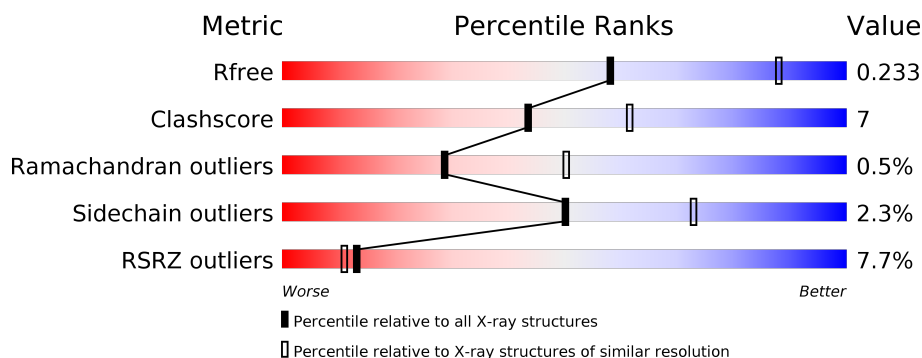
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.57 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	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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 on 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	<div> <div>6%</div> <div> <div></div> <div>65%</div> <div>12%</div> <div>•</div> <div>22%</div> </div> </div>
2	B	937	<div> <div>7%</div> <div> <div></div> <div>72%</div> <div>13%</div> <div>•</div> <div>14%</div> </div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10500 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 Polycomb Protein EED.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	2	0
			3706	2366	639	682	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 Histone-lysine N-methyltransferase EZH2, Polycomb protein SUZ12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	809	Total	C	N	O	S	0	0	0
			6515	4096	1185	1193	41			

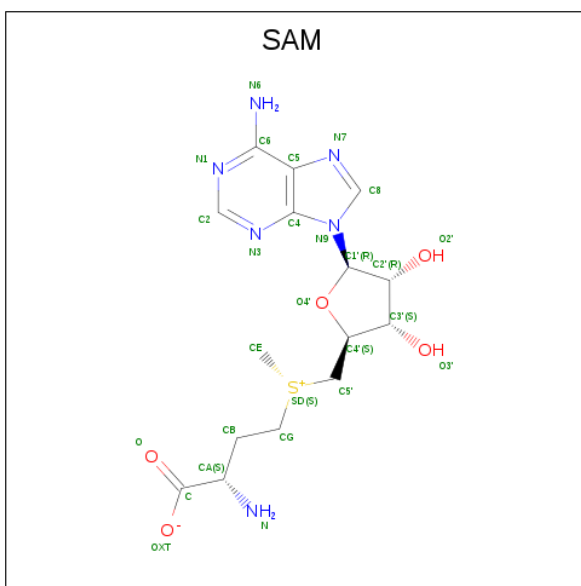
There are 15 discrepancies between the modelled and reference sequences:

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	-	linker	UNP G0SDW4
B	2525	VAL	-	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 (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula:  $C_{15}H_{22}N_6O_5S$ ).

