



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 07:43 AM EDT

PDB ID : 2X38 / pdb_00002x38
Title : The crystal structure of the murine class IA PI 3-kinase p110delta in complex with IC87114.
Authors : Berndt, A.; Miller, S.; Williams, O.; Lee, D.D.; Houseman, B.T.; Pacold, J.I.; Gorrec, F.; Hon, W.-C.; Liu, Y.; Rommel, C.; Gaillard, P.; Ruckle, T.; Schwarz, M.K.; Shokat, K.M.; Shaw, J.P.; Williams, R.L.
Deposited on : 2010-01-22
Resolution : 2.20 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](#) ①) 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

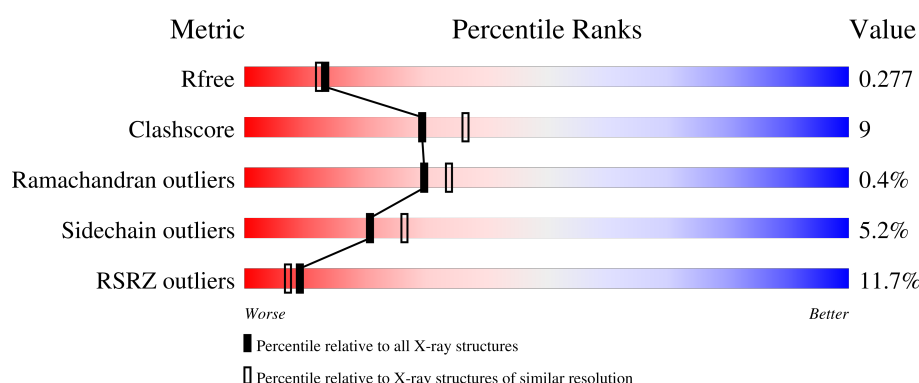
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	940	10% 69% 17% • 13%

2 Entry composition [i](#)

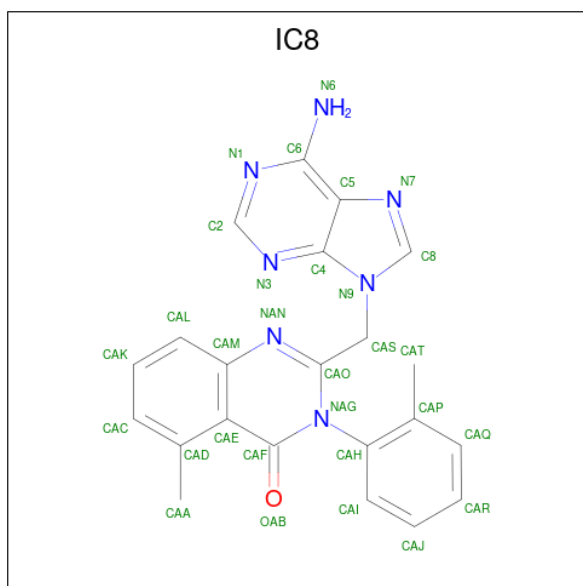
There are 3 unique types of molecules in this entry. The entry contains 6709 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT DELTA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	822	6639	4257	1127	1200	55	0	1	0

- Molecule 2 is 2-[(6-AMINO-9H-PURIN-9-YL)METHYL]-5-METHYL-3-(2-METHYLPHENYL)QUINAZOLIN-4(3H)-ONE (CCD ID: IC8) (formula: C₂₂H₁₉N₇O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	30	22	7	1	0	0

