



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:10 PM UTC

PDB ID : 5WFC / pdb_00005wfc
Title : Humanized mutant of the Chaetomium thermophilum Polycomb Repressive Complex 2 bound to the inhibitor GSK343
Authors : Bratkowski, M.A.; Liu, X.
Deposited on : 2017-07-11
Resolution : 2.28 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

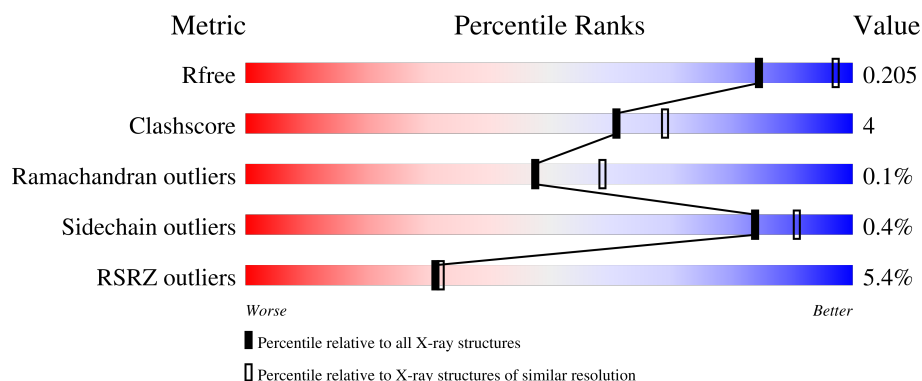
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 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	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	4% 69% 6% 24%
2	B	936	4% 73% 9% 18%
3	D	11	27% 45% 18% 36%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10563 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	460	3643	2328	628	668	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

Continued on next page...

Continued from previous page...

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	769	Total	C	N	O	S	0	0	0
			6185	3898	1116	1130	41			

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

Continued on next page...

Continued from previous page...

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

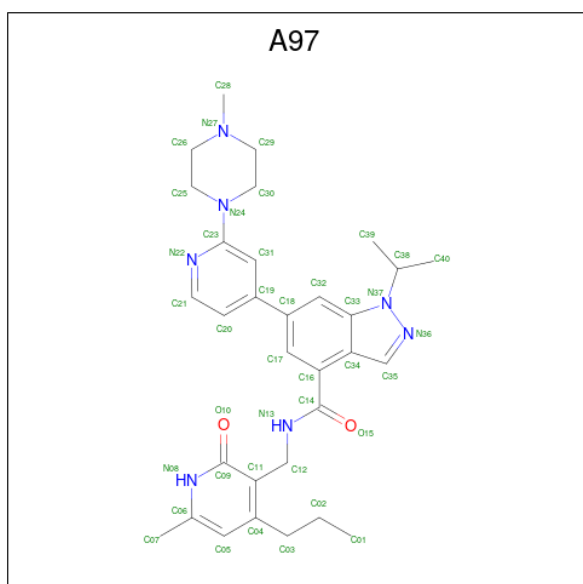
- Molecule 3 is a protein called Histone H3.1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	D	7	Total	C	N	O	0	0	0
			51	32	11	8			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 5 is N-[(6-methyl-2-oxo-4-propyl-1,2-dihydropyridin-3-yl)methyl]-6-[2-(4-methylpiperazin-1-yl)pyridin-4-yl]-1-(propan-2-yl)-1H-indazole-4-carboxamide (CCD ID: A97) (formula: C₃₁H₃₉N₇O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			40	31	7	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	258	Total 258	O 258	0	0
6	B	377	Total 377	O 377	0	0
6	D	1	Total 1	O 1	0	0

- Molecule 3: Histone H3.1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	117.59Å 137.79Å 222.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.72 – 2.28 44.72 – 2.28	Depositor EDS
% Data completeness (in resolution range)	96.5 (44.72-2.28) 96.5 (44.72-2.28)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.67 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, R_{free}	0.167 , 0.203 0.169 , 0.205	Depositor DCC
R_{free} test set	4072 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10563	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, M3L, A97