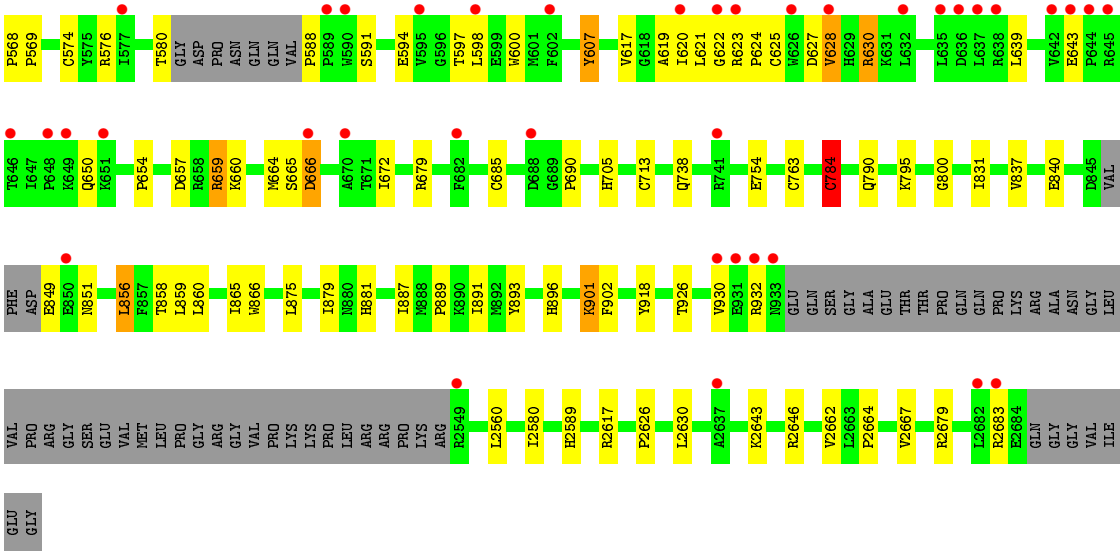


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	92	Total	O	0	0
			92	92		
5	B	152	Total	O	0	0
			152	152		





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.45Å 138.01Å 223.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.32 – 2.57 47.32 – 2.57	Depositor EDS
% Data completeness (in resolution range)	95.4 (47.32-2.57) 95.4 (47.32-2.57)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 2.58Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, $R_{free}$	0.174 , 0.233 0.174 , 0.233	Depositor DCC
$R_{free}$ test set	2733 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.0	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 50.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10500	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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: ZN, SAM

