



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 09:31 AM EDT

PDB ID : 5WF7  
Title : Chaetomium thermophilum Polycomb Repressive Complex 2 bound to GSK126  
Authors : Bratkowski, M.A.; Liu, X.  
Deposited on : 2017-07-11  
Resolution : 2.50 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

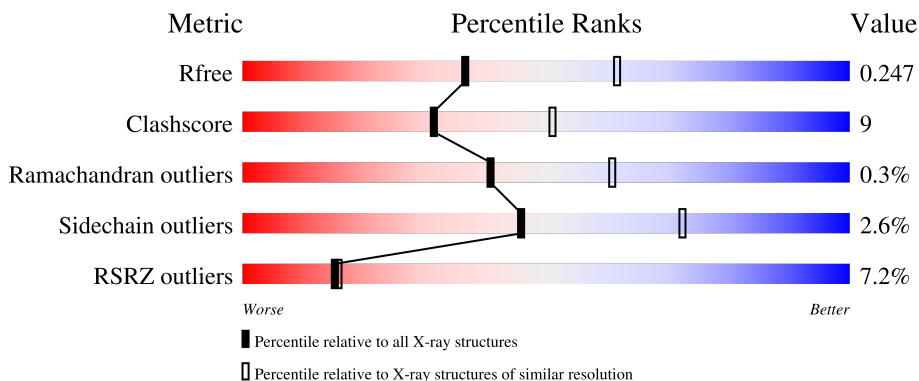
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	 4% 62% 13% 25%
2	B	937	 7% 63% 18% 18%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10065 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
			Total	C	N	O	S			
1	A	453	3579	2289	614	657	19	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-39	MET	-	initiating methionine	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 chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	765	6151	3885	1112	1114	40	0	0	0

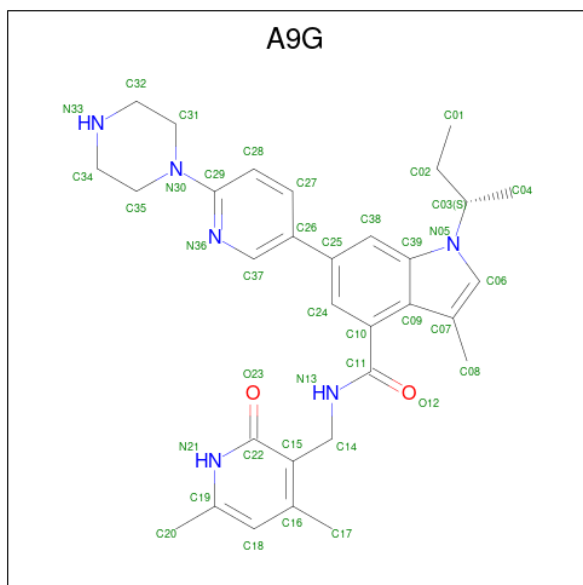
There are 15 discrepancies between the modelled and reference sequences:

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 1-[(2S)-butan-2-yl]-N-[(4,6-dimethyl-2-oxo-1,2-dihydropyridin-3-yl)methyl]-3-methyl-6-[6-(piperazin-1-yl)pyridin-3-yl]-1H-indole-4-carboxamide (three-letter code: A9G) (formula: C<sub>31</sub>H<sub>38</sub>N<sub>6</sub>O<sub>2</sub>).