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	0.35	0/3753	0.54	0/5106
2	B	0.33	0/6325	0.50	0/8541
3	D	1.03	1/39 (2.6%)	0.39	0/52
All	All	0.34	1/10117 (0.0%)	0.52	0/13699

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	27	M3L	C-N	6.01	1.41	1.33

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	3643	0	3510	25	0
2	B	6185	0	6076	60	0
3	D	51	0	58	1	0
4	B	8	0	0	0	0
5	B	40	0	0	0	0
6	A	258	0	0	3	0
6	B	377	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	1	0	0	0	0
All	All	10563	0	9644	83	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 4.

All (83) 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:248:LYS:HD2	2:B:249:SER:H	1.30	0.91
2:B:2683:ARG:O	2:B:2684:GLU:C	2.21	0.84
2:B:401:PHE:HB2	2:B:428:MET:HE1	1.69	0.75
2:B:412:MET:HE2	2:B:417:LYS:HG2	1.71	0.71
2:B:248:LYS:HD2	2:B:249:SER:N	2.07	0.68
1:A:22:ASP:OD2	1:A:36:ASP:HA	1.94	0.67
2:B:891:ILE:HD13	2:B:900:ILE:HG12	1.76	0.66
2:B:476:LYS:HE2	2:B:2596:PHE:CE1	2.32	0.65
2:B:248:LYS:CD	2:B:249:SER:H	2.09	0.64
1:A:326:GLN:OE1	3:D:26:ARG:NH1	2.30	0.62
2:B:309:GLU:HG2	2:B:2580:ILE:HG12	1.83	0.60
1:A:186:HIS:CG	1:A:190:LEU:HD21	2.39	0.58
2:B:479:LYS:NZ	6:B:8105:HOH:O	2.34	0.56
2:B:248:LYS:HE2	2:B:249:SER:HB3	1.86	0.56
2:B:419:ASN:HB3	2:B:472:ILE:HG12	1.86	0.56
2:B:407:GLU:OE2	2:B:407:GLU:N	2.35	0.56
1:A:289:THR:HG22	6:A:717:HOH:O	2.05	0.55
1:A:512:LYS:NZ	1:A:513:ALA:O	2.39	0.55
2:B:413:THR:HG23	2:B:414:PRO:O	2.08	0.54
1:A:237:SER:HB2	1:A:295:THR:HG23	1.89	0.54
1:A:493:GLU:CD	1:A:493:GLU:H	2.17	0.53
2:B:475:ASN:O	2:B:526:GLN:NE2	2.41	0.52
2:B:612:ARG:HG3	2:B:612:ARG:HH11	1.75	0.52
2:B:595:VAL:O	2:B:599:GLU:HG3	2.10	0.52
1:A:536:TRP:CZ3	1:A:550:GLN:HB2	2.45	0.51
2:B:2682:LEU:O	2:B:2683:ARG:C	2.53	0.51
1:A:178:VAL:HG12	1:A:224:MET:HE3	1.91	0.50
1:A:491:SER:HB2	1:A:493:GLU:OE2	2.11	0.50
2:B:614:GLU:HB3	2:B:625:CYS:SG	2.52	0.49
2:B:453:LYS:HD3	2:B:454:LEU:N	2.28	0.49
2:B:520:GLU:HB3	2:B:528:ARG:HG3	1.95	0.49
1:A:83:ILE:HB	2:B:288:TYR:CE2	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:574:CYS:HA	2:B:625:CYS:HB3	1.95	0.48
1:A:39:GLU:HB3	1:A:542:ASN:HA	1.94	0.48
2:B:370:GLN:HG2	2:B:456:ARG:O	2.14	0.48
1:A:13:ARG:HD2	2:B:275:GLU:HA	1.95	0.48
2:B:889:PRO:HB3	2:B:902:PHE:CE1	2.49	0.47