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	0.43	0/3818	0.63	1/5195 (0.0%)
2	B	0.46	2/6664 (0.0%)	0.58	2/9006 (0.0%)
All	All	0.45	2/10482 (0.0%)	0.60	3/14201 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	784	CYS	CB-SG	-9.27	1.66	1.82
2	B	622	GLY	C-N	5.49	1.46	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	630	ARG	NE-CZ-NH2	-5.40	117.60	120.30
2	B	784	CYS	CA-CB-SG	5.21	123.38	114.00
1	A	37	LEU	CA-CB-CG	-5.03	103.73	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3706	0	3574	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	6515	0	6403	92	0
3	B	8	0	0	0	0
4	B	27	0	22	0	0
5	A	92	0	0	2	0
5	B	152	0	0	5	0
All	All	10500	0	9999	136	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (136) 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:881:HIS:HD2	2:B:918:TYR:H	1.07	1.00
2:B:881:HIS:CD2	2:B:918:TYR:H	1.95	0.84
2:B:591:SER:HB3	2:B:594:GLU:HG3	1.63	0.80
2:B:270:LYS:NZ	5:B:8101:HOH:O	2.10	0.80
2:B:837:VAL:HG13	2:B:926:THR:HG22	1.67	0.76
2:B:550:ILE:HG13	2:B:551:GLU:OE1	1.86	0.74
2:B:309:GLU:HG2	2:B:2580:ILE:HG12	1.77	0.67
2:B:763:CYS:HB2	2:B:784:CYS:HB2	1.75	0.67
1:A:25:LYS:HD3	1:A:25:LYS:H	1.60	0.66
1:A:319:HIS:HB2	1:A:510:LEU:HB3	1.77	0.65
2:B:394:THR:HG22	2:B:396:SER:H	1.63	0.63
1:A:34:SER:HB2	1:A:37:LEU:HD12	1.79	0.63
2:B:515:ASP:OD2	2:B:2589:HIS:HD2	1.82	0.63
2:B:252:ILE:HD12	2:B:287:GLN:HB3	1.81	0.62
2:B:831:ILE:HD11	2:B:856:LEU:HD21	1.82	0.62
2:B:419:ASN:HB3	2:B:472:ILE:HG12	1.82	0.61
2:B:643:GLU:H	2:B:643:GLU:CD	2.03	0.61
2:B:297:ARG:NH2	5:B:8105:HOH:O	2.31	0.61
2:B:248:LYS:HG3	2:B:249:SER:N	2.16	0.60
1:A:60:THR:HG23	5:A:607:HOH:O	1.99	0.60
2:B:517:GLU:OE2	2:B:2589:HIS:HE1	1.83	0.60
1:A:408:LYS:NZ	1:A:412:LEU:O	2.30	0.60
2:B:932:ARG:NH2	5:B:8103:HOH:O	2.34	0.60
2:B:567:HIS:O	2:B:576:ARG:NH2	2.35	0.59
2:B:860:LEU:HD12	2:B:865:ILE:HD12	1.83	0.59
2:B:451:GLN:NE2	2:B:456:ARG:HD2	2.17	0.58
1:A:248:VAL:HG23	1:A:257:SER:HB3	1.84	0.58
2:B:567:HIS:HB3	2:B:568:PRO:HD2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:643:GLU:N	2:B:643:GLU:OE1	2.23	0.58
1:A:186:HIS:CG	1:A:190:LEU:HD21	2.40	0.57
2:B:598:LEU:HD22	2:B:628:VAL:HG23	1.87	0.57
1:A:294:GLN:NE2	5:A:603:HOH:O	2.38	0.56
2:B:421:LEU:HD13	2:B:425:SER:HA	1.87	0.56
1:A:15:ARG:HH22	2:B:271:GLN:HE21	1.54	0.56
2:B:412:MET:HG2	2:B:473:PHE:HE2	1.70	0.55
2:B:412:MET:HG2	2:B:473:PHE:CE2	2.42	0.55
2:B:881:HIS:HD2	2:B:918:TYR:N	1.91	0.55
2:B:418:SER:N	5:B:8107:HOH:O	2.39	0.55
1:A:60:THR:HG21	1:A:98:SER:HB3	1.87	0.54
1:A:93:GLU:HG3	1:A:117:GLU:H	1.72	0.54
2:B:198:THR:O	2:B:202:ILE:HG13	2.07	0.54
2:B:248:LYS:NZ	2:B:249:SER:H	2.06	0.54
1:A:8:GLU:HG3	1:A:9:TRP:CD1	2.44	0.53
1:A:292:THR:HG22	2:B:320:GLN:NE2	2.24	0.53
1:A:181:LEU:HD13	1:A:214:TRP:CG	2.44	0.52
2:B:754:GLU:OE1	2:B:790:GLN:HG3	2.09	0.52
1:A:75:ASP:HB3	1:A:78:ALA:HB2	1.90	0.52
2:B:415:GLN:HA	2:B:418:SER:HB3	1.91	0.52
2:B:657:ASP:OD2	2:B:660:LYS:HG3	2.09	0.52
1:A:386:GLN:HG2	1:A:407:MET:HB3	1.92	0.52
1:A:515:ARG:HD3	1:A:517:LEU:HD21	1.92	0.51
2:B:569:PRO:N	2:B:576:ARG:HH21	2.10	0.50
2:B:650:GLN:OE1	2:B:690:PRO:HB3	2.11	0.50
2:B:430:SER:O	2:B:434:VAL:HG23	2.13	0.49
1:A:20:PHE:HB3	1:A:544:ASN:HB3	1.95	0.49
1:A:263:ASP:C	1:A:320:THR:HG22	2.32	0.49
2:B:197:TRP:CE3	2:B:202:ILE:HG12	2.46	0.49
2:B:672:ILE:HG23	2:B:705:HIS:HB2	1.94	0.49
2:B:580:THR:HA	2:B:630:ARG:HG3	1.95	0.49
2:B:551:GLU:OE1	2:B:551:GLU:N	2.46	0.48
1:A:380:ARG:HH11	1:A:380:ARG:HG2	1.77	0.48