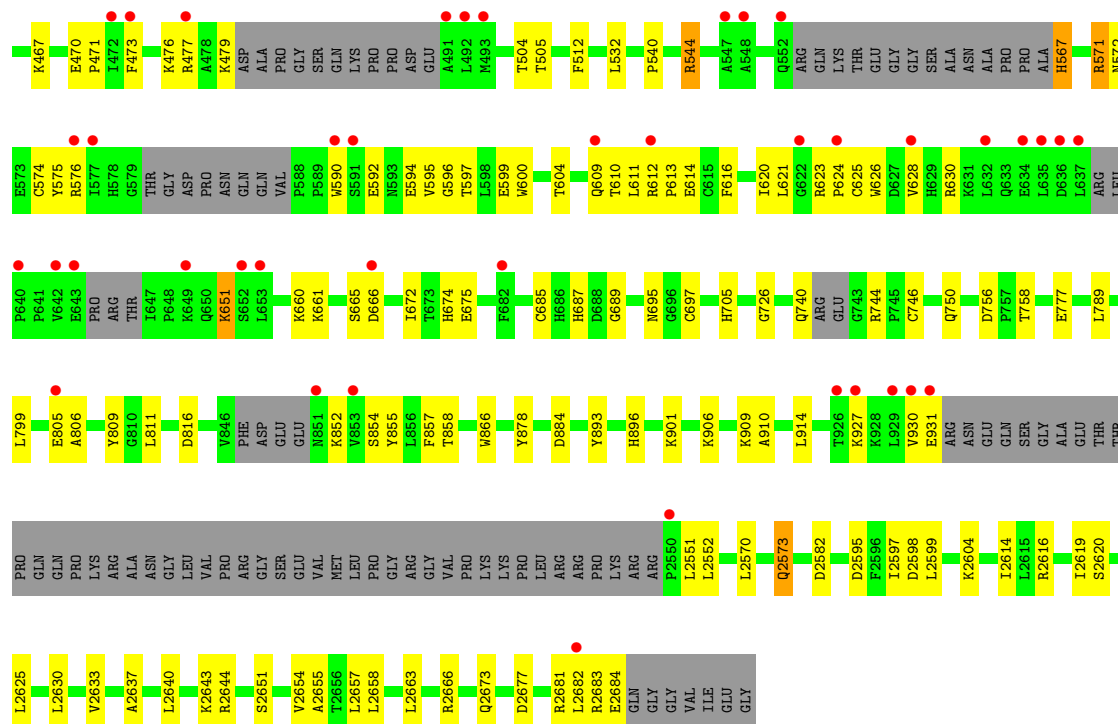


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
4	B	1	Total	C	N	O	0	0
			39	31	6	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	134	Total	O	0	0
			134	134		
5	B	154	Total	O	0	0
			154	154		





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.88Å 136.30Å 223.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.14 – 2.50 44.14 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.5 (44.14-2.50) 93.5 (44.14-2.50)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.35 (at 2.48Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, $R_{free}$	0.191 , 0.247 0.191 , 0.247	Depositor DCC
$R_{free}$ test set	2875 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	37.0	Xtrriage
Anisotropy	0.125	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 50.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10065	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: A9G, 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	0.48	0/3683	0.64	0/5013
2	B	0.44	0/6290	0.61	0/8491
All	All	0.46	0/9973	0.62	0/13504

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 [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	3579	0	3437	54	0
2	B	6151	0	6065	128	0
3	B	8	0	0	0	0
4	B	39	0	0	0	0
5	A	134	0	0	1	0
5	B	154	0	0	6	0
All	All	10065	0	9502	174	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 9.

