



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:19 AM UTC

PDB ID : 5WFD / pdb_00005wfd
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

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

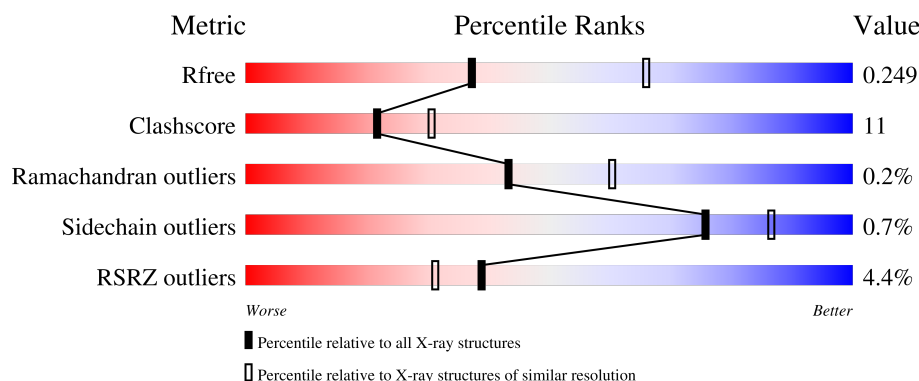
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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% 63%13%23%
2	B	936	5% 64%18%17%

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
1	A	466	Total	C	N	O	S	0	2	0
			3682	2354	635	674	19			

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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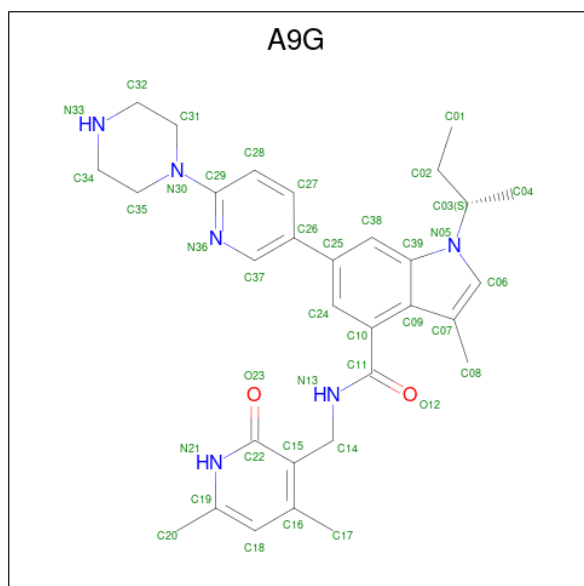
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Chain	Residue	Modelled	Actual	Comment	Reference
B	2525	VAL	-	linker	UNP G0SDW4
B	2526	PRO	-	linker	UNP G0SDW4
B	2527	ARG	-	linker	UNP G0SDW4
B	2528	GLY	-	linker	UNP G0SDW4
B	2529	SER	-	linker	UNP G0SDW4

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- 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 (CCD ID: A9G) (formula: C₃₁H₃₈N₆O₂).



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, R_{free}	0.181 , 0.240 0.194 , 0.249	Depositor DCC
R_{free} test set	2476 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	42.1	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9956	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: 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	0.44	0/3794	0.64	0/5163
2	B	0.43	0/6368	0.63	0/8602
All	All	0.44	0/10162	0.63	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	76	0
2	B	6227	0	6113	141	0
3	B	8	0	0	0	0
4	B	39	0	0	1	0
All	All	9956	0	9670	212	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 11.

All (212) 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:HD2	2:B:651:LYS:O	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
1:A:68:CYS:HG	1:A:83:ILE:HG12	1.55	0.71
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:493:MET:HE3	2:B:546:TRP:HH2	1.58	0.67
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
1:A:350:SER:C	1:A:519:ILE:HD12	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:493:MET:HE3	2:B:546:TRP:CH2	2.33	0.62
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
2:B:594:GLU:HB2	2:B:621:LEU:CD2	2.31	0.60
2:B:601:MET:HE2	2:B:616:PHE:CD2	2.36	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
2:B:651:LYS:HD2	2:B:651:LYS:C	2.29	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:412:MET:HE3	2:B:417:LYS:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:414:PRO:HA	2:B:417:LYS:HZ3	1.74	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: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
1:A:263:ASP:C	1:A:320:THR:HG22	2.34	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:408:SER:OG	2:B:412:MET:HE2	2.12	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:493:MET:HE1	2:B:603:ALA:HB1	1.98	0.46
2:B:843:ARG:HB3	4:B:8009:A9G:C04	2.45	0.46
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:HG23	1:A:320:THR:O	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
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
1:A:93:GLU:CD	1:A:117:GLU:HB2	2.42	0.44
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:N	2:B:584:ASN:ND2	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:295:THR:HG22	1:A:311:MET:HE3	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:CE	2:B:417:LYS:HB3	2.48	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:349:LYS:C	1:A:350:SER:OG	2.63	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:HD2	1:A:332:ARG:HA	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:664:MET:HE2	2:B:664:MET:HB3	1.92	0.40
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:333:MET:HE2	1:A:333:MET:HB2	1.92	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 [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	460/605 (76%)	443 (96%)	16 (4%)	1 (0%)	43	60
2	B	750/936 (80%)	710 (95%)	39 (5%)	1 (0%)	48	66
All	All	1210/1541 (78%)	1153 (95%)	55 (4%)	2 (0%)	43	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	718	GLU
1	A	350	SER

