



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 16, 2022 – 12:17 PM EDT

PDB ID : 5WFD  
Title : Humanized mutant of the Chaetomium thermophilum Polycomb Repressive Complex 2 bound to the inhibitor GSK126  
Authors : Bratkowski, M.A.; Liu, X.  
Deposited on : 2017-07-11  
Resolution : 2.65 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	:	2.27
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)	:	2.27

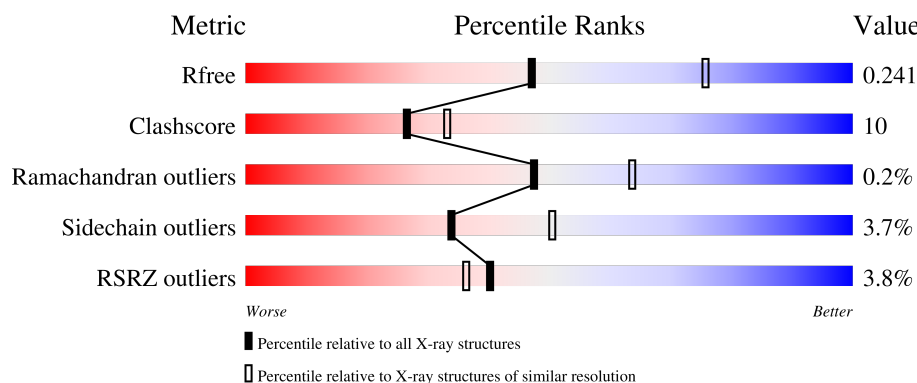
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

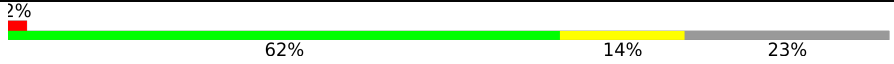

The reported resolution of this entry is 2.65 Å.

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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	605	
2	B	936	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9956 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	466	3682	2354	635	674	19	0	2	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
2	B	774	Total	C	N	O	S	0	0	0
			6227	3925	1125	1137	40			

There are 23 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	302	ILE	PRO	engineered mutation	UNP G0SDW4
B	304	TYR	ARG	engineered mutation	UNP G0SDW4
B	?	-	GLU	deletion	UNP G0SDW4
B	850	LYS	GLU	engineered mutation	UNP G0SDW4
B	851	TYR	ASN	engineered mutation	UNP G0SDW4
B	852	MET	LYS	engineered mutation	UNP G0SDW4
B	853	CYS	VAL	engineered mutation	UNP G0SDW4
B	855	PHE	TYR	engineered mutation	UNP G0SDW4
B	2524	LEU	-	linker	UNP G0SDW4

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Chain	Residue	Modelled	Actual	Comment	Reference
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

- | Mol | Chain | Residues | Atoms           | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 3   | B     | 8        | Total Zn<br>8 8 | 0       | 0       |

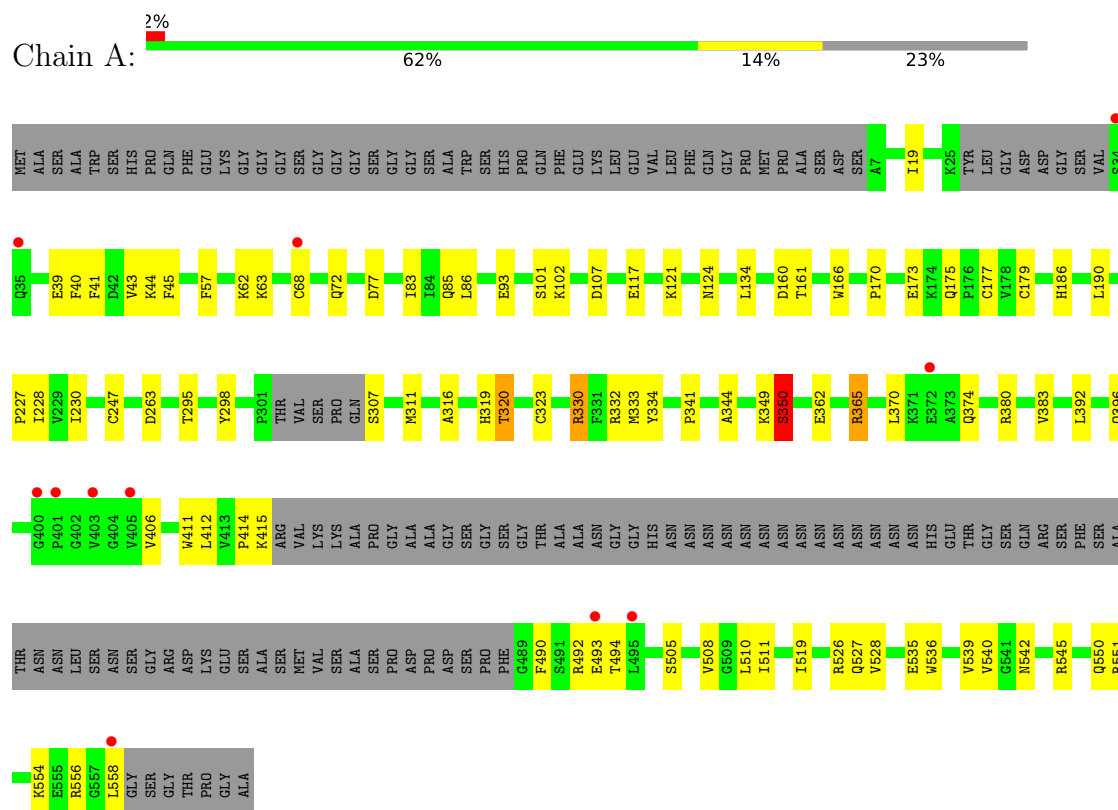
- 
- A9G
- Chemical structure diagram of A9G, showing a complex molecule with various rings and substituents. The structure includes a piperidine ring (N33, C31, C32, C34, C35, N30), a pyridine ring (N36, C29, C28, C27, C26, C37), a benzimidazole system (C25, C38, C39, C06, C07, C08, C09, C10, C11, O12, N13, C14, C15, C16, C17, C18, C19, C20, N21, C22, O23), and a substituted benzene ring (C01, C02, C03(S), C04, N05). The structure is labeled with atom IDs (N33, C31, C32, C34, C35, N30, C29, C28, C27, C26, C25, C38, C39, C06, C07, C08, C09, C10, C11, O12, N13, C14, C15, C16, C17, C18, C19, C20, N21, C22, O23, C01, C02, C03(S), C04, N05).