2:B:412:MET:HG2	2:B:473:PHE:CE2	2.49	0.47
1:A:181:LEU:HD13	1:A:214:TRP:CG	2.50	0.47
1:A:217:PRO:HD3	1:A:230:ILE:HD11	1.96	0.47
2:B:575:TYR:CE1	2:B:576:ARG:HG3	2.50	0.47
2:B:2555:LYS:HG3	2:B:2571:PRO:HB3	1.97	0.47
2:B:413:THR:O	2:B:416:GLN:HB2	2.16	0.46
2:B:412:MET:HG2	2:B:473:PHE:HE2	1.80	0.46
2:B:601:MET:HE2	2:B:616:PHE:CD2	2.50	0.46
2:B:444:TRP:CZ2	2:B:462:ILE:HD12	2.50	0.46
2:B:266:ASP:OD1	2:B:287:GLN:HG2	2.16	0.46
2:B:453:LYS:HD3	2:B:454:LEU:H	1.79	0.46
2:B:738:GLN:HA	2:B:749:VAL:HG11	1.98	0.45
2:B:394:THR:HG22	2:B:396:SER:N	2.32	0.45
1:A:42:ASP:OD1	1:A:527:GLN:HG2	2.17	0.45
2:B:650:GLN:OE1	2:B:690:PRO:HB3	2.17	0.45
2:B:551:GLU:HG2	2:B:551:GLU:O	2.16	0.45
2:B:2592:ASN:HB3	6:B:8237:HOH:O	2.17	0.45
2:B:2599:LEU:O	2:B:2604:LYS:HE3	2.17	0.44
2:B:550:ILE:HD11	2:B:607:TYR:CD2	2.53	0.44
1:A:129:LYS:HB3	1:A:129:LYS:HE2	1.66	0.44
1:A:307:SER:N	6:A:612:HOH:O	2.51	0.44
1:A:76:LYS:HG2	1:A:555:GLU:HB3	2.00	0.43
2:B:893:TYR:CE2	2:B:896:HIS:HA	2.54	0.43
1:A:7:ALA:N	6:A:610:HOH:O	2.50	0.43
2:B:209:LEU:O	2:B:212:GLU:HG2	2.19	0.43
2:B:709:CYS:N	2:B:722:LEU:O	2.49	0.42
2:B:660:LYS:O	2:B:744:ARG:NH1	2.43	0.42
1:A:334:TYR:O	1:A:341:PRO:HA	2.19	0.42
2:B:597:THR:HA	2:B:600:TRP:CZ2	2.55	0.42
1:A:413:VAL:HA	1:A:414:PRO:HD3	1.93	0.42
2:B:2682:LEU:O	2:B:2684:GLU:N	2.53	0.42
2:B:377:LEU:HD12	2:B:457:VAL:HG11	2.02	0.41
2:B:571:ARG:HD3	6:B:8351:HOH:O	2.20	0.41
2:B:789:LEU:HD11	2:B:901:LYS:HB3	2.02	0.41
2:B:806:ALA:N	6:B:8125:HOH:O	2.51	0.41
2:B:408:SER:O	2:B:412:MET:HB2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:476:LYS:HA	2:B:476:LYS:HD2	1.81	0.41
2:B:394:THR:HG22	2:B:396:SER:H	1.86	0.41
2:B:2598:ASP:OD1	2:B:2598:ASP:N	2.53	0.41
2:B:394:THR:HB	2:B:397:ASN:HB2	2.02	0.41
1:A:344:ALA:HB3	1:A:528:VAL:HG11	2.03	0.41
1:A:393:ALA:N	1:A:396:GLN:HG3	2.36	0.41
2:B:2682:LEU:C	2:B:2684:GLU:N	2.77	0.41
2:B:591:SER:OG	2:B:594:GLU:HG3	2.20	0.40
1:A:36:ASP:O	1:A:37:LEU:HD13	2.21	0.40
2:B:828:GLY:HA2	2:B:872:TYR:O	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	452/605 (75%)	442 (98%)	9 (2%)	1 (0%)	43	53
2	B	749/936 (80%)	726 (97%)	23 (3%)	0	100	100
3	D	4/11 (36%)	4 (100%)	0	0	100	100
All	All	1205/1552 (78%)	1172 (97%)	32 (3%)	1 (0%)	48	59