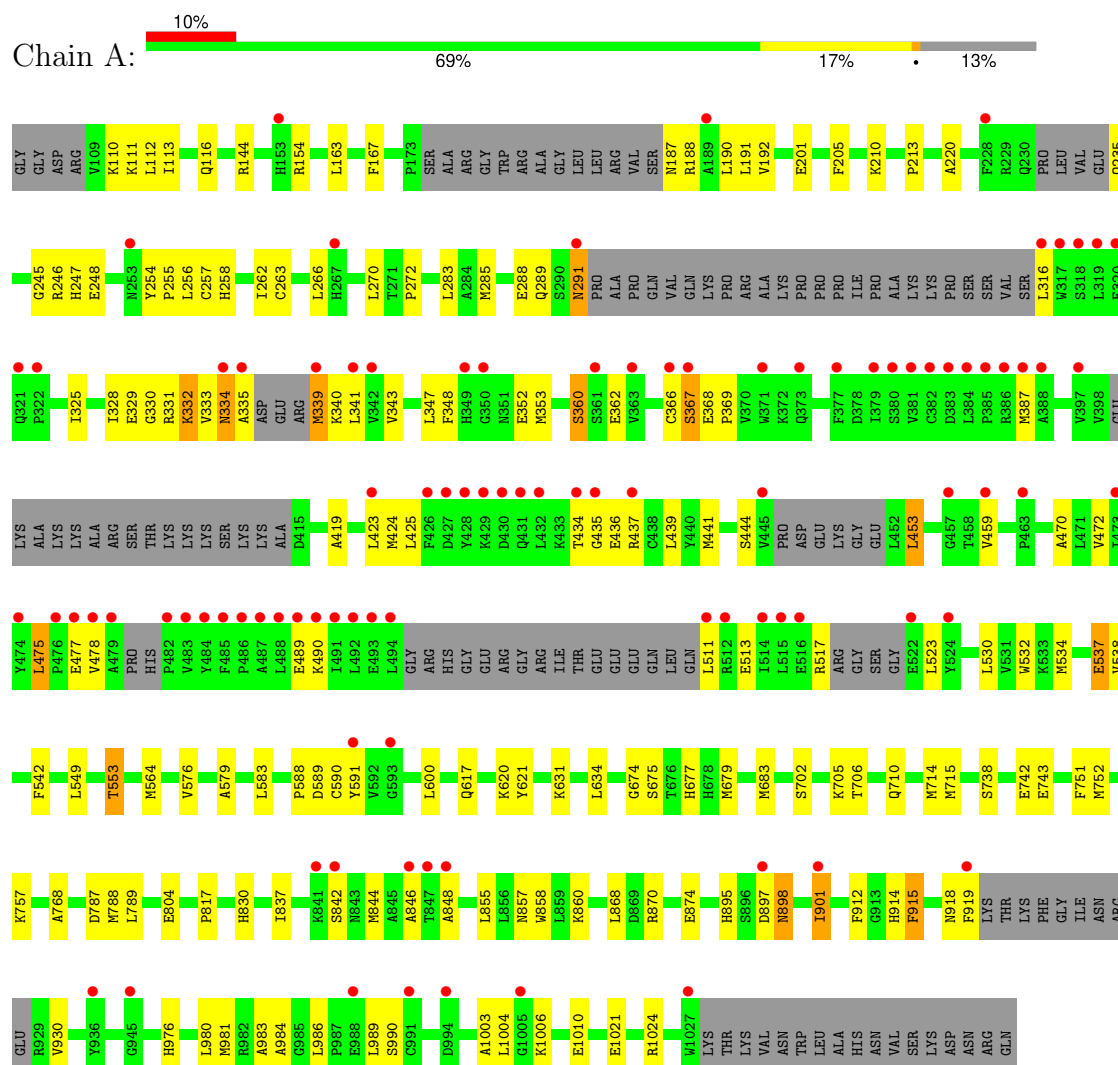
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	40	Total	O	0	0
			40	40		

3 Residue-property plots

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: PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT DELTA ISOFORM



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.42Å 64.66Å 116.90Å 90.00° 103.39° 90.00°	Depositor
Resolution (Å)	56.89 – 2.20 56.89 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.1 (56.89-2.20) 98.0 (56.89-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.5.0046	Depositor
R, R_{free}	0.239 , 0.277 0.238 , 0.277	Depositor DCC
R_{free} test set	1578 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6709	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.98% 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: IC8

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	0.65	0/6782	0.88	5/9150 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	334	ASN	N-CA-C	7.95	118.39	107.73
1	A	444	SER	N-CA-C	6.24	118.57	110.53
1	A	930	VAL	N-CA-C	6.19	113.95	108.63
1	A	235	GLN	CA-C-N	5.92	126.07	119.32
1	A	235	GLN	C-N-CA	5.92	126.07	119.32