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

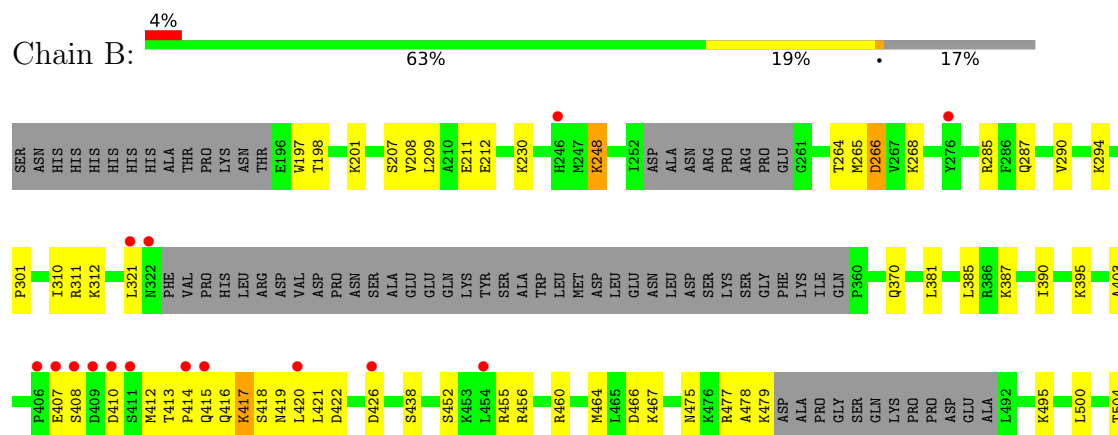
### 3 Residue-property plots [i](#)

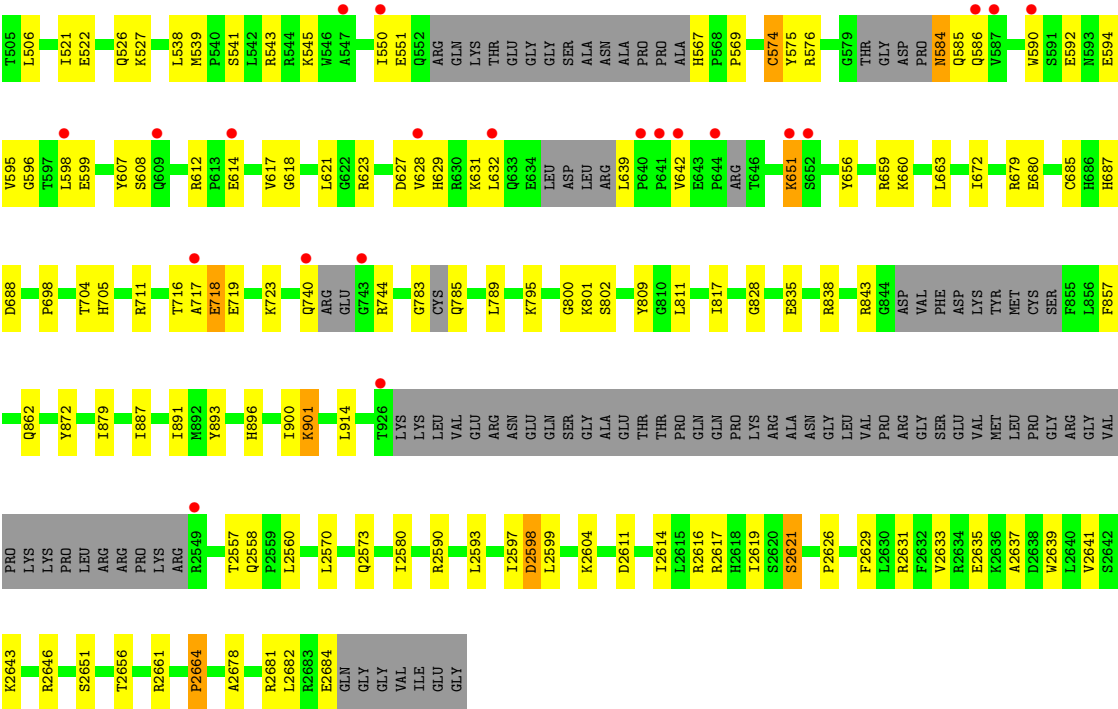
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Polycomb Protein EED