All (174) 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:612:ARG:HG2	2:B:614:GLU:OE2	1.44	1.17
2:B:626:TRP:HE3	2:B:630:ARG:NH2	1.43	1.16
2:B:394:THR:HG22	2:B:397:ASN:HB2	1.41	1.02
2:B:612:ARG:HG3	2:B:613:PRO:HD2	1.46	0.96
2:B:626:TRP:CE3	2:B:630:ARG:NH2	2.31	0.96
1:A:77:ASP:HB2	2:B:280:ARG:HH11	1.31	0.95
2:B:604:THR:HG21	2:B:2655:ALA:HA	1.48	0.94
2:B:197:TRP:CE3	2:B:202:ILE:HG22	2.10	0.86
2:B:626:TRP:HE3	2:B:630:ARG:HH22	0.86	0.85
2:B:540:PRO:O	2:B:544:ARG:HD2	1.79	0.82
2:B:202:ILE:HD11	2:B:439:MET:O	1.83	0.77
1:A:242:ASN:O	2:B:361:ARG:NH2	2.18	0.76
1:A:395:ALA:HB1	1:A:405:VAL:HG21	1.68	0.74
1:A:225:GLU:OE1	5:A:601:HOH:O	2.07	0.73
2:B:2551:LEU:C	2:B:2552:LEU:HD12	2.08	0.73
1:A:365:ARG:NH1	2:B:226:GLU:OE1	2.22	0.72
2:B:574:CYS:SG	2:B:576:ARG:HG2	2.29	0.72
2:B:2640:LEU:O	5:B:8101:HOH:O	2.07	0.71
2:B:197:TRP:NE1	2:B:390:ILE:HD12	2.06	0.70
2:B:540:PRO:O	2:B:544:ARG:CD	2.41	0.68
1:A:77:ASP:HB2	2:B:280:ARG:NH1	2.09	0.67
1:A:106:THR:OG1	1:A:108:GLN:HG2	1.95	0.65
2:B:268:LYS:HE3	5:B:8157:HOH:O	1.97	0.65
2:B:609:GLN:HG3	2:B:610:THR:HG23	1.79	0.65
1:A:380:ARG:O	1:A:380:ARG:HG3	1.97	0.64
2:B:660:LYS:O	2:B:744:ARG:NH1	2.31	0.64
1:A:290:ASP:OD2	1:A:293:LYS:NZ	2.31	0.63
2:B:222:ASN:O	2:B:226:GLU:HG3	2.01	0.60
2:B:394:THR:HG23	2:B:397:ASN:H	1.66	0.60
2:B:209:LEU:O	2:B:212:GLU:HG2	2.01	0.60
2:B:2614:ILE:HD11	2:B:2619:ILE:HD12	1.83	0.59
2:B:2614:ILE:HD11	2:B:2619:ILE:CD1	2.33	0.59
2:B:665:SER:OG	2:B:666:ASP:N	2.36	0.59
2:B:2654:VAL:HG23	2:B:2663:LEU:HD23	1.84	0.59
2:B:394:THR:CG2	2:B:397:ASN:HB2	2.26	0.58
2:B:574:CYS:HA	2:B:625:CYS:HB3	1.85	0.58
1:A:179:CYS:SG	1:A:230:ILE:HD12	2.44	0.58
2:B:672:ILE:HG23	2:B:705:HIS:HB2	1.86	0.58
2:B:2570:LEU:HD12	2:B:2573:GLN:OE1	2.05	0.57
1:A:40:PHE:HB3	1:A:540:VAL:HB	1.87	0.57
1:A:186:HIS:CG	1:A:190:LEU:HD21	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:GLN:HG2	1:A:407:MET:HB3	1.88	0.56
2:B:2625:LEU:HD21	2:B:2657:LEU:HD13	1.88	0.56
2:B:651:LYS:H	2:B:651:LYS:HD2	1.71	0.56
1:A:398:VAL:HG12	1:A:399:HIS:CE1	2.41	0.55
1:A:307:SER:N	2:B:467:LYS:HE2	2.21	0.55
2:B:884:ASP:OD2	2:B:906:LYS:NZ	2.37	0.55
1:A:120:VAL:HB	1:A:134:LEU:HB2	1.86	0.55
2:B:592:GLU:HA	2:B:595:VAL:HG12	1.88	0.55
1:A:9:TRP:CH2	1:A:362:GLU:HG3	2.42	0.54
2:B:575:TYR:HD1	2:B:625:CYS:SG	2.31	0.54
2:B:893:TYR:CE2	2:B:896:HIS:HA	2.43	0.54
2:B:432:GLN:O	2:B:432:GLN:HG3	2.07	0.54
2:B:567:HIS:O	2:B:576:ARG:NH1	2.41	0.54
2:B:396:SER:O	2:B:400:ARG:HG3	2.08	0.53
2:B:661:LYS:HG2	2:B:726:GLY:O	2.08	0.53
2:B:467:LYS:NZ	5:B:8104:HOH:O	2.33	0.53
2:B:612:ARG:CG	2:B:614:GLU:OE2	2.38	0.53
2:B:571:ARG:NH1	2:B:2673:GLN:HG3	2.23	0.53
1:A:366:PHE:CZ	1:A:408:LYS:HG3	2.44	0.53