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	6639	0	6619	112	0
2	A	30	0	19	2	0
3	A	40	0	0	3	0
All	All	6709	0	6638	114	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 (114) 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:837:ILE:CD1	1:A:901:ILE:HD11	1.73	1.18
1:A:549:LEU:HG	1:A:564:MET:HE1	1.10	1.10
1:A:366:CYS:O	1:A:367:SER:HB2	1.67	0.94
1:A:549:LEU:CG	1:A:564:MET:HE1	1.98	0.92
1:A:837:ILE:HD11	1:A:901:ILE:HD11	1.49	0.92
1:A:837:ILE:HD12	1:A:901:ILE:HD11	1.54	0.87
1:A:549:LEU:HG	1:A:564:MET:CE	2.01	0.86
1:A:367:SER:HB3	1:A:368:GLU:C	2.00	0.85
1:A:367:SER:HB3	1:A:369:PRO:N	1.91	0.85
1:A:245:GLY:HA3	1:A:768:ALA:HB2	1.59	0.84
1:A:830:HIS:HD2	3:A:2033:HOH:O	1.64	0.81
1:A:328:ILE:HB	1:A:472:VAL:HG23	1.63	0.79
1:A:617:GLN:NE2	1:A:984:ALA:HA	1.98	0.78
1:A:583:LEU:HD11	1:A:600:LEU:HD11	1.68	0.74
1:A:110:LYS:NZ	1:A:144:ARG:HH12	1.88	0.72
1:A:366:CYS:O	1:A:367:SER:CB	2.40	0.69
1:A:848:ALA:HB2	1:A:857:ASN:ND2	2.09	0.67
1:A:617:GLN:HE21	1:A:984:ALA:HA	1.58	0.66
1:A:553:THR:CG2	1:A:564:MET:HE3	2.25	0.66
1:A:110:LYS:HZ3	1:A:144:ARG:HH12	1.42	0.65
1:A:895:HIS:H	1:A:898:ASN:HD21	1.45	0.65
1:A:532:TRP:HZ3	1:A:564:MET:HE2	1.60	0.64
1:A:588:PRO:HB3	3:A:2004:HOH:O	1.96	0.64
1:A:192:VAL:HG13	1:A:272:PRO:HB2	1.80	0.62
1:A:167:PHE:HZ	1:A:285:MET:HE1	1.64	0.62
1:A:113:ILE:HA	1:A:116:GLN:HE21	1.65	0.62
1:A:870:ARG:NH2	1:A:874:GLU:OE2	2.32	0.61
1:A:914:HIS:HB3	1:A:918:ASN:O	2.01	0.61
1:A:710:GLN:O	1:A:714:MET:HG2	2.02	0.59
1:A:285:MET:O	1:A:288:GLU:HG2	2.03	0.58
1:A:187:ASN:N	1:A:210:LYS:HD3	2.19	0.58
1:A:256:LEU:O	1:A:262:ILE:HB	2.04	0.58
1:A:837:ILE:CD1	1:A:901:ILE:CD1	2.67	0.57
1:A:553:THR:HG21	1:A:564:MET:HE3	1.86	0.56
1:A:842:SER:O	1:A:844:MET:HE2	2.06	0.56
1:A:706:THR:OG1	1:A:710:GLN:OE1	2.23	0.56
1:A:387:MET:HG3	1:A:589:ASP:HA	1.88	0.56
1:A:860:LYS:HG2	1:A:868:LEU:HD22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:915:PHE:CD2	1:A:915:PHE:C	2.84	0.55
2:A:2028:IC8:HAA3	2:A:2028:IC8:OAB	2.06	0.55
1:A:334:ASN:ND2	1:A:335:ALA:H	2.05	0.55
1:A:787:ASP:OD1	1:A:912:PHE:O	2.23	0.55
1:A:328:ILE:HG22	1:A:329:GLU:HG2	1.89	0.55
1:A:436:GLU:O	1:A:437:ARG:HD2	2.06	0.54
1:A:387:MET:HE3	1:A:590:CYS:H	1.72	0.54
1:A:702:SER:O	1:A:706:THR:HG22	2.08	0.54
1:A:789:LEU:HD13	1:A:981:MET:HE2	1.90	0.54
1:A:191:LEU:O	1:A:272:PRO:HD2	2.09	0.53
1:A:332:LYS:NZ	1:A:341:LEU:HD21	2.23	0.53
1:A:617:GLN:HE22	1:A:620:LYS:NZ	2.08	0.52
1:A:419:ALA:HB3	1:A:441:MET:HE3	1.92	0.52
1:A:329:GLU:HB2	1:A:369:PRO:O	2.10	0.52
1:A:858:TRP:CZ3	1:A:901:ILE:HD13	2.45	0.51
1:A:255:PRO:HG2	1:A:258:HIS:CD2	2.46	0.51
1:A:553:THR:CG2	1:A:564:MET:CE	2.88	0.50