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	393	ALA

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	389/495 (79%)	389 (100%)	0	100	100
2	B	672/815 (82%)	668 (99%)	4 (1%)	78	87
3	D	3/6 (50%)	3 (100%)	0	100	100
All	All	1064/1316 (81%)	1060 (100%)	4 (0%)	84	91

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	264	THR
2	B	621	LEU
2	B	628	VAL
2	B	2683	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	394	GLN
1	A	397	GLN
2	B	318	ASN
2	B	468	ASN
2	B	549	GLN
2	B	629	HIS
2	B	880	ASN
2	B	895	ASN
2	B	921	ASN
2	B	2573	GLN
2	B	2577	GLN
2	B	2618	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\# Z > 2$
3	M3L	D	27	3	10,11,12	0.55	0	9,14,16	0.49	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	M3L	D	27	3	-	0/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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
5	A97	B	8009	-	42,44,44	2.91	17 (40%)	55,63,63	4.15	21 (38%)

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
5	A97	B	8009	-	-	4/23/34/34	0/5/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	8009	A97	O10-C09	7.06	1.37	1.23
5	B	8009	A97	C23-N24	7.03	1.53	1.37
5	B	8009	A97	C33-N37	6.89	1.45	1.37
5	B	8009	A97	C30-N24	5.64	1.56	1.46
5	B	8009	A97	C35-N36	5.21	1.37	1.32
5	B	8009	A97	C34-C35	4.68	1.47	1.42
5	B	8009	A97	C25-N24	4.47	1.54	1.46
5	B	8009	A97	C05-C06	3.43	1.44	1.36
5	B	8009	A97	C32-C33	3.36	1.45	1.39
5	B	8009	A97	C16-C34	2.94	1.45	1.41
5	B	8009	A97	C31-C23	2.89	1.43	1.39
5	B	8009	A97	C14-N13	2.86	1.40	1.33
5	B	8009	A97	C20-C21	2.74	1.43	1.38
5	B	8009	A97	C03-C04	2.70	1.58	1.51
5	B	8009	A97	C07-C06	2.53	1.54	1.49
5	B	8009	A97	O15-C14	2.42	1.29	1.23
5	B	8009	A97	C17-C18	2.15	1.43	1.39

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	8009	A97	C19-C31-C23	18.95	124.83	118.17
5	B	8009	A97	C11-C09-N08	15.09	127.17	115.70
5	B	8009	A97	O10-C09-C11	-7.04	115.88	124.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	8009	A97	C09-N08-C06	-6.77	118.09	125.36
5	B	8009	A97	N22-C23-N24	6.57	126.15	116.76
5	B	8009	A97	C31-C23-N24	-6.27	114.78	122.35
5	B	8009	A97	C12-N13-C14	4.59	132.38	121.29
5	B	8009	A97	C35-N36-N37	4.15	108.79	105.95
5	B	8009	A97	C29-C30-N24	4.15	119.52	110.78
5	B	8009	A97	C03-C04-C11	-3.32	119.89	122.42
5	B	8009	A97	C34-C33-N37	3.24	108.24	106.61
5	B	8009	A97	C20-C19-C31	-3.09	113.99	118.23
5	B	8009	A97	C30-C29-N27	2.96	115.61	110.86
5	B	8009	A97	C16-C14-N13	2.77	122.70	117.32
5	B	8009	A97	C16-C17-C18	2.67	125.79	120.82
5	B	8009	A97	C32-C33-C34	-2.53	120.12	122.99
5	B	8009	A97	C02-C03-C04	2.26	122.53	114.35
5	B	8009	A97	C31-C23-N22	-2.25	119.07	122.82
5	B	8009	A97	C38-N37-N36	-2.24	117.29	119.66
5	B	8009	A97	C28-N27-C29	-2.16	106.51	110.63
5	B	8009	A97	O15-C14-C16	-2.13	117.13	121.03

There are no chirality outliers.