#### • Molecule 2: Histone-lysine-N-methyltransferase EZH2, Polycomb protein SUZ12 chimera





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.53Å 136.97Å 223.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.15 – 2.65 46.15 – 2.65	Depositor EDS
% Data completeness (in resolution range)	95.8 (46.15-2.65) 95.8 (46.15-2.65)	Depositor EDS
$R_{merge}$	0.21	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.59 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, $R_{free}$	0.181 , 0.240 0.182 , 0.241	Depositor DCC
$R_{free}$ test set	2476 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.1	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 42.2	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	0.93	EDS
Total number of atoms	9956	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, A9G

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	0.51	0/3794	0.66	0/5163
2	B	0.48	0/6368	0.63	0/8602
All	All	0.49	0/10162	0.64	0/13765

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3682	0	3557	73	0
2	B	6227	0	6113	134	0
3	B	8	0	0	0	0
4	B	39	0	0	1	0
All	All	9956	0	9670	202	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 10.

All (202) 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:68:CYS:SG	1:A:83:ILE:HG12	1.90	1.10
1:A:68:CYS:SG	1:A:83:ILE:CG1	2.56	0.92
1:A:72:GLN:OE1	1:A:554:LYS:NZ	2.03	0.91
2:B:415:GLN:HA	2:B:418:SER:HB3	1.53	0.91
2:B:717:ALA:HB2	2:B:723:LYS:HG2	1.57	0.85
2:B:594:GLU:HB3	2:B:621:LEU:HD21	1.58	0.84
2:B:594:GLU:CB	2:B:621:LEU:HD21	2.07	0.83
2:B:651:LYS:O	2:B:651:LYS:HD2	1.79	0.83
1:A:307:SER:HB3	2:B:467:LYS:HG2	1.60	0.83
2:B:198:THR:HG23	2:B:201:LYS:H	1.46	0.81
1:A:93:GLU:OE1	1:A:121:LYS:NZ	2.14	0.80
1:A:528:VAL:HG22	1:A:539:VAL:HG22	1.61	0.79
2:B:421:LEU:HD23	2:B:426:ASP:OD1	1.83	0.78
1:A:41:PHE:HE2	1:A:62:LYS:HE2	1.49	0.78
2:B:835:GLU:OE2	2:B:838:ARG:NH1	2.19	0.76
2:B:585:GLN:HG3	2:B:586:GLN:H	1.51	0.75
2:B:412:MET:HE3	2:B:417:LYS:HB3	1.68	0.74
2:B:679:ARG:HH11	2:B:679:ARG:HB3	1.55	0.70
1:A:160:ASP:O	1:A:161:THR:HB	1.93	0.69
2:B:475:ASN:HA	2:B:477:ARG:CZ	2.21	0.69
1:A:411:TRP:CZ3	1:A:412:LEU:CD1	2.76	0.69
2:B:679:ARG:HB3	2:B:679:ARG:NH1	2.07	0.69
2:B:495:LYS:HE2	2:B:599:GLU:OE2	1.92	0.68
2:B:716:THR:O	2:B:718:GLU:N	2.26	0.68
1:A:186:HIS:CG	1:A:190:LEU:HD21	2.28	0.68
1:A:392:LEU:O	1:A:396:GLN:HG3	1.93	0.68
2:B:2643:LYS:HB2	2:B:2646:ARG:HG3	1.75	0.68
2:B:266:ASP:OD2	2:B:285:ARG:HD2	1.94	0.66
2:B:265:MET:HG3	2:B:290:VAL:HG21	1.77	0.66
2:B:801:LYS:NZ	2:B:802:SER:O	2.28	0.66
2:B:569:PRO:HA	2:B:576:ARG:HH11	1.60	0.66
2:B:592:GLU:HA	2:B:595:VAL:HG22	1.78	0.66
2:B:2599:LEU:HB2	2:B:2604:LYS:HZ3	1.59	0.66
2:B:594:GLU:CB	2:B:621:LEU:CD2	2.74	0.65
2:B:679:ARG:HH11	2:B:679:ARG:CB	2.09	0.65
1:A:350:SER:O	1:A:519:ILE:HB	1.96	0.65
1:A:415:LYS:HE3	1:A:493:GLU:HB3	1.79	0.65
2:B:717:ALA:HB2	2:B:723:LYS:CG	2.26	0.64
1:A:370:LEU:O	1:A:374:GLN:HG3	1.98	0.64
2:B:500:LEU:HD13	2:B:2656:THR:HG22	1.80	0.63
2:B:585:GLN:CG	2:B:586:GLN:H	2.11	0.63
2:B:672:ILE:HD13	2:B:704:THR:HG22	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:569:PRO:HB3	2:B:576:ARG:HD3	1.82	0.62
2:B:717:ALA:HB2	2:B:723:LYS:HB3	1.81	0.62
1:A:68:CYS:SG	1:A:83:ILE:HG13	2.39	0.62
1:A:350:SER:C	1:A:519:ILE:HD12	2.21	0.61
2:B:594:GLU:HB2	2:B:621:LEU:CD2	2.31	0.60
2:B:420:LEU:HB3	2:B:421:LEU:HD12	1.84	0.59
1:A:177:CYS:O	1:A:227:PRO:HB3	2.03	0.59
2:B:569:PRO:HA	2:B:576:ARG:NH1	2.18	0.59
1:A:350:SER:O	1:A:519:ILE:CB	2.51	0.59
2:B:198:THR:CG2	2:B:201:LYS:H	2.16	0.58