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	393/495 (79%)	390 (99%)	3 (1%)	73	85
2	B	677/815 (83%)	673 (99%)	4 (1%)	78	88
All	All	1070/1310 (82%)	1063 (99%)	7 (1%)	76	86

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	320	THR
1	A	349	LYS
1	A	350	SER
2	B	266	ASP
2	B	584	ASN
2	B	628	VAL
2	B	651	LYS

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

Mol	Chain	Res	Type
2	B	222	ASN
2	B	306	HIS
2	B	584	ASN
2	B	695	ASN
2	B	780	HIS
2	B	880	ASN
2	B	921	ASN
2	B	924	ASN
2	B	2558	GLN

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 oligosaccharides 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	-	40,43,43	2.46	15 (37%)	52,62,62	2.60	18 (34%)

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	-	-	3/22/31/31	0/5/5/5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	8009	A9G	O23-C22	6.22	1.35	1.23
4	B	8009	A9G	C29-N30	5.69	1.50	1.37
4	B	8009	A9G	C10-C11	4.74	1.59	1.50
4	B	8009	A9G	C24-C25	4.13	1.46	1.39
4	B	8009	A9G	C11-N13	4.12	1.42	1.33
4	B	8009	A9G	C09-C39	4.08	1.48	1.41
4	B	8009	A9G	C35-N30	3.38	1.52	1.46
4	B	8009	A9G	C06-N05	3.33	1.43	1.38
4	B	8009	A9G	C31-N30	3.07	1.52	1.46
4	B	8009	A9G	C18-C19	2.73	1.42	1.36
4	B	8009	A9G	C20-C19	2.38	1.54	1.49
4	B	8009	A9G	C08-C07	2.37	1.55	1.50
4	B	8009	A9G	C28-C29	2.37	1.44	1.39
4	B	8009	A9G	O12-C11	-2.24	1.18	1.23
4	B	8009	A9G	C19-N21	2.07	1.40	1.37

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	8009	A9G	C15-C22-N21	9.89	123.22	115.70
4	B	8009	A9G	O23-C22-C15	-7.99	114.71	124.56
4	B	8009	A9G	N36-C29-N30	4.88	123.73	116.76
4	B	8009	A9G	C22-N21-C19	-4.77	120.24	125.36
4	B	8009	A9G	C28-C29-N36	-3.83	115.90	123.46
4	B	8009	A9G	C14-N13-C11	3.50	129.75	121.29
4	B	8009	A9G	C27-C26-C25	3.17	126.73	121.25
4	B	8009	A9G	C28-C27-C26	3.10	125.10	121.12
4	B	8009	A9G	C34-C35-N30	2.72	116.31	110.38
4	B	8009	A9G	C27-C26-C37	-2.72	110.82	116.76
4	B	8009	A9G	C37-N36-C29	2.68	121.80	117.41
4	B	8009	A9G	C25-C38-C39	2.62	123.58	119.47
4	B	8009	A9G	C32-C31-N30	2.58	115.99	110.38
4	B	8009	A9G	C08-C07-C09	-2.51	125.23	128.58
4	B	8009	A9G	C10-C09-C07	2.40	139.54	135.48
4	B	8009	A9G	C10-C09-C39	-2.23	115.25	121.35
4	B	8009	A9G	C38-C25-C24	-2.15	115.21	118.35
4	B	8009	A9G	C17-C16-C18	2.11	123.15	118.63

There are no chirality outliers.