2:B:574:CYS:HA	2:B:625:CYS:HB3	1.95	0.48
2:B:377:LEU:HD12	2:B:457:VAL:HG11	1.95	0.48
2:B:849:GLU:HG3	2:B:851:ASN:H	1.79	0.48
1:A:320:THR:O	1:A:320:THR:CG2	2.62	0.47
2:B:840:GLU:OE1	2:B:926:THR:HG23	2.15	0.47
2:B:265:MET:HG2	2:B:290:VAL:HG21	1.96	0.47
2:B:619:ALA:O	2:B:2679:ARG:NH2	2.47	0.46
1:A:217:PRO:HD3	1:A:230:ILE:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:926:THR:O	2:B:930:VAL:HG13	2.16	0.46
2:B:248:LYS:HG3	2:B:249:SER:H	1.80	0.46
2:B:211:GLU:O	2:B:214:PRO:HD2	2.16	0.46
2:B:2630:LEU:HD11	2:B:2667:VAL:HG12	1.98	0.45
1:A:411:TRP:CZ3	1:A:412:LEU:HD13	2.52	0.45
1:A:151:PRO:HD3	2:B:237:HIS:CD2	2.52	0.45
2:B:859:LEU:HD12	2:B:891:ILE:HD12	1.99	0.45
1:A:16:THR:OG1	2:B:271:GLN:NE2	2.49	0.45
1:A:161:THR:HG22	1:A:161:THR:O	2.17	0.45
2:B:394:THR:HG22	2:B:396:SER:N	2.29	0.45
2:B:607:TYR:CE1	2:B:639:LEU:HD13	2.51	0.45
2:B:195:THR:HG23	2:B:196:GLU:H	1.81	0.45
2:B:795:LYS:HA	2:B:795:LYS:HD2	1.80	0.45
1:A:25:LYS:HB2	1:A:34:SER:O	2.17	0.44
2:B:412:MET:C	2:B:417:LYS:HZ3	2.20	0.44
2:B:588:PRO:O	2:B:623:ARG:NH2	2.51	0.43
2:B:643:GLU:N	2:B:643:GLU:CD	2.71	0.43
2:B:665:SER:OG	2:B:666:ASP:N	2.49	0.43
2:B:875:LEU:HA	2:B:875:LEU:HD23	1.82	0.43
2:B:893:TYR:CE2	2:B:896:HIS:HA	2.53	0.43
2:B:451:GLN:HE22	2:B:456:ARG:NH1	2.17	0.43
1:A:42:ASP:OD1	1:A:527:GLN:HG2	2.18	0.43
2:B:858:THR:HA	2:B:866:TRP:CD1	2.54	0.43
1:A:300:THR:HA	1:A:301:PRO:HD3	1.87	0.43
1:A:124:ASN:ND2	1:A:127:GLU:OE1	2.49	0.43
2:B:264:THR:HG21	2:B:287:GLN:OE1	2.19	0.43
2:B:517:GLU:OE2	2:B:2589:HIS:CE1	2.68	0.43
2:B:2664:PRO:O	2:B:2667:VAL:HG22	2.19	0.43
2:B:413:THR:O	2:B:416:GLN:HB2	2.19	0.42
1:A:75:ASP:HB3	1:A:78:ALA:CB	2.49	0.42
2:B:476:LYS:HA	2:B:476:LYS:HD2	1.83	0.42
1:A:25:LYS:HD3	1:A:25:LYS:N	2.32	0.42
2:B:879:ILE:HD13	2:B:887:ILE:HD11	2.00	0.42
2:B:417:LYS:O	2:B:421:LEU:HD23	2.20	0.42
2:B:617:VAL:HG13	2:B:621:LEU:HD12	2.01	0.42
2:B:659:ARG:HD2	2:B:659:ARG:HA	1.91	0.42
2:B:889:PRO:HA	2:B:901:LYS:O	2.19	0.42
2:B:624:PRO:O	2:B:627:ASP:HB3	2.20	0.42
1:A:135:VAL:HG21	2:B:297:ARG:HB3	2.01	0.42
1:A:163:ILE:HD12	1:A:190:LEU:HD13	2.01	0.42
1:A:398:VAL:HG12	1:A:398:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:VAL:HA	1:A:58:ALA:O	2.20	0.41
2:B:889:PRO:HB3	2:B:902:PHE:CE1	2.55	0.41
1:A:535:GLU:HG2	1:A:536:TRP:CD1	2.55	0.41
1:A:15:ARG:NH2	2:B:271:GLN:HE21	2.16	0.41
2:B:377:LEU:HD12	2:B:457:VAL:CG1	2.50	0.41
2:B:901:LYS:O	2:B:901:LYS:HG2	2.20	0.41
2:B:685:CYS:HB2	2:B:713:CYS:HB3	2.01	0.41
2:B:221:VAL:O	2:B:225:LEU:HG	2.21	0.41
1:A:386:GLN:HG3	1:A:408:LYS:O	2.21	0.41
1:A:64:HIS:CD2	1:A:88:ARG:HB2	2.55	0.41
2:B:2643:LYS:HB3	2:B:2646:ARG:HD2	2.03	0.41
2:B:597:THR:HA	2:B:600:TRP:CE2	2.56	0.41
2:B:2626:PRO:HG3	2:B:2664:PRO:HD3	2.02	0.41
1:A:394:GLN:O	1:A:398:VAL:HG23	2.21	0.41
1:A:262:GLU:O	1:A:264:THR:HG23	2.20	0.41
1:A:46:TYR:CE1	1:A:109:PRO:HB3	2.55	0.41
1:A:492:ARG:HG2	1:A:492:ARG:NH1	2.36	0.41
2:B:455:ARG:NH1	5:B:8121:HOH:O	2.54	0.41
1:A:320:THR:O	1:A:320:THR:HG23	2.21	0.41
1:A:391:SER:O	1:A:393:ALA:N	2.53	0.41
1:A:56:VAL:HG22	1:A:69:ARG:HB2	2.02	0.41
2:B:800:GLY:HA3	2:B:2560:LEU:HD23	2.03	0.41
1:A:334:TYR:O	1:A:341:PRO:HA	2.21	0.40
1:A:316:ALA:HB1	1:A:511:ILE:HD11	2.03	0.40
2:B:654:PRO:O	2:B:664:MET:HG3	2.21	0.40
1:A:95:ASN:HA	1:A:115:GLY:HA3	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	464/605 (77%)	442 (95%)	18 (4%)	4 (1%)	17	34
2	B	793/937 (85%)	759 (96%)	32 (4%)	2 (0%)	41	62
All	All	1257/1542 (82%)	1201 (96%)	50 (4%)	6 (0%)	29	50