1:A:367:SER:CB	1:A:368:GLU:C	2.80	0.50
1:A:837:ILE:HD11	1:A:901:ILE:CD1	2.32	0.50
1:A:246:ARG:NH1	1:A:248:GLU:OE1	2.45	0.50
1:A:617:GLN:HE21	1:A:984:ALA:CA	2.25	0.50
1:A:343:VAL:H	1:A:360:SER:HB2	1.77	0.49
1:A:513:GLU:OE1	1:A:542:PHE:HZ	1.95	0.49
1:A:915:PHE:C	1:A:915:PHE:HD2	2.20	0.49
1:A:332:LYS:HE3	1:A:332:LYS:C	2.38	0.48
1:A:589:ASP:OD2	1:A:591:TYR:HB2	2.13	0.48
1:A:332:LYS:HZ2	1:A:341:LEU:HD21	1.79	0.48
1:A:289:GLN:HG2	1:A:677:HIS:CD2	2.49	0.47
1:A:553:THR:HG21	1:A:564:MET:CE	2.43	0.47
1:A:489:GLU:HG3	1:A:490:LYS:HE2	1.97	0.47
1:A:679:MET:O	1:A:683:MET:HG3	2.13	0.47
1:A:984:ALA:HB1	1:A:986:LEU:HD13	1.96	0.47
1:A:213:PRO:HD3	1:A:254:TYR:O	2.14	0.47
1:A:579:ALA:HB1	1:A:600:LEU:HG	1.97	0.46
1:A:330:GLY:HA2	1:A:470:ALA:O	2.16	0.46
1:A:534:MET:HA	1:A:534:MET:HE2	1.97	0.46
1:A:367:SER:HB3	1:A:369:PRO:CA	2.46	0.46
1:A:553:THR:HG22	1:A:564:MET:HE3	1.97	0.46
1:A:291:ASN:HD21	1:A:675:SER:HA	1.80	0.45
1:A:205:PHE:CZ	1:A:220:ALA:HA	2.51	0.45
1:A:205:PHE:HZ	1:A:220:ALA:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:513:GLU:HG2	1:A:542:PHE:CZ	2.52	0.45
1:A:154:ARG:NH2	1:A:674:GLY:O	2.50	0.45
1:A:621:TYR:CZ	1:A:983:ALA:HB2	2.51	0.45
1:A:247:HIS:HB2	1:A:738:SER:HA	1.97	0.45
1:A:1021:GLU:HA	1:A:1024:ARG:HH11	1.82	0.45
1:A:846:ALA:HA	1:A:857:ASN:HB3	1.98	0.45
1:A:976:HIS:O	1:A:980:LEU:HG	2.18	0.43
1:A:553:THR:HG22	1:A:564:MET:CE	2.48	0.43
1:A:348:PHE:CE1	1:A:353:MET:HG2	2.53	0.43
1:A:583:LEU:HD11	1:A:600:LEU:CD1	2.44	0.43
1:A:981:MET:HB3	1:A:989:LEU:HD21	2.00	0.43
2:A:2028:IC8:OAB	2:A:2028:IC8:CAA	2.65	0.43
1:A:163:LEU:HD23	1:A:167:PHE:HD2	1.83	0.43
1:A:895:HIS:H	1:A:898:ASN:ND2	2.15	0.43
1:A:435:GLY:HA2	1:A:475:LEU:O	2.19	0.43
1:A:1006:LYS:HB3	1:A:1010:GLU:HB2	2.00	0.43
1:A:715:MET:HE1	1:A:751:PHE:HD2	1.84	0.43
1:A:1003:ALA:HB1	1:A:1006:LYS:HD2	2.01	0.43
1:A:257:CYS:O	1:A:263:CYS:HB2	2.18	0.42
1:A:424:MET:SD	1:A:459:VAL:HG11	2.60	0.42
1:A:895:HIS:CE1	1:A:897:ASP:HB2	2.55	0.42
1:A:870:ARG:HA	1:A:870:ARG:HD2	1.96	0.41
1:A:347:LEU:HD22	1:A:425:LEU:HD11	2.02	0.41
1:A:534:MET:O	1:A:538:VAL:HG23	2.20	0.41
1:A:434:THR:HG21	1:A:477:GLU:HA	2.03	0.41
1:A:439:LEU:O	1:A:470:ALA:HA	2.21	0.41
1:A:339:MET:N	3:A:2002:HOH:O	2.53	0.41
1:A:534:MET:SD	1:A:537:GLU:HG3	2.61	0.41
1:A:340:LYS:HG2	1:A:362:GLU:HB3	2.03	0.41
1:A:490:LYS:HA	1:A:490:LYS:HD3	1.96	0.41
1:A:325:ILE:HG22	1:A:475:LEU:HD12	2.03	0.40
1:A:453:LEU:HD12	1:A:453:LEU:HA	1.92	0.40
1:A:788:MET:HE2	1:A:817:PRO:HG2	2.03	0.40
1:A:860:LYS:HG2	1:A:868:LEU:CD2	2.51	0.40
1:A:752:MET:O	1:A:757:LYS:HA	2.21	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	801/940 (85%)	774 (97%)	24 (3%)	3 (0%)	30	34