All (4) torsion outliers are listed below:

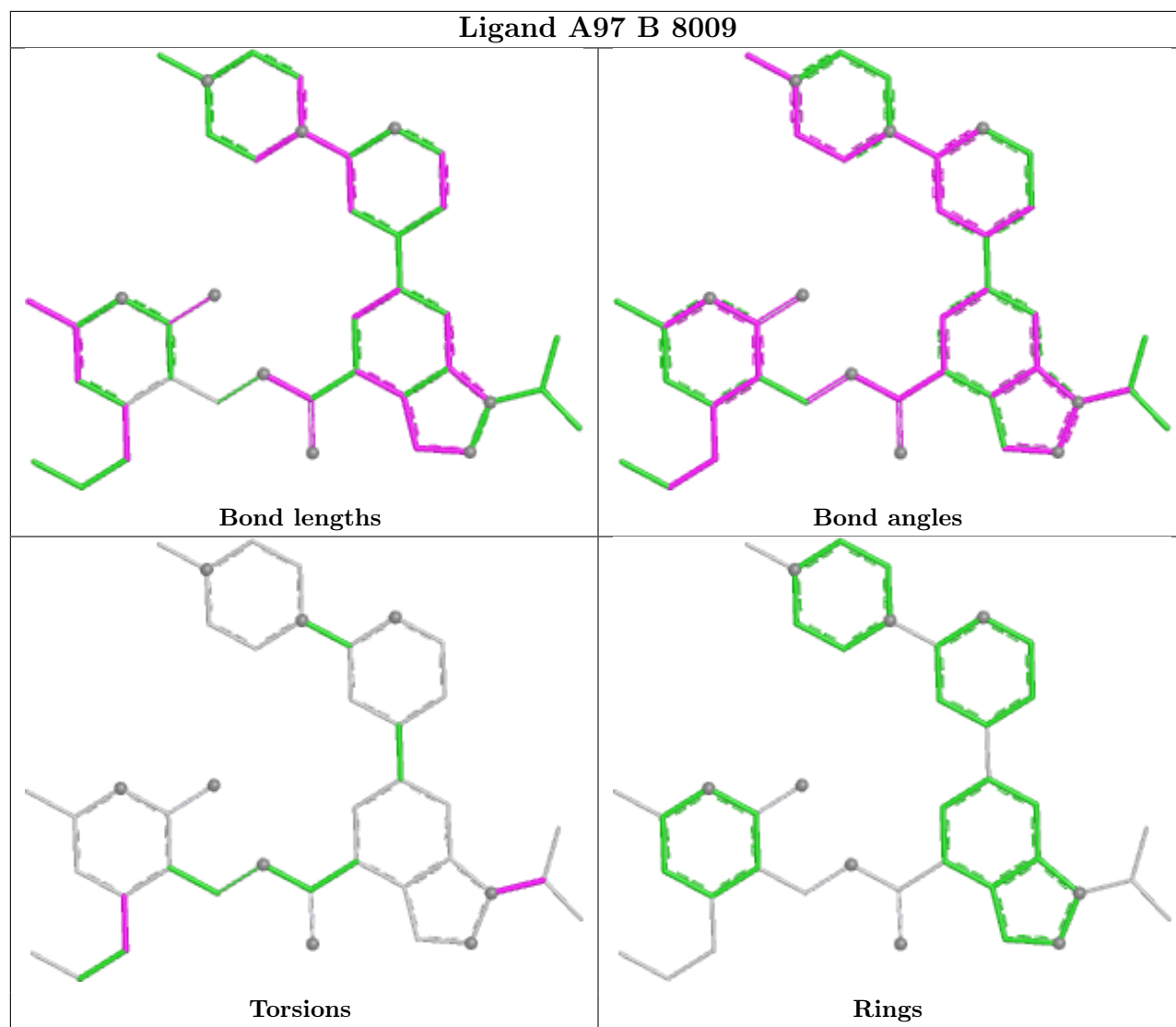
Mol	Chain	Res	Type	Atoms
5	B	8009	A97	C02-C03-C04-C11
5	B	8009	A97	C02-C03-C04-C05
5	B	8009	A97	C39-C38-N37-C33
5	B	8009	A97	C40-C38-N37-C33