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	310	ALA
1	A	393	ALA
2	B	666	ASP
2	B	2683	ARG
1	A	309	PRO
1	A	392	LEU

### 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	396/495 (80%)	387 (98%)	9 (2%)	50	73
2	B	709/816 (87%)	693 (98%)	16 (2%)	50	73
All	All	1105/1311 (84%)	1080 (98%)	25 (2%)	50	73

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	TYR
1	A	25	LYS
1	A	34	SER
1	A	36	ASP
1	A	107	ASP
1	A	175	GLN
1	A	320	THR
1	A	351	LYS
1	A	385	ASP
2	B	255	ASN

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Mol	Chain	Res	Type
2	B	270	LYS
2	B	297	ARG
2	B	312	LYS
2	B	361	ARG
2	B	607	TYR
2	B	620	ILE
2	B	628	VAL
2	B	659	ARG
2	B	679	ARG
2	B	738	GLN
2	B	784	CYS
2	B	856	LEU
2	B	901	LYS
2	B	2617	ARG
2	B	2662	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	119	ASN
1	A	209	GLN
2	B	271	GLN
2	B	432	GLN
2	B	451	GLN
2	B	662	GLN
2	B	881	HIS
2	B	2589	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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	SAM	B	8009	-	21,29,29	1.27	2 (9%)	18,42,42	1.47	1 (5%)

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	SAM	B	8009	-	-	2/8/33/33	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	8009	SAM	C2-N3	4.12	1.38	1.32
4	B	8009	SAM	C2-N1	2.56	1.38	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	8009	SAM	N3-C2-N1	-5.08	120.73	128.68

There are no chirality outliers.

All (2) torsion outliers are listed below:

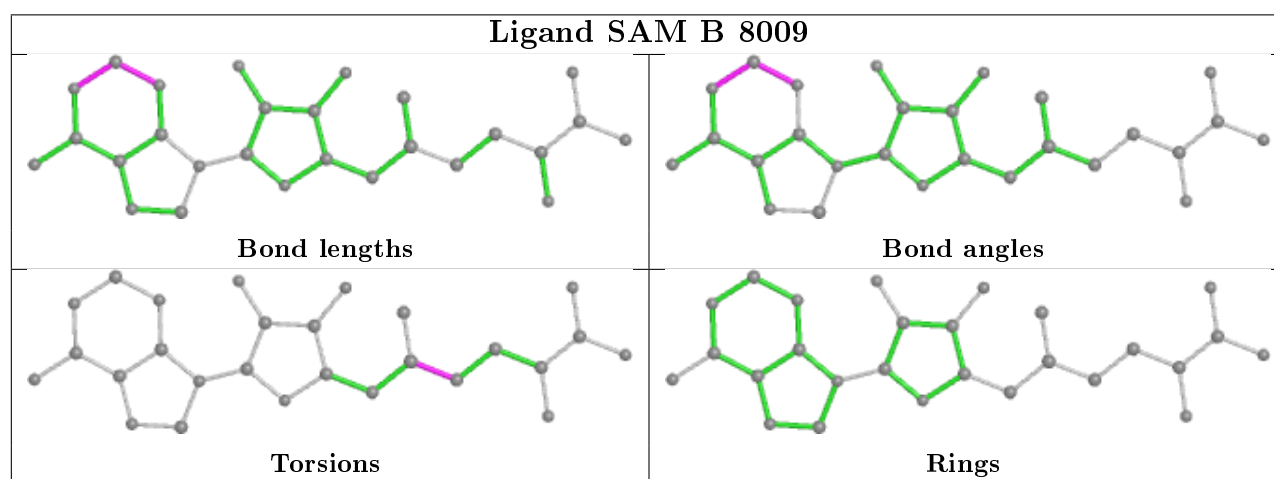
Mol	Chain	Res	Type	Atoms
4	B	8009	SAM	CB-CG-SD-CE
4	B	8009	SAM	CB-CG-SD-C5'

There are no ring outliers.