2:B:685:CYS:HB2	2:B:687:HIS:CD2	2.45	0.52
2:B:571:ARG:HD2	5:B:8105:HOH:O	2.08	0.52
1:A:181:LEU:HD13	1:A:214:TRP:CG	2.45	0.52
2:B:397:ASN:OD1	2:B:400:ARG:HD2	2.11	0.51
2:B:927:LYS:O	2:B:931:GLU:HG2	2.10	0.51
2:B:2682:LEU:C	2:B:2684:GLU:H	2.15	0.51
1:A:177:CYS:O	1:A:227:PRO:HB3	2.11	0.51
2:B:443:ALA:HA	2:B:446:ARG:HB3	1.92	0.51
2:B:789:LEU:HD11	2:B:901:LYS:HB3	1.91	0.51
2:B:476:LYS:HG2	2:B:2595:ASP:HB3	1.93	0.50
2:B:689:GLY:HA3	2:B:695:ASN:OD1	2.11	0.50
2:B:927:LYS:HA	2:B:930:VAL:HG22	1.93	0.50
2:B:811:LEU:HD23	2:B:914:LEU:HD12	1.94	0.50
2:B:816:ASP:OD1	2:B:909:LYS:HG2	2.12	0.50
2:B:612:ARG:HG3	2:B:613:PRO:CD	2.32	0.50
1:A:137:HIS:NE2	1:A:156:SER:HB2	2.27	0.50
1:A:380:ARG:NH1	1:A:404:GLY:N	2.60	0.50
1:A:391:SER:O	1:A:393:ALA:N	2.45	0.50
1:A:360:PHE:CE1	1:A:504:LEU:HD21	2.47	0.49
2:B:597:THR:HA	2:B:600:TRP:CZ2	2.47	0.49
2:B:512:PHE:CD2	2:B:2625:LEU:HD13	2.47	0.49
2:B:366:ALA:HA	2:B:454:LEU:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:444:TRP:CD1	2:B:459:LEU:HB2	2.47	0.49
2:B:590:TRP:HA	2:B:623:ARG:NH2	2.27	0.48
1:A:98:SER:HA	1:A:112:CYS:O	2.14	0.48
2:B:614:GLU:HB3	2:B:625:CYS:SG	2.53	0.48
2:B:746:CYS:O	2:B:750:GLN:HG3	2.13	0.48
2:B:597:THR:HA	2:B:600:TRP:CE2	2.49	0.48
1:A:13:ARG:NH2	2:B:275:GLU:HG3	2.30	0.47
2:B:198:THR:O	2:B:202:ILE:HG23	2.13	0.47
2:B:592:GLU:HA	2:B:595:VAL:CG1	2.44	0.47
2:B:604:THR:HG21	2:B:2655:ALA:CA	2.31	0.47
2:B:799:LEU:HD13	2:B:878:TYR:CD2	2.50	0.47
1:A:40:PHE:CB	1:A:540:VAL:HB	2.44	0.47
1:A:334:TYR:O	1:A:341:PRO:HA	2.15	0.47
2:B:630:ARG:HB2	2:B:630:ARG:HH21	1.80	0.47
2:B:666:ASP:N	2:B:666:ASP:OD1	2.43	0.47
2:B:221:VAL:O	2:B:225:LEU:HG	2.15	0.46
1:A:386:GLN:HA	1:A:390:ILE:HD11	1.97	0.46
2:B:504:THR:HG22	2:B:532:LEU:HD12	1.97	0.46
1:A:75:ASP:HB3	1:A:78:ALA:HB2	1.97	0.46
1:A:248:VAL:HG23	1:A:257:SER:HB3	1.98	0.46
2:B:374:ALA:HB2	2:B:457:VAL:HG21	1.97	0.46
2:B:2551:LEU:O	2:B:2552:LEU:HD12	2.15	0.46
1:A:307:SER:N	2:B:467:LYS:HG2	2.31	0.46
2:B:651:LYS:H	2:B:651:LYS:CD	2.28	0.46
2:B:572:ASN:OD1	2:B:624:PRO:HA	2.16	0.46
2:B:2643:LYS:NZ	5:B:8113:HOH:O	2.49	0.46
1:A:13:ARG:HH22	2:B:275:GLU:HG3	1.81	0.45
1:A:179:CYS:HB2	1:A:219:PHE:CE1	2.52	0.45
1:A:310:ALA:HB1	1:A:312:PHE:O	2.16	0.45
2:B:390:ILE:HB	2:B:393:CYS:HB2	1.98	0.45
2:B:630:ARG:NH2	2:B:630:ARG:HB2	2.31	0.45
1:A:93:GLU:CD	1:A:117:GLU:HB2	2.38	0.45
2:B:444:TRP:CZ2	2:B:462:ILE:HD12	2.52	0.45
2:B:470:GLU:HB3	2:B:471:PRO:HD3	1.99	0.44
2:B:852:LYS:HD3	2:B:855:TYR:CE1	2.53	0.44
2:B:909:LYS:HD3	2:B:910:ALA:O	2.17	0.44
2:B:2597:ILE:HD12	2:B:2598:ASP:N	2.32	0.44
1:A:235:PHE:HD2	1:A:297:SER:HB2	1.81	0.44
1:A:334:TYR:HB2	1:A:530:TRP:CD2	2.52	0.44