1:A:41:PHE:CE2	1:A:62:LYS:HE2	2.35	0.58
1:A:411:TRP:CZ3	1:A:412:LEU:HD11	2.38	0.57
1:A:247:CYS:HB2	1:A:330:ARG:HG3	1.86	0.57
2:B:607:TYR:HE1	2:B:639:LEU:HD12	1.69	0.57
2:B:2682:LEU:O	2:B:2684:GLU:N	2.33	0.57
1:A:350:SER:O	1:A:519:ILE:CG1	2.52	0.57
2:B:594:GLU:HB2	2:B:621:LEU:HD21	1.82	0.56
2:B:408:SER:O	2:B:412:MET:HB2	2.05	0.56
1:A:350:SER:O	1:A:519:ILE:HD12	2.05	0.56
1:A:414:PRO:HA	1:A:494:THR:HG23	1.87	0.56
2:B:594:GLU:HB3	2:B:621:LEU:CD2	2.30	0.56
2:B:2593:LEU:HD11	2:B:2611:ASP:OD2	2.04	0.56
2:B:717:ALA:CB	2:B:723:LYS:HB3	2.35	0.56
1:A:102:LYS:HE3	1:A:107:ASP:OD1	2.05	0.56
1:A:411:TRP:CE3	1:A:412:LEU:CD1	2.89	0.56
2:B:607:TYR:CE1	2:B:639:LEU:HD12	2.40	0.56
2:B:656:TYR:HB2	2:B:663:LEU:HD23	1.88	0.55
2:B:550:ILE:HD13	2:B:642:VAL:HG23	1.88	0.55
1:A:39:GLU:HG2	1:A:542:ASN:HA	1.89	0.55
1:A:307:SER:HB3	2:B:467:LYS:CG	2.36	0.55
2:B:311:ARG:NH1	2:B:2580:ILE:HD12	2.21	0.55
2:B:2631:ARG:O	2:B:2635:GLU:HG3	2.07	0.55
2:B:608:SER:O	2:B:612:ARG:NH1	2.39	0.55
2:B:598:LEU:HD12	2:B:617:VAL:HG21	1.90	0.54
2:B:264:THR:HG22	2:B:287:GLN:OE1	2.08	0.54
2:B:575:TYR:HD2	2:B:629:HIS:ND1	2.06	0.53
2:B:717:ALA:HB2	2:B:723:LYS:CB	2.38	0.53
1:A:307:SER:HB2	2:B:466:ASP:HA	1.91	0.53
2:B:301:PRO:HB2	2:B:809:TYR:CE2	2.44	0.53
1:A:43:VAL:O	1:A:44:LYS:HG2	2.09	0.53
2:B:651:LYS:HD2	2:B:651:LYS:C	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:208:VAL:O	2:B:211:GLU:HG2	2.09	0.53
2:B:2678:ALA:HA	2:B:2681:ARG:CZ	2.39	0.53
1:A:319:HIS:HB2	1:A:510:LEU:HB3	1.91	0.52
1:A:542:ASN:O	1:A:545:ARG:HG3	2.10	0.52
2:B:310:ILE:HD12	2:B:312:LYS:O	2.08	0.52
1:A:39:GLU:CG	1:A:542:ASN:HA	2.40	0.52
2:B:598:LEU:HD21	2:B:632:LEU:HD13	1.92	0.52
2:B:685:CYS:HB2	2:B:687:HIS:CD2	2.45	0.51
1:A:380:ARG:HB2	1:A:380:ARG:NH1	2.27	0.50
2:B:2619:ILE:HG22	2:B:2621:SER:H	1.76	0.50
1:A:179:CYS:SG	1:A:230:ILE:HD12	2.52	0.50
2:B:197:TRP:NE1	2:B:390:ILE:HG12	2.27	0.50
2:B:417:LYS:O	2:B:421:LEU:HD13	2.11	0.50
2:B:704:THR:HG23	2:B:705:HIS:ND1	2.26	0.50
1:A:349:LYS:O	1:A:350:SER:CB	2.59	0.50
2:B:197:TRP:CE2	2:B:390:ILE:HG12	2.47	0.49
2:B:321:LEU:HD22	2:B:838:ARG:HG2	1.93	0.49
2:B:614:GLU:OE2	2:B:632:LEU:HD23	2.12	0.49
2:B:413:THR:HB	2:B:416:GLN:HB2	1.93	0.49
1:A:101:SER:OG	1:A:102:LYS:N	2.43	0.48
2:B:2616:ARG:HH21	2:B:2617:ARG:HH12	1.59	0.48
2:B:403:ALA:HB1	2:B:421:LEU:HD11	1.95	0.48
2:B:672:ILE:O	2:B:679:ARG:HD2	2.14	0.48
1:A:40:PHE:HB3	1:A:540:VAL:HB	1.94	0.48
2:B:475:ASN:O	2:B:526:GLN:NE2	2.47	0.48
2:B:2629:PHE:O	2:B:2633:VAL:HG23	2.13	0.48
2:B:478:ALA:H	2:B:2598:ASP:HB2	1.79	0.47
2:B:395:LYS:HE2	2:B:466:ASP:OD1	2.14	0.47
2:B:584:ASN:HB2	2:B:585:GLN:H	1.50	0.47
2:B:789:LEU:HD11	2:B:901:LYS:HB3	1.96	0.47
2:B:539:MET:HB3	2:B:543:ARG:NH1	2.30	0.47
1:A:380:ARG:CB	1:A:380:ARG:HH11	2.27	0.47
2:B:521:ILE:HD13	2:B:527:LYS:HB2	1.97	0.47
2:B:569:PRO:HB3	2:B:576:ARG:CD	2.45	0.47
2:B:783:GLY:O	2:B:785:GLN:N	2.48	0.47
1:A:45:PHE:CD2	1:A:57:PHE:HB3	2.50	0.47
1:A:263:ASP:C	1:A:320:THR:HG22	2.34	0.47
1:A:316:ALA:HB1	1:A:511:ILE:HD11	1.96	0.47
2:B:618:GLY:O	2:B:621:LEU:O	2.33	0.47
2:B:414:PRO:O	2:B:415:GLN:HB2	2.15	0.46
2:B:843:ARG:HB3	4:B:8009:A9G:C04	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:421:LEU:HD12	2:B:421:LEU:N	2.31	0.46
2:B:545:LYS:HG3	2:B:2661:ARG:HG2	1.97	0.46
2:B:550:ILE:HG13	2:B:551:GLU:N	2.31	0.46
2:B:550:ILE:HG13	2:B:551:GLU:HG2	1.98	0.46
2:B:550:ILE:HD13	2:B:642:VAL:CG2	2.46	0.46
2:B:594:GLU:OE1	2:B:621:LEU:HD22	2.16	0.46
2:B:2626:PRO:HG3	2:B:2664:PRO:HD3	1.97	0.46
1:A:320:THR:O	1:A:320:THR:HG23	2.16	0.46