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, 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	460/605 (76%)	-0.29	24 (5%) 33 33	12, 29, 82, 109	2 (0%)
2	B	769/936 (82%)	0.04	40 (5%) 33 33	16, 40, 77, 109	0
3	D	6/11 (54%)	1.93	3 (50%) 0 0	46, 54, 70, 80	0
All	All	1235/1552 (79%)	-0.08	67 (5%) 31 32	12, 36, 80, 109	2 (0%)

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	579	GLY	6.6
1	A	557	GLY	5.7
2	B	743	GLY	5.1
1	A	301	PRO	4.4
2	B	421	LEU	4.3
3	D	30	PRO	4.0
1	A	400	GLY	3.9
1	A	309	PRO	3.9
1	A	25	LYS	3.9
1	A	379	GLY	3.7
2	B	844	GLY	3.6
2	B	647	ILE	3.6
2	B	567	HIS	3.5
2	B	2684	GLU	3.4
1	A	36	ASP	3.4
2	B	622	GLY	3.3
2	B	628	VAL	3.2
2	B	321	LEU	3.2
1	A	34	SER	3.1
2	B	196	GLU	3.1
1	A	390	ILE	3.0
1	A	405	VAL	3.0
1	A	399	HIS	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	2550	PRO	3.0
3	D	29	ALA	2.9
1	A	37	LEU	2.9
2	B	360	PRO	2.8
3	D	24	ALA	2.8
1	A	307	SER	2.8
2	B	2683	ARG	2.8
1	A	414	PRO	2.8
2	B	454	LEU	2.7
2	B	276	TYR	2.6
1	A	489	GLY	2.6
1	A	388	GLN	2.5
2	B	474	ASP	2.5
2	B	453	LYS	2.5
2	B	929	LEU	2.5
2	B	587	VAL	2.5
2	B	568	PRO	2.5
2	B	648	PRO	2.3
1	A	389	GLY	2.3
2	B	425	SER	2.3
1	A	393	ALA	2.3
2	B	806	ALA	2.3
1	A	381	VAL	2.2
2	B	528	ARG	2.2
2	B	649	LYS	2.2
2	B	854	SER	2.2
2	B	455	ARG	2.2
2	B	739	ARG	2.2
2	B	414	PRO	2.2
2	B	664	MET	2.2
2	B	589	PRO	2.2
2	B	261	GLY	2.2
1	A	373	ALA	2.2
2	B	413	THR	2.2
2	B	322	ASN	2.1
1	A	397	GLN	2.1
1	A	556	ARG	2.1
2	B	740	GLN	2.1
2	B	412	MET	2.1
2	B	578	HIS	2.1
1	A	35	GLN	2.0
2	B	492	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	391	SER	2.0
2	B	451	GLN	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	M3L	D	27	12/13	0.88	0.14	35,43,48,51	0