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	367	SER
1	A	742	GLU
1	A	478	VAL

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	729/827 (88%)	691 (95%)	38 (5%)	21	26

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	LYS
1	A	112	LEU
1	A	188	ARG
1	A	190	LEU
1	A	201	GLU
1	A	266	LEU
1	A	270	LEU
1	A	283	LEU

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Mol	Chain	Res	Type
1	A	291	ASN
1	A	316	LEU
1	A	331	ARG
1	A	332	LYS
1	A	333	VAL
1	A	339	MET
1	A	352	GLU
1	A	360	SER
1	A	423	LEU
1	A	453	LEU
1	A	475	LEU
1	A	511	LEU
1	A	517	ARG
1	A	523	LEU
1	A	530	LEU
1	A	537	GLU
1	A	553	THR
1	A	576	VAL
1	A	631	LYS
1	A	634	LEU
1	A	705	LYS
1	A	743	GLU
1	A	804	GLU
1	A	855	LEU
1	A	898	ASN
1	A	901	ILE
1	A	915	PHE
1	A	919	PHE
1	A	990	SER
1	A	1004	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	247	HIS
1	A	273	HIS
1	A	278	HIS
1	A	289	GLN
1	A	291	ASN
1	A	334	ASN
1	A	344	GLN
1	A	536	HIS

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Mol	Chain	Res	Type
1	A	539	GLN
1	A	617	GLN
1	A	792	GLN
1	A	830	HIS
1	A	898	ASN
1	A	906	GLN
1	A	918	ASN
1	A	948	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand 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	$\# Z > 2$
2	IC8	A	2028	-	34,34,34	1.94	8 (23%)	44,50,50	2.60	14 (31%)

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
2	IC8	A	2028	-	-	0/6/8/8	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2028	IC8	CAS-CAO	6.98	1.56	1.49
2	A	2028	IC8	C4-N9	-4.60	1.32	1.37
2	A	2028	IC8	CAE-CAF	-3.65	1.39	1.47
2	A	2028	IC8	CAH-NAG	-2.71	1.40	1.44
2	A	2028	IC8	C5-N7	-2.52	1.34	1.39
2	A	2028	IC8	CAM-NAN	-2.35	1.35	1.39
2	A	2028	IC8	CAO-NAN	2.27	1.33	1.29
2	A	2028	IC8	CAA-CAD	2.05	1.54	1.51