2:B:611:LEU:HD12	2:B:612:ARG:H	1.81	0.44
1:A:408:LYS:HE2	1:A:408:LYS:HB3	1.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:460:ARG:O	2:B:464:MET:HG2	2.18	0.43
2:B:620:ILE:HD13	2:B:620:ILE:HA	1.82	0.43
1:A:377:TYR:HB3	1:A:380:ARG:HG3	2.00	0.43
2:B:2633:VAL:O	2:B:2637:ALA:HB2	2.18	0.43
2:B:2677:ASP:O	2:B:2681:ARG:HB2	2.17	0.43
2:B:2582:ASP:OD2	2:B:2616:ARG:NE	2.50	0.43
2:B:301:PRO:HB2	2:B:809:TYR:CE2	2.53	0.43
2:B:370:GLN:HG2	2:B:456:ARG:O	2.18	0.43
2:B:927:LYS:HA	2:B:927:LYS:HD3	1.76	0.43
1:A:293:LYS:HD3	1:A:293:LYS:HA	1.80	0.43
2:B:479:LYS:HA	2:B:505:THR:HG21	2.01	0.43
2:B:756:ASP:OD1	2:B:758:THR:N	2.44	0.43
2:B:2643:LYS:HG3	5:B:8113:HOH:O	2.18	0.43
2:B:390:ILE:O	2:B:393:CYS:HB2	2.19	0.43
2:B:202:ILE:HG21	2:B:202:ILE:HD13	1.52	0.43
2:B:197:TRP:CE2	2:B:390:ILE:HD12	2.54	0.42
2:B:2663:LEU:HD12	2:B:2663:LEU:HA	1.90	0.42
2:B:2682:LEU:O	2:B:2684:GLU:N	2.38	0.42
2:B:2599:LEU:HB2	2:B:2604:LYS:HE2	2.00	0.42
2:B:2630:LEU:HA	2:B:2633:VAL:HG12	2.01	0.42
2:B:2683:ARG:C	2:B:2684:GLU:OE1	2.58	0.42
2:B:265:MET:HG2	2:B:290:VAL:HG21	2.01	0.42
2:B:805:GLU:O	2:B:805:GLU:HG3	2.19	0.42
2:B:594:GLU:HB3	2:B:621:LEU:HD21	2.01	0.42
2:B:596:GLY:HA2	2:B:599:GLU:OE1	2.20	0.42
2:B:687:HIS:NE2	2:B:697:CYS:HB2	2.34	0.42
1:A:371:LYS:HB2	1:A:371:LYS:HE2	1.83	0.42
2:B:200:ASP:OD1	2:B:200:ASP:N	2.52	0.41
2:B:441:THR:O	2:B:444:TRP:HB3	2.21	0.41
1:A:54:PRO:HA	1:A:55:PRO:HD3	1.93	0.41
1:A:266:VAL:HG12	1:A:268:TRP:HD1	1.84	0.41
2:B:616:PHE:CZ	2:B:2654:VAL:HG11	2.56	0.41
1:A:42:ASP:OD1	1:A:527:GLN:HG2	2.20	0.41
1:A:413:VAL:O	1:A:498:TRP:NE1	2.47	0.41
2:B:364:LYS:HG3	2:B:365:ILE:N	2.34	0.41
2:B:604:THR:CG2	2:B:2658:LEU:HB2	2.51	0.41
1:A:235:PHE:CD2	1:A:297:SER:HB2	2.55	0.41
1:A:308:ARG:HG2	1:A:309:PRO:HD2	2.02	0.41
1:A:93:GLU:HG3	1:A:117:GLU:H	1.85	0.41
1:A:246:ASP:OD2	1:A:328:PHE:N	2.54	0.41
1:A:381:VAL:HA	1:A:404:GLY:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:442:GLU:O	2:B:443:ALA:CB	2.69	0.41
2:B:858:THR:HA	2:B:866:TRP:CD1	2.56	0.41
2:B:240:LYS:HD3	2:B:240:LYS:HA	1.87	0.41
1:A:13:ARG:HA	1:A:13:ARG:HD3	1.88	0.40
1:A:365:ARG:HG3	1:A:365:ARG:HH21	1.86	0.40
2:B:2682:LEU:O	2:B:2682:LEU:HD23	2.22	0.40
2:B:202:ILE:HD11	2:B:439:MET:C	2.40	0.40
1:A:25:LYS:HD3	1:A:25:LYS:HA	1.84	0.40
2:B:208:VAL:O	2:B:211:GLU:HB2	2.22	0.40
2:B:674:HIS:CD2	2:B:675:GLU:HG2	2.56	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	443/605 (73%)	425 (96%)	17 (4%)	1 (0%)	47 68
2	B	739/937 (79%)	706 (96%)	30 (4%)	3 (0%)	34 54
All	All	1182/1542 (77%)	1131 (96%)	47 (4%)	4 (0%)	41 61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	443	ALA
2	B	806	ALA
1	A	393	ALA
2	B	260	GLU