No monomer is involved in short contacts.

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	470/605 (77%)	0.33	34 (7%)	15 13	23, 39, 94, 129	0
2	B	809/937 (86%)	0.34	64 (7%)	12 10	24, 51, 98, 132	0
All	All	1279/1542 (82%)	0.34	98 (7%)	13 11	23, 47, 98, 132	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	403	VAL	7.1
2	B	645	ARG	6.6
2	B	628	VAL	6.0
1	A	401	PRO	5.1
2	B	410	ASP	5.0
2	B	637	LEU	4.9
2	B	2682	LEU	4.7
2	B	358	ILE	4.7
1	A	390	ILE	4.6
2	B	644	PRO	4.3
2	B	622	GLY	4.3
2	B	577	ILE	4.2
1	A	394	GLN	4.1
2	B	326	HIS	4.1
2	B	646	THR	4.1
1	A	387	GLY	4.0
1	A	392	LEU	3.9
1	A	398	VAL	3.8
1	A	397	GLN	3.7
2	B	359	GLN	3.7
1	A	382	VAL	3.7
2	B	590	TRP	3.6
2	B	850	GLU	3.6
2	B	408	SER	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	638	ARG	3.4
1	A	372	GLU	3.4
1	A	400	GLY	3.4
2	B	255	ASN	3.4
1	A	6	SER	3.3
2	B	635	LEU	3.3
2	B	632	LEU	3.3
2	B	418	SER	3.3
1	A	399	HIS	3.3
1	A	389	GLY	3.2
2	B	598	LEU	3.2
1	A	393	ALA	3.1
1	A	405	VAL	3.1
1	A	391	SER	3.1
2	B	323	PHE	3.0
2	B	930	VAL	2.9
2	B	415	GLN	2.9
2	B	195	THR	2.9
2	B	550	ILE	2.9
2	B	454	LEU	2.9
2	B	643	GLU	2.9
2	B	666	ASP	2.8
2	B	452	SER	2.8
2	B	595	VAL	2.8
1	A	395	ALA	2.8
1	A	375	GLN	2.8
1	A	388	GLN	2.8
2	B	2637	ALA	2.7
2	B	649	LYS	2.7
1	A	5	ASP	2.7
2	B	357	LYS	2.7
1	A	368	ALA	2.6
1	A	396	GLN	2.6
1	A	381	VAL	2.6
2	B	2549	ARG	2.5
2	B	407	GLU	2.5
1	A	374	GLN	2.5
2	B	602	PHE	2.5
1	A	415	LYS	2.5
2	B	491	ALA	2.5
1	A	404	GLY	2.4
1	A	35	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	406	VAL	2.4
1	A	556	ARG	2.4
2	B	406	PRO	2.4
2	B	741	ARG	2.4
1	A	497	ALA	2.3
2	B	276	TYR	2.3
1	A	492	ARG	2.3
2	B	2683	ARG	2.3
2	B	412	MET	2.3
2	B	933	ASN	2.3
2	B	931	GLU	2.3
2	B	420	LEU	2.3
2	B	414	PRO	2.2
2	B	682	PHE	2.2
2	B	648	PRO	2.2
1	A	378	ASN	2.2
2	B	932	ARG	2.2
2	B	642	VAL	2.2
2	B	626	TRP	2.2
2	B	688	ASP	2.2
2	B	623	ARG	2.1
2	B	450	ASP	2.1
2	B	196	GLU	2.1
2	B	620	ILE	2.1
2	B	551	GLU	2.1
2	B	651	LYS	2.1
2	B	636	ASP	2.1
2	B	589	PRO	2.1
1	A	36	ASP	2.0
2	B	360	PRO	2.0
2	B	670	ALA	2.0
2	B	495	LYS	2.0