1:A:320:THR:O	1:A:320:THR:CG2	2.63	0.46
2:B:574:CYS:SG	2:B:576:ARG:HD2	2.56	0.46
2:B:800:GLY:HA3	2:B:2560:LEU:HD23	1.98	0.45
1:A:295:THR:C	1:A:311:MET:HE3	2.37	0.45
2:B:879:ILE:HD13	2:B:887:ILE:HD11	1.98	0.45
2:B:209:LEU:O	2:B:212:GLU:HG2	2.16	0.45
2:B:419:ASN:HA	2:B:422:ASP:HB3	1.97	0.45
1:A:380:ARG:NH1	1:A:380:ARG:CB	2.79	0.45
1:A:93:GLU:HG3	1:A:117:GLU:H	1.81	0.45
1:A:19:ILE:HD12	2:B:268:LYS:HE2	1.99	0.45
2:B:685:CYS:HB3	2:B:698:PRO:HD2	1.98	0.45
2:B:407:GLU:HB2	2:B:460:ARG:NH1	2.33	0.44
2:B:891:ILE:CD1	2:B:900:ILE:HG12	2.47	0.44
1:A:320:THR:HG23	1:A:323:CYS:SG	2.57	0.44
1:A:349:LYS:O	1:A:349:LYS:HG2	2.17	0.44
1:A:380:ARG:HH11	1:A:380:ARG:HB3	1.81	0.44
2:B:567:HIS:O	2:B:576:ARG:NH2	2.49	0.44
2:B:584:ASN:ND2	2:B:584:ASN:N	2.65	0.44
2:B:623:ARG:HD3	2:B:627:ASP:OD2	2.17	0.44
1:A:383:VAL:HG12	1:A:406:VAL:HG22	1.99	0.44
2:B:660:LYS:O	2:B:744:ARG:NH1	2.44	0.44
1:A:333:MET:HE2	1:A:333:MET:HB2	1.89	0.44
2:B:381:LEU:O	2:B:385:LEU:HG	2.17	0.44
2:B:538:LEU:HD12	2:B:538:LEU:HA	1.78	0.43
1:A:508:VAL:HG21	2:B:455:ARG:HD2	1.99	0.43
1:A:344:ALA:HB3	1:A:528:VAL:HG11	2.00	0.43
2:B:266:ASP:OD1	2:B:287:GLN:NE2	2.51	0.43
1:A:41:PHE:CD1	1:A:526:ARG:HD2	2.54	0.43
2:B:2614:ILE:HD12	2:B:2614:ILE:HA	1.79	0.43
2:B:2614:ILE:HD11	2:B:2619:ILE:HD11	2.01	0.42
1:A:41:PHE:CE1	1:A:526:ARG:HD2	2.54	0.42
1:A:179:CYS:HA	1:A:228:ILE:O	2.19	0.42
1:A:334:TYR:O	1:A:341:PRO:HA	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:LYS:O	1:A:350:SER:OG	2.35	0.42
2:B:893:TYR:CE1	2:B:896:HIS:HA	2.55	0.42
2:B:412:MET:HE3	2:B:417:LYS:CB	2.44	0.42
2:B:403:ALA:HB2	2:B:420:LEU:HD13	2.01	0.42
2:B:2637:ALA:O	2:B:2641:VAL:HG22	2.20	0.42
1:A:550:GLN:HG2	1:A:551:ARG:N	2.35	0.42
2:B:795:LYS:HD2	2:B:817:ILE:HG12	2.02	0.42
1:A:362:GLU:OE2	1:A:365:ARG:NH2	2.52	0.42
2:B:828:GLY:HA2	2:B:872:TYR:O	2.20	0.42
1:A:41:PHE:O	1:A:330:ARG:NH1	2.53	0.41
1:A:134:LEU:HD13	1:A:166:TRP:CG	2.55	0.41
1:A:43:VAL:H	1:A:527:GLN:HG2	1.85	0.41
1:A:332:ARG:HA	1:A:332:ARG:HD2	1.74	0.41
1:A:349:LYS:HE3	1:A:349:LYS:HB3	1.63	0.41
1:A:350:SER:O	1:A:519:ILE:CD1	2.67	0.41
2:B:460:ARG:O	2:B:464:MET:HG2	2.20	0.41
1:A:170:PRO:O	1:A:173:GLU:HG3	2.20	0.41
1:A:383:VAL:HG21	1:A:490:PHE:CZ	2.55	0.41
2:B:590:TRP:CG	2:B:631:LYS:HD3	2.56	0.41
2:B:811:LEU:HD23	2:B:914:LEU:HD12	2.03	0.41
1:A:535:GLU:HG2	1:A:536:TRP:CD1	2.56	0.41
2:B:230:LYS:HA	2:B:230:LYS:HD3	1.73	0.41
2:B:475:ASN:HA	2:B:477:ARG:NH1	2.36	0.41
2:B:596:GLY:HA2	2:B:599:GLU:OE2	2.21	0.41
2:B:2570:LEU:O	2:B:2573:GLN:HG2	2.20	0.41
2:B:2639:TRP:CH2	2:B:2646:ARG:HD3	2.55	0.41
1:A:85:GLN:HG3	1:A:86:LEU:N	2.36	0.41
2:B:248:LYS:HA	2:B:248:LYS:HD2	1.95	0.41
2:B:370:GLN:HG2	2:B:456:ARG:O	2.21	0.41
2:B:2678:ALA:HA	2:B:2681:ARG:NH1	2.36	0.41
2:B:680:GLU:HG2	2:B:862:GLN:HG3	2.04	0.40
2:B:2557:THR:HG23	2:B:2558:GLN:HG2	2.02	0.40
2:B:506:LEU:HD23	2:B:506:LEU:HA	1.90	0.40
2:B:2597:ILE:HD12	2:B:2597:ILE:HA	1.87	0.40
2:B:500:LEU:O	2:B:504:THR:HG23	2.22	0.40
1:A:190:LEU:HA	1:A:190:LEU:HD23	1.85	0.40
2:B:716:THR:OG1	2:B:719:GLU:HG3	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	460/605 (76%)	443 (96%)	16 (4%)	1 (0%)	47	64
2	B	750/936 (80%)	710 (95%)	39 (5%)	1 (0%)	51	69
All	All	1210/1541 (78%)	1153 (95%)	55 (4%)	2 (0%)	47	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	718	GLU
1	A	350	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	393/495 (79%)	380 (97%)	13 (3%)	38	54
2	B	677/815 (83%)	650 (96%)	27 (4%)	31	47
All	All	1070/1310 (82%)	1030 (96%)	40 (4%)	34	50