### 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	382/495 (77%)	376 (98%)	6 (2%)	62 84
2	B	667/816 (82%)	646 (97%)	21 (3%)	40 67
All	All	1049/1311 (80%)	1022 (97%)	27 (3%)	46 72

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	175	GLN
1	A	300	THR
1	A	380	ARG
1	A	385	ASP
1	A	512	LYS
1	A	515	ARG
2	B	200	ASP
2	B	230	LYS
2	B	264	THR
2	B	362	SER
2	B	446	ARG
2	B	473	PHE
2	B	477	ARG
2	B	544	ARG
2	B	567	HIS
2	B	571	ARG
2	B	628	VAL
2	B	651	LYS
2	B	740	GLN
2	B	777	GLU
2	B	854	SER
2	B	857	PHE
2	B	2573	GLN
2	B	2620	SER
2	B	2644	ARG
2	B	2651	SER
2	B	2666	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides 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	A9G	B	8009	-	37,43,43	3.03	18 (48%)	46,62,62	2.56	15 (32%)

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	A9G	B	8009	-	-	2/19/31/31	0/5/5/5

All (18) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	8009	A9G	C29-N30	7.07	1.51	1.37
4	B	8009	A9G	C10-C11	6.52	1.61	1.50
4	B	8009	A9G	O23-C22	6.42	1.35	1.23
4	B	8009	A9G	C35-N30	5.30	1.55	1.46
4	B	8009	A9G	C11-N13	4.81	1.44	1.33
4	B	8009	A9G	C06-N05	4.48	1.44	1.38
4	B	8009	A9G	C31-N30	4.21	1.53	1.46
4	B	8009	A9G	C09-C39	4.07	1.47	1.42
4	B	8009	A9G	C20-C19	3.87	1.57	1.50
4	B	8009	A9G	C02-C03	3.05	1.66	1.49
4	B	8009	A9G	C18-C19	2.89	1.43	1.36
4	B	8009	A9G	C35-C34	2.89	1.58	1.51
4	B	8009	A9G	C24-C25	2.87	1.44	1.39
4	B	8009	A9G	O12-C11	-2.60	1.18	1.23
4	B	8009	A9G	C31-C32	2.50	1.57	1.51
4	B	8009	A9G	C28-C29	2.47	1.45	1.39
4	B	8009	A9G	C08-C07	2.11	1.55	1.51
4	B	8009	A9G	C37-C26	2.11	1.43	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	8009	A9G	C15-C22-N21	9.71	122.94	115.69
4	B	8009	A9G	O23-C22-C15	-6.31	116.84	124.54
4	B	8009	A9G	N36-C29-N30	4.49	123.51	116.79
4	B	8009	A9G	C28-C29-N36	-4.14	115.82	123.41
4	B	8009	A9G	C22-N21-C19	-3.95	121.38	125.20
4	B	8009	A9G	C07-C06-N05	3.52	111.82	107.49
4	B	8009	A9G	C32-C31-N30	3.17	117.35	110.48
4	B	8009	A9G	C27-C26-C25	3.02	126.58	121.36
4	B	8009	A9G	C10-C11-N13	2.68	119.92	116.30
4	B	8009	A9G	C38-C25-C26	2.66	127.12	121.05
4	B	8009	A9G	C37-N36-C29	2.62	122.08	117.30
4	B	8009	A9G	C28-C27-C26	2.49	124.72	121.13
4	B	8009	A9G	C27-C26-C37	-2.24	111.23	116.76
4	B	8009	A9G	C17-C16-C18	2.21	123.25	118.60
4	B	8009	A9G	C18-C19-N21	-2.03	116.67	119.13

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	8009	A9G	C01-C02-C03-C04

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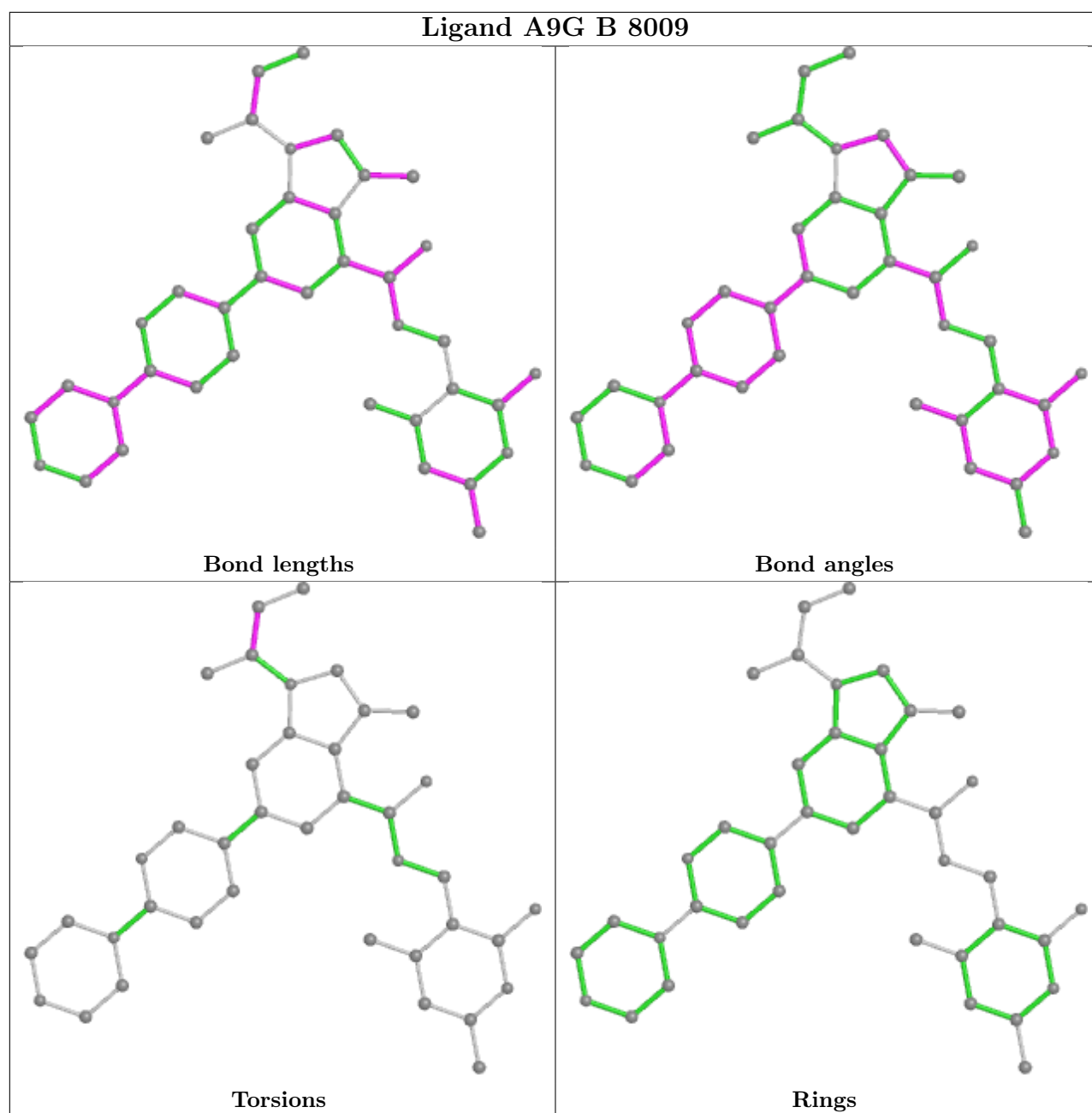
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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
4	B	8009	A9G	C01-C02-C03-N05