## 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](#)

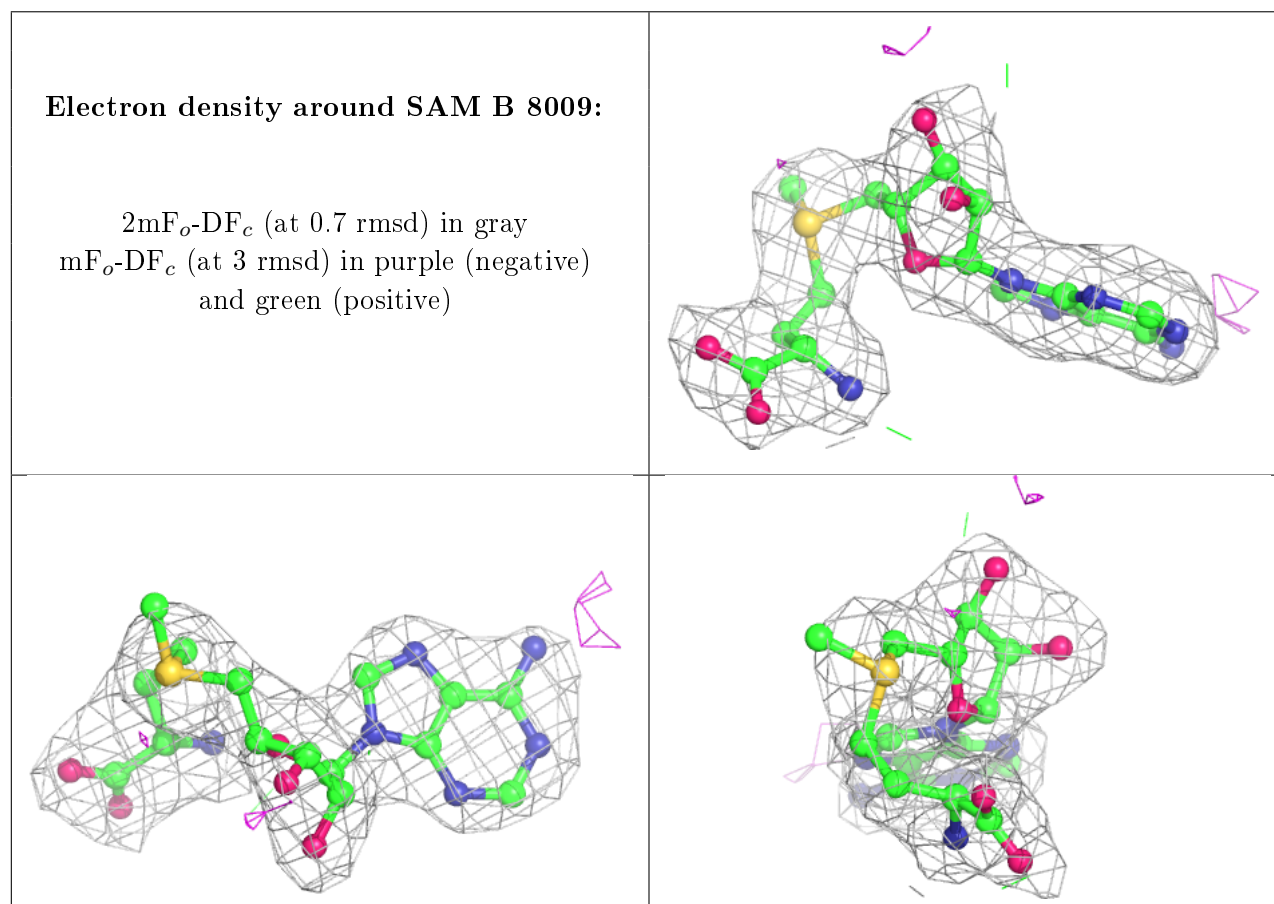
There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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
4	SAM	B	8009	27/27	0.95	0.14	31,42,54,56	0
3	ZN	B	8005	1/1	0.98	0.08	48,48,48,48	0
3	ZN	B	8007	1/1	0.99	0.15	32,32,32,32	0
3	ZN	B	8008	1/1	0.99	0.04	73,73,73,73	0
3	ZN	B	8002	1/1	0.99	0.13	33,33,33,33	0
3	ZN	B	8001	1/1	1.00	0.15	36,36,36,36	0
3	ZN	B	8003	1/1	1.00	0.14	40,40,40,40	0
3	ZN	B	8006	1/1	1.00	0.11	49,49,49,49	0
3	ZN	B	8004	1/1	1.00	0.08	52,52,52,52	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.