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2028	IC8	N9-C8-N7	-7.04	107.65	114.16
2	A	2028	IC8	C4-N9-C8	6.63	110.52	105.75
2	A	2028	IC8	N1-C2-N3	-5.50	120.25	128.58
2	A	2028	IC8	CAE-CAF-NAG	5.39	121.14	115.14
2	A	2028	IC8	N3-C4-N9	5.38	133.53	126.87
2	A	2028	IC8	C5-C4-N3	-4.25	120.86	126.72
2	A	2028	IC8	C2-N3-C4	3.51	120.41	111.83
2	A	2028	IC8	CAP-CAH-NAG	3.48	123.08	118.69
2	A	2028	IC8	CAO-CAS-N9	-2.93	107.70	111.63
2	A	2028	IC8	CAM-NAN-CAO	2.77	123.99	117.26
2	A	2028	IC8	CAH-NAG-CAF	2.53	119.75	117.21
2	A	2028	IC8	C5-N7-C8	2.53	107.42	103.45
2	A	2028	IC8	OAB-CAF-CAE	-2.35	119.31	124.19
2	A	2028	IC8	NAG-CAO-NAN	-2.06	118.31	124.36

There are no chirality outliers.

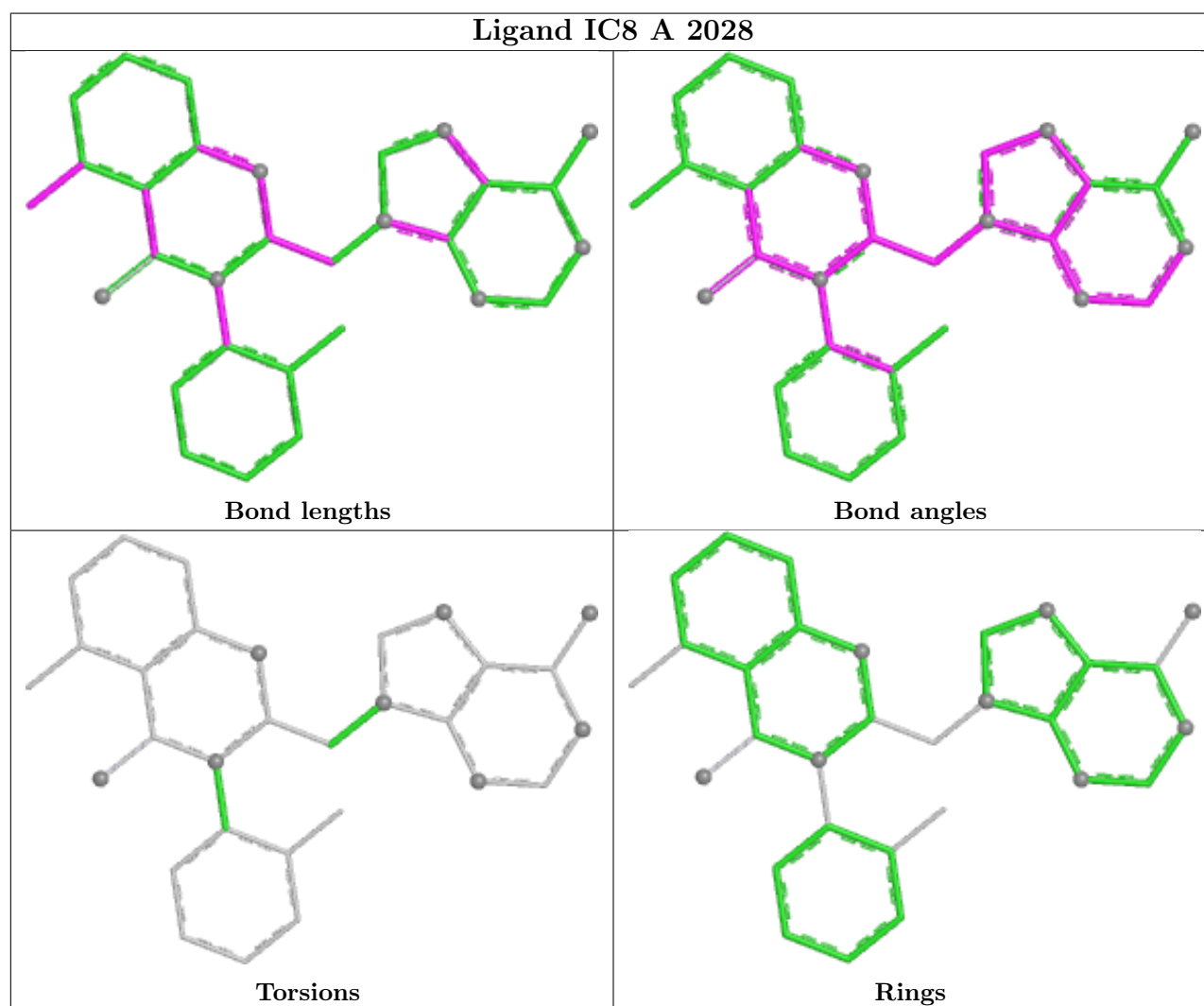
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2028	IC8	2	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 ⓘ