All (3) 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
4	B	8009	A9G	C02-C03-N05-C06

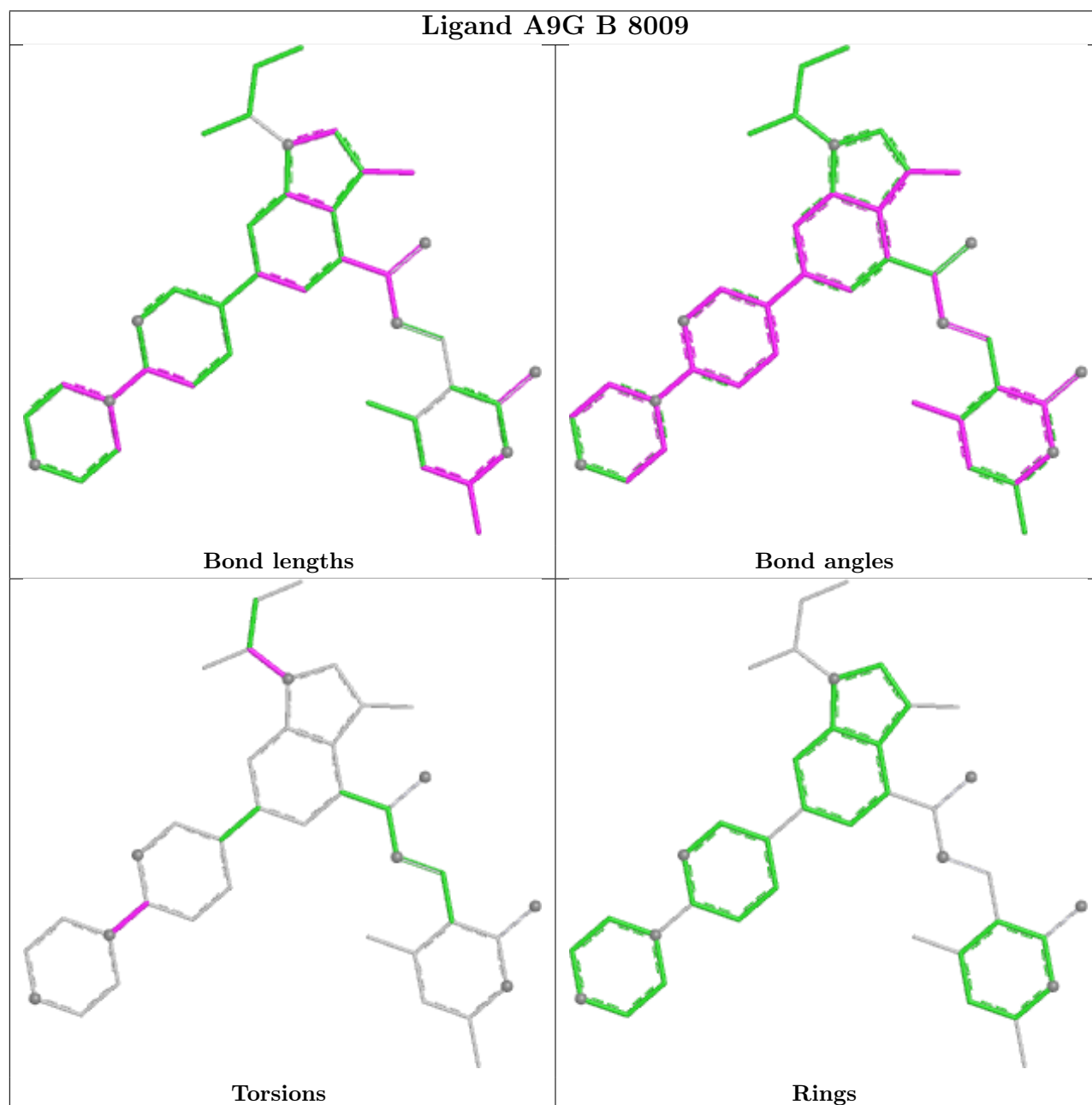
There are no ring outliers.