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	LYS
1	A	77	ASP
1	A	124	ASN
1	A	175	GLN

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Mol	Chain	Res	Type
1	A	298	TYR
1	A	320	THR
1	A	330	ARG
1	A	350	SER
1	A	365	ARG
1	A	492	ARG
1	A	505	SER
1	A	556	ARG
1	A	558	LEU
2	B	207	SER
2	B	248	LYS
2	B	266	ASP
2	B	294	LYS
2	B	387	LYS
2	B	410	ASP
2	B	417	LYS
2	B	438	SER
2	B	452	SER
2	B	479	LYS
2	B	522	GLU
2	B	541	SER
2	B	574	CYS
2	B	584	ASN
2	B	628	VAL
2	B	651	LYS
2	B	659	ARG
2	B	688	ASP
2	B	711	ARG
2	B	740	GLN
2	B	857	PHE
2	B	901	LYS
2	B	2590	ARG
2	B	2598	ASP
2	B	2621	SER
2	B	2651	SER
2	B	2664	PRO

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



### 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 monosaccharides 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	A9G	B	8009	-	39,43,43	2.64	18 (46%)	48,62,62	1.92	14 (29%)

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	-	-	2/21/31/31	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	6.35	1.50	1.37
4	B	8009	A9G	C10-C11	5.44	1.59	1.50
4	B	8009	A9G	C22-N21	4.40	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	8009	A9G	O23-C22	4.30	1.35	1.24
4	B	8009	A9G	C09-C39	4.20	1.48	1.42
4	B	8009	A9G	C24-C25	4.14	1.46	1.39
4	B	8009	A9G	C11-N13	4.13	1.42	1.33
4	B	8009	A9G	C06-N05	3.88	1.43	1.38
4	B	8009	A9G	C35-N30	3.68	1.52	1.46
4	B	8009	A9G	C31-N30	3.35	1.52	1.46
4	B	8009	A9G	C19-N21	3.01	1.40	1.34
4	B	8009	A9G	O12-C11	-2.55	1.18	1.23
4	B	8009	A9G	C14-N13	-2.39	1.41	1.46
4	B	8009	A9G	C28-C29	2.34	1.44	1.39
4	B	8009	A9G	C08-C07	2.20	1.55	1.51
4	B	8009	A9G	C18-C19	2.08	1.42	1.38
4	B	8009	A9G	C35-C34	2.05	1.56	1.51
4	B	8009	A9G	C24-C10	2.01	1.41	1.37