6.3 Carbohydrates [i](#)

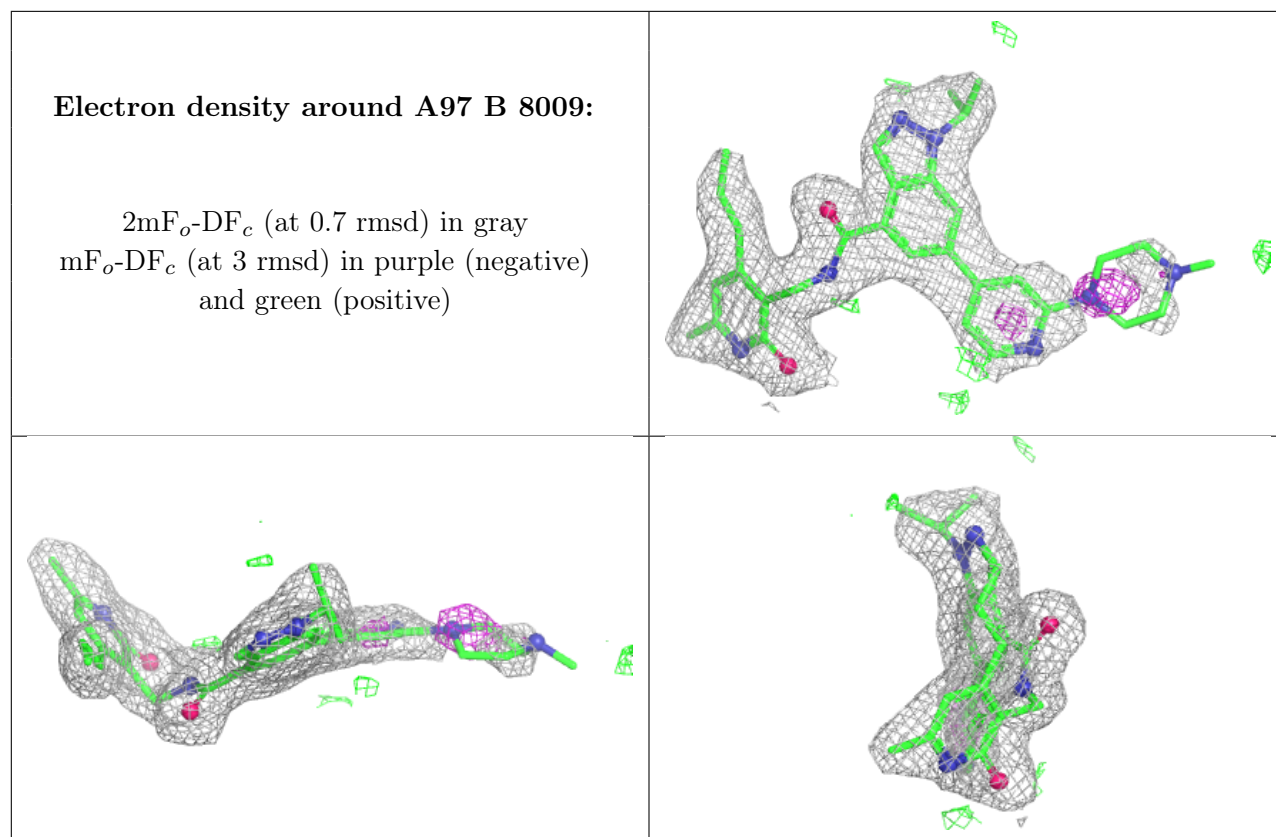
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	A97	B	8009	40/40	0.90	0.14	24,41,74,75	0
4	ZN	B	8005	1/1	0.99	0.02	36,36,36,36	0
4	ZN	B	8006	1/1	0.99	0.02	33,33,33,33	0
4	ZN	B	8008	1/1	0.99	0.05	55,55,55,55	0
4	ZN	B	8004	1/1	0.99	0.02	37,37,37,37	0
4	ZN	B	8003	1/1	1.00	0.02	30,30,30,30	0
4	ZN	B	8007	1/1	1.00	0.04	23,23,23,23	0
4	ZN	B	8001	1/1	1.00	0.04	28,28,28,28	0
4	ZN	B	8002	1/1	1.00	0.05	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.