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	453/605 (74%)	0.18	22 (4%) 29 31	18, 35, 95, 126	0
2	B	765/937 (81%)	0.33	66 (8%) 10 10	18, 53, 93, 137	0
All	All	1218/1542 (78%)	0.27	88 (7%) 15 16	18, 47, 94, 137	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	930	VAL	6.2
2	B	637	LEU	5.6
2	B	929	LEU	5.0
2	B	491	ALA	4.9
1	A	389	GLY	4.8
2	B	635	LEU	4.5
1	A	379	GLY	4.5
1	A	384	VAL	4.3
1	A	489	GLY	4.2
1	A	375	GLN	4.1
2	B	931	GLU	4.1
2	B	577	ILE	4.1
2	B	454	LEU	4.0
2	B	436	ASN	3.9
2	B	439	MET	3.8
1	A	393	ALA	3.8
2	B	649	LYS	3.8
2	B	666	ASP	3.6
2	B	927	LYS	3.5
1	A	380	ARG	3.4
2	B	452	SER	3.4
2	B	473	PHE	3.4
1	A	492	ARG	3.4
2	B	472	ILE	3.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	636	ASP	3.4
2	B	492	LEU	3.3
2	B	433	ALA	3.3
1	A	372	GLU	3.2
2	B	643	GLU	3.2
1	A	378	ASN	3.2
2	B	642	VAL	3.2
2	B	276	TYR	3.1
2	B	652	SER	3.1
2	B	632	LEU	3.0
2	B	653	LEU	3.0
1	A	405	VAL	2.9
1	A	493	GLU	2.9
2	B	590	TRP	2.9
1	A	370	LEU	2.9
2	B	851	ASN	2.8
1	A	381	VAL	2.7
2	B	393	CYS	2.7
2	B	640	PRO	2.7
2	B	552	GLN	2.7
2	B	444	TRP	2.7
2	B	323	PHE	2.6
2	B	609	GLN	2.6
2	B	431	PRO	2.6
2	B	447	VAL	2.6
2	B	576	ARG	2.6
2	B	634	GLU	2.6
2	B	2682	LEU	2.5
2	B	2550	PRO	2.5
2	B	322	ASN	2.5
2	B	682	PHE	2.5
2	B	197	TRP	2.5
2	B	453	LYS	2.5
1	A	398	VAL	2.4
1	A	392	LEU	2.4
2	B	198	THR	2.4
1	A	495	LEU	2.4
2	B	622	GLY	2.3
2	B	401	PHE	2.3
1	A	373	ALA	2.3
2	B	591	SER	2.3
2	B	360	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	493	MET	2.2
2	B	477	ARG	2.2
2	B	628	VAL	2.2
2	B	451	GLN	2.2
2	B	437	ALA	2.2
2	B	548	ALA	2.2
2	B	438	SER	2.2
2	B	363	GLN	2.2
2	B	547	ALA	2.2
2	B	926	THR	2.2
1	A	394	GLN	2.1
2	B	612	ARG	2.1
1	A	374	GLN	2.1
1	A	397	GLN	2.1
2	B	402	MET	2.1
2	B	624	PRO	2.1
2	B	208	VAL	2.1
2	B	853	VAL	2.1
2	B	324	VAL	2.0
1	A	395	ALA	2.0
2	B	201	LYS	2.0
2	B	805	GLU	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 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.