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, 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	466/605 (77%)	-0.27	12 (2%) 57 51	13, 35, 87, 123	2 (0%)
2	B	774/936 (82%)	0.07	43 (5%) 30 24	19, 48, 97, 137	0
All	All	1240/1541 (80%)	-0.06	55 (4%) 39 31	13, 43, 95, 137	2 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	558	LEU	5.8
2	B	717	ALA	5.5
2	B	740	GLN	5.5
1	A	68	CYS	5.0
2	B	743	GLY	4.4
2	B	644	PRO	4.0
2	B	855	PHE	3.9
2	B	567	HIS	3.6
2	B	628	VAL	3.6
2	B	408	SER	3.5
2	B	584	ASN	3.4
2	B	568	PRO	3.4
2	B	579	GLY	3.2
1	A	403	VAL	3.0
1	A	349	LYS	3.0
2	B	926	THR	3.0
2	B	639	LEU	2.9
1	A	350	SER	2.9
2	B	492	LEU	2.9
1	A	37	LEU	2.9
2	B	479	LYS	2.8
1	A	7	ALA	2.8
2	B	414	PRO	2.7
2	B	651	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	454	LEU	2.7
2	B	630	ARG	2.7
2	B	650	GLN	2.6
2	B	783	GLY	2.6
1	A	301	PRO	2.6
2	B	587	VAL	2.6
2	B	2550	PRO	2.6
2	B	610	THR	2.5
2	B	652	SER	2.5
2	B	647	ILE	2.5
2	B	739	ARG	2.4
2	B	276	TYR	2.4
2	B	643	GLU	2.4
2	B	467	LYS	2.4
1	A	36	ASP	2.3
2	B	569	PRO	2.3
2	B	640	PRO	2.3
2	B	575	TYR	2.3
2	B	417	LYS	2.3
1	A	401	PRO	2.3
2	B	2598	ASP	2.3
2	B	406	PRO	2.2
2	B	275	GLU	2.2
2	B	805	GLU	2.2
2	B	586	GLN	2.2
1	A	415	LYS	2.2
2	B	585	GLN	2.2
2	B	201	LYS	2.1
2	B	407	GLU	2.1
2	B	196	GLU	2.0
1	A	402	GLY	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 oligosaccharides in this entry.

6.4 Ligands

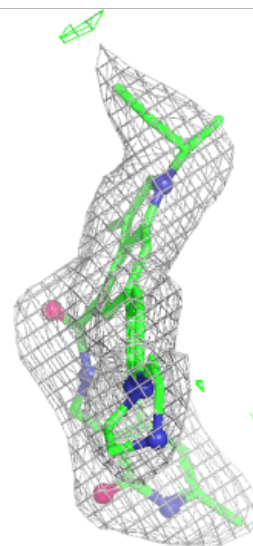
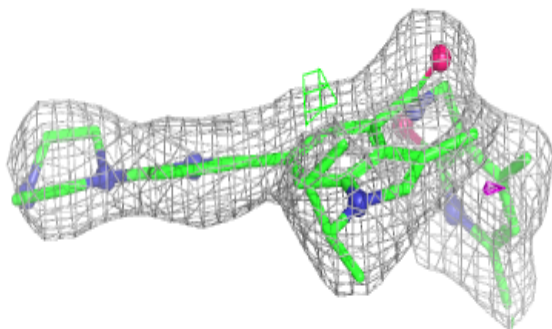
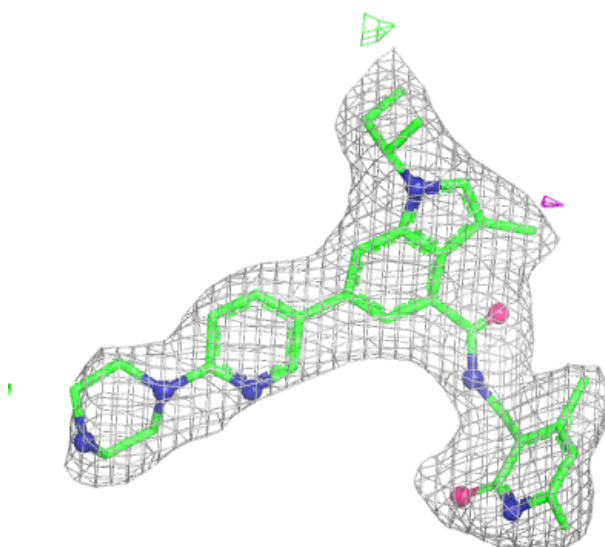
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A9G	B	8009	39/39	0.94	0.09	16,37,67,73	0
3	ZN	B	8008	1/1	0.96	0.06	88,88,88,88	0
3	ZN	B	8002	1/1	0.98	0.06	34,34,34,34	0
3	ZN	B	8006	1/1	0.99	0.04	44,44,44,44	0
3	ZN	B	8001	1/1	0.99	0.03	34,34,34,34	0
3	ZN	B	8005	1/1	0.99	0.02	44,44,44,44	0
3	ZN	B	8007	1/1	1.00	0.01	28,28,28,28	0
3	ZN	B	8003	1/1	1.00	0.02	42,42,42,42	0
3	ZN	B	8004	1/1	1.00	0.02	43,43,43,43	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.