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	822/940 (87%)	0.74	96 (11%) 9 7	8, 21, 35, 53	1 (0%)

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	479	ALA	8.0
1	A	494	LEU	7.2
1	A	428	TYR	6.7
1	A	511	LEU	6.3
1	A	482	PRO	6.0
1	A	487	ALA	5.7
1	A	846	ALA	5.7
1	A	317	TRP	5.6
1	A	484	TYR	5.6
1	A	334	ASN	5.5
1	A	341	LEU	4.8
1	A	485	PHE	4.7
1	A	386	ARG	4.6
1	A	318	SER	4.5
1	A	435	GLY	4.3
1	A	388	ALA	4.3
1	A	490	LYS	4.3
1	A	491	ILE	4.3
1	A	429	LYS	4.2
1	A	486	PRO	4.2
1	A	445	VAL	4.1
1	A	367	SER	4.0
1	A	478	VAL	4.0
1	A	430	ASP	3.9
1	A	319	LEU	3.8
1	A	434	THR	3.7
1	A	591	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	477	GLU	3.6
1	A	483	VAL	3.6
1	A	350	GLY	3.5
1	A	384	LEU	3.4
1	A	228	PHE	3.3
1	A	366	CYS	3.3
1	A	335	ALA	3.2
1	A	382	CYS	3.1
1	A	489	GLU	3.1
1	A	493	GLU	3.0
1	A	488	LEU	3.0
1	A	387	MET	3.0
1	A	431	GLN	2.9
1	A	1027	TRP	2.9
1	A	593	GLY	2.9
1	A	492	LEU	2.9
1	A	514	ILE	2.8
1	A	381	VAL	2.8
1	A	361	SER	2.8
1	A	474	TYR	2.7
1	A	349	HIS	2.7
1	A	919	PHE	2.7
1	A	342	VAL	2.7
1	A	373	GLN	2.6
1	A	383	ASP	2.6
1	A	991	CYS	2.6
1	A	1005	GLY	2.6
1	A	397	VAL	2.5
1	A	363	VAL	2.5
1	A	153	HIS	2.5
1	A	267	HIS	2.4
1	A	522	GLU	2.4
1	A	385	PRO	2.4
1	A	945	GLY	2.4
1	A	320	GLU	2.4
1	A	473	ILE	2.4
1	A	426	PHE	2.3
1	A	524	TYR	2.3
1	A	842	SER	2.3
1	A	377	PHE	2.3
1	A	897	ASP	2.3
1	A	427	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	994	ASP	2.2
1	A	848	ALA	2.2
1	A	432	LEU	2.2
1	A	379	ILE	2.2
1	A	476	PRO	2.2
1	A	189	ALA	2.2
1	A	380	SER	2.2
1	A	936	TYR	2.2
1	A	459	VAL	2.2
1	A	988	GLU	2.2
1	A	371	TRP	2.1
1	A	253	ASN	2.1
1	A	339	MET	2.1
1	A	423	LEU	2.1
1	A	437	ARG	2.1
1	A	512	ARG	2.1
1	A	841	LYS	2.1
1	A	457	GLY	2.1
1	A	847	THR	2.1
1	A	515	LEU	2.1
1	A	322	PRO	2.1
1	A	516	GLU	2.0
1	A	291	ASN	2.0
1	A	321	GLN	2.0
1	A	316	LEU	2.0
1	A	463	PRO	2.0
1	A	901	ILE	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.