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	8009	A9G	N36-C29-N30	4.63	123.73	116.79
4	B	8009	A9G	C17-C16-C15	-4.11	116.99	122.01
4	B	8009	A9G	C28-C29-N36	-4.09	115.90	123.41
4	B	8009	A9G	C14-N13-C11	3.36	129.75	121.81
4	B	8009	A9G	C27-C26-C25	3.10	126.73	121.36
4	B	8009	A9G	C14-C15-C16	3.06	123.53	119.75
4	B	8009	A9G	C07-C06-N05	3.02	111.21	107.49
4	B	8009	A9G	C18-C19-N21	-2.92	117.24	121.49
4	B	8009	A9G	C28-C27-C26	2.75	125.10	121.13
4	B	8009	A9G	C34-C35-N30	2.69	116.31	110.48
4	B	8009	A9G	C32-C31-N30	2.54	115.99	110.48
4	B	8009	A9G	C37-N36-C29	2.46	121.80	117.30
4	B	8009	A9G	C27-C26-C37	-2.41	110.82	116.76
4	B	8009	A9G	C19-N21-C22	2.38	120.24	116.89

There are no chirality outliers.

All (2) torsion outliers are listed below:

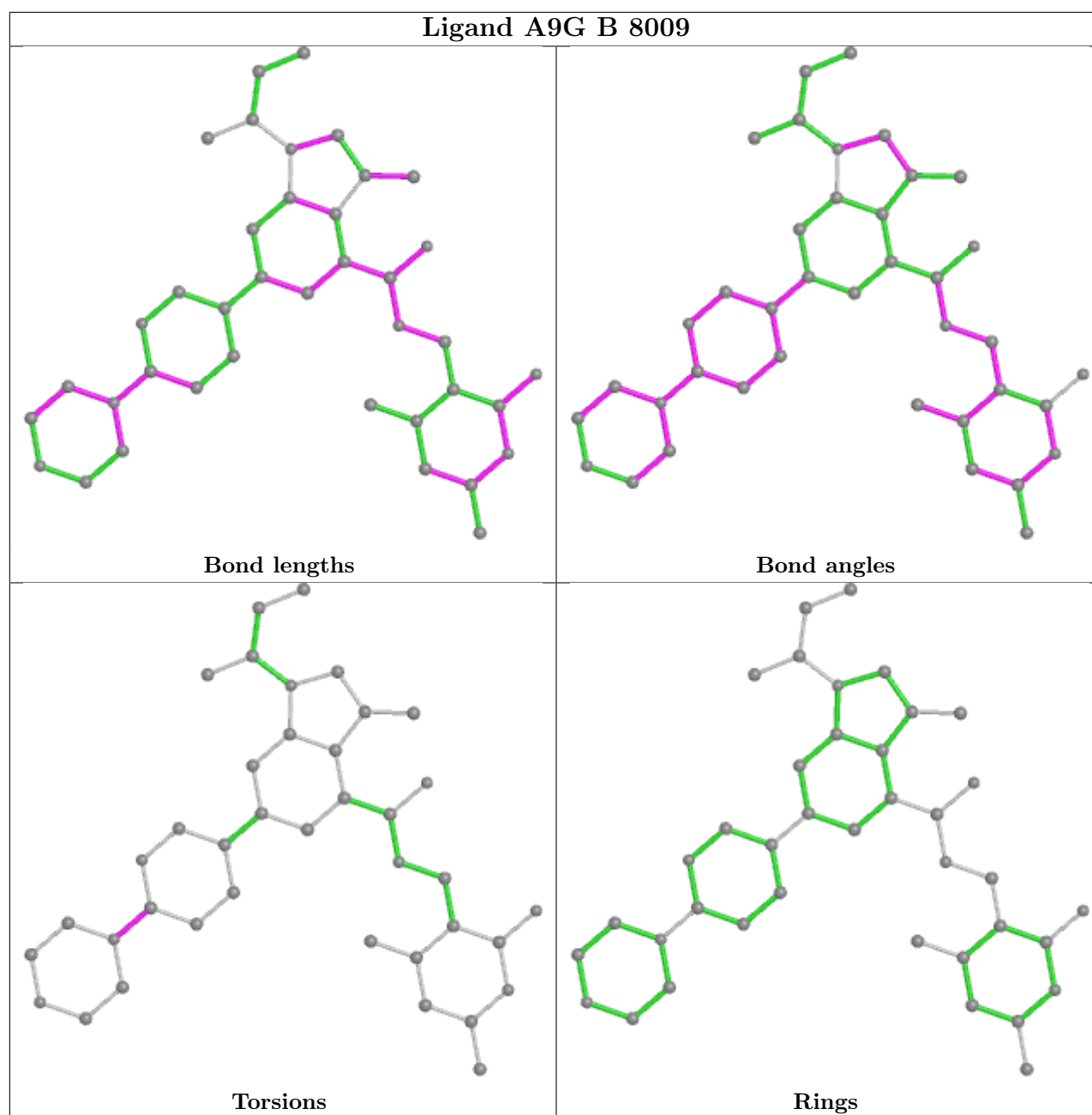
Mol	Chain	Res	Type	Atoms
4	B	8009	A9G	C28-C29-N30-C35
4	B	8009	A9G	N36-C29-N30-C35