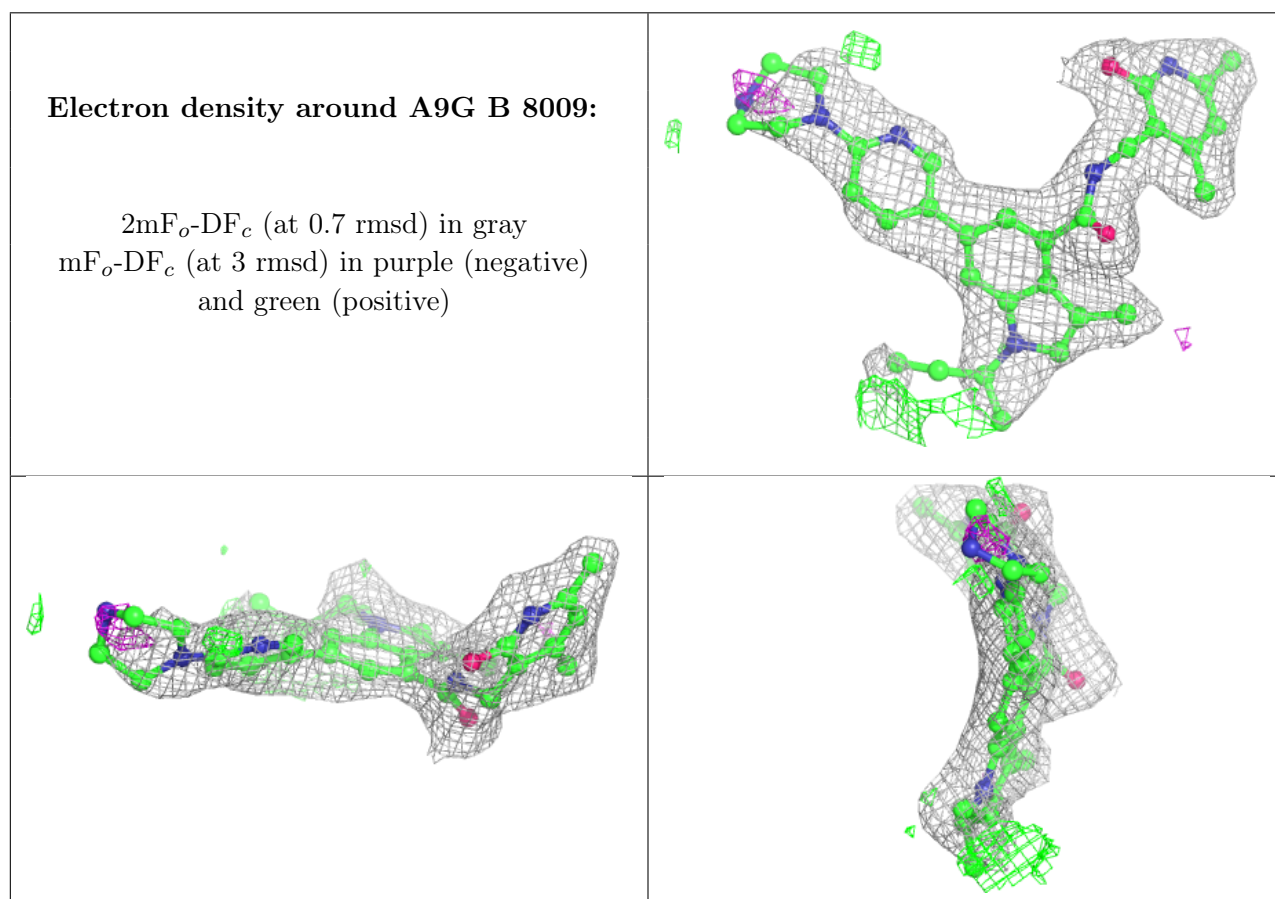
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	A9G	B	8009	39/39	0.89	0.18	27,46,69,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	B	8008	1/1	0.97	0.06	64,64,64,64	0
3	ZN	B	8006	1/1	0.98	0.09	48,48,48,48	0
3	ZN	B	8005	1/1	0.99	0.06	53,53,53,53	0
3	ZN	B	8001	1/1	0.99	0.12	44,44,44,44	0
3	ZN	B	8002	1/1	0.99	0.13	44,44,44,44	0
3	ZN	B	8004	1/1	0.99	0.06	52,52,52,52	0
3	ZN	B	8003	1/1	1.00	0.14	47,47,47,47	0
3	ZN	B	8007	1/1	1.00	0.10	30,30,30,30	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.