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	8009	A9G	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	466/605 (77%)	-0.12	11 (2%) 59 54	17, 35, 87, 123	0
2	B	774/936 (82%)	-0.01	36 (4%) 31 28	19, 48, 97, 137	0
All	All	1240/1541 (80%)	-0.05	47 (3%) 40 36	17, 43, 95, 137	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	403	VAL	5.5
2	B	408	SER	5.0
2	B	628	VAL	4.6
2	B	926	THR	4.5
2	B	586	GLN	4.2
2	B	415	GLN	4.0
2	B	410	ASP	3.6
1	A	558	LEU	3.3
2	B	407	GLU	3.2
2	B	651	LYS	3.2
2	B	590	TRP	3.1
2	B	454	LEU	3.0
1	A	35	GLN	2.9
1	A	68	CYS	2.9
2	B	743	GLY	2.8
2	B	420	LEU	2.8
1	A	405	VAL	2.7
2	B	642	VAL	2.7
2	B	411	SER	2.7
1	A	401	PRO	2.6
2	B	426	ASP	2.6
2	B	547	ALA	2.6
2	B	609	GLN	2.6
2	B	641	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	409	ASP	2.5
1	A	400	GLY	2.5
2	B	246	HIS	2.5
1	A	495	LEU	2.3
2	B	740	GLN	2.3
2	B	406	PRO	2.3
2	B	632	LEU	2.3
2	B	717	ALA	2.2
2	B	587	VAL	2.2
2	B	640	PRO	2.2
2	B	550	ILE	2.2
1	A	372	GLU	2.2
2	B	276	TYR	2.1
2	B	414	PRO	2.1
2	B	644	PRO	2.1
1	A	34	SER	2.1
2	B	2549	ARG	2.1
2	B	614	GLU	2.1
2	B	321	LEU	2.1
2	B	322	ASN	2.0
2	B	598	LEU	2.0
2	B	652	SER	2.0
1	A	493	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.

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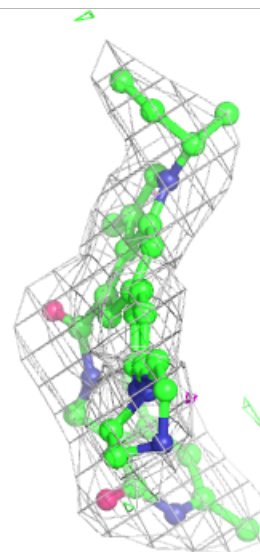
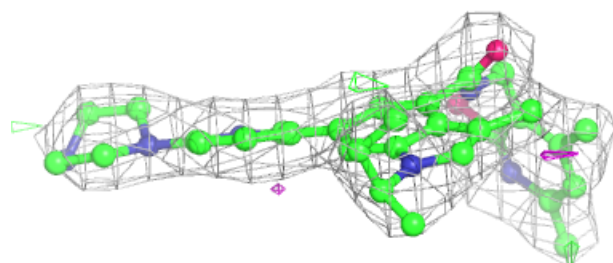
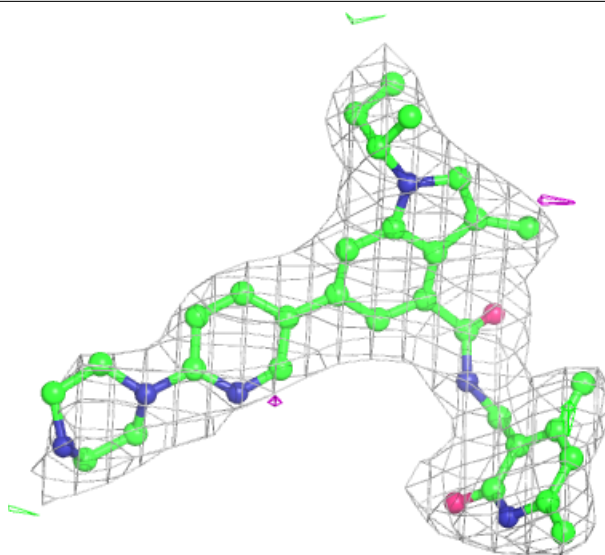
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	B	8008	1/1	0.93	0.06	88,88,88,88	0
4	A9G	B	8009	39/39	0.95	0.16	16,37,67,73	0
3	ZN	B	8002	1/1	0.97	0.18	34,34,34,34	0
3	ZN	B	8005	1/1	0.99	0.11	44,44,44,44	0
3	ZN	B	8006	1/1	0.99	0.14	44,44,44,44	0
3	ZN	B	8001	1/1	0.99	0.12	34,34,34,34	0
3	ZN	B	8004	1/1	0.99	0.12	43,43,43,43	0
3	ZN	B	8003	1/1	1.00	0.14	42,42,42,42	0
3	ZN	B	8007	1/1	1.00	0.13	28,28,28,28	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 A9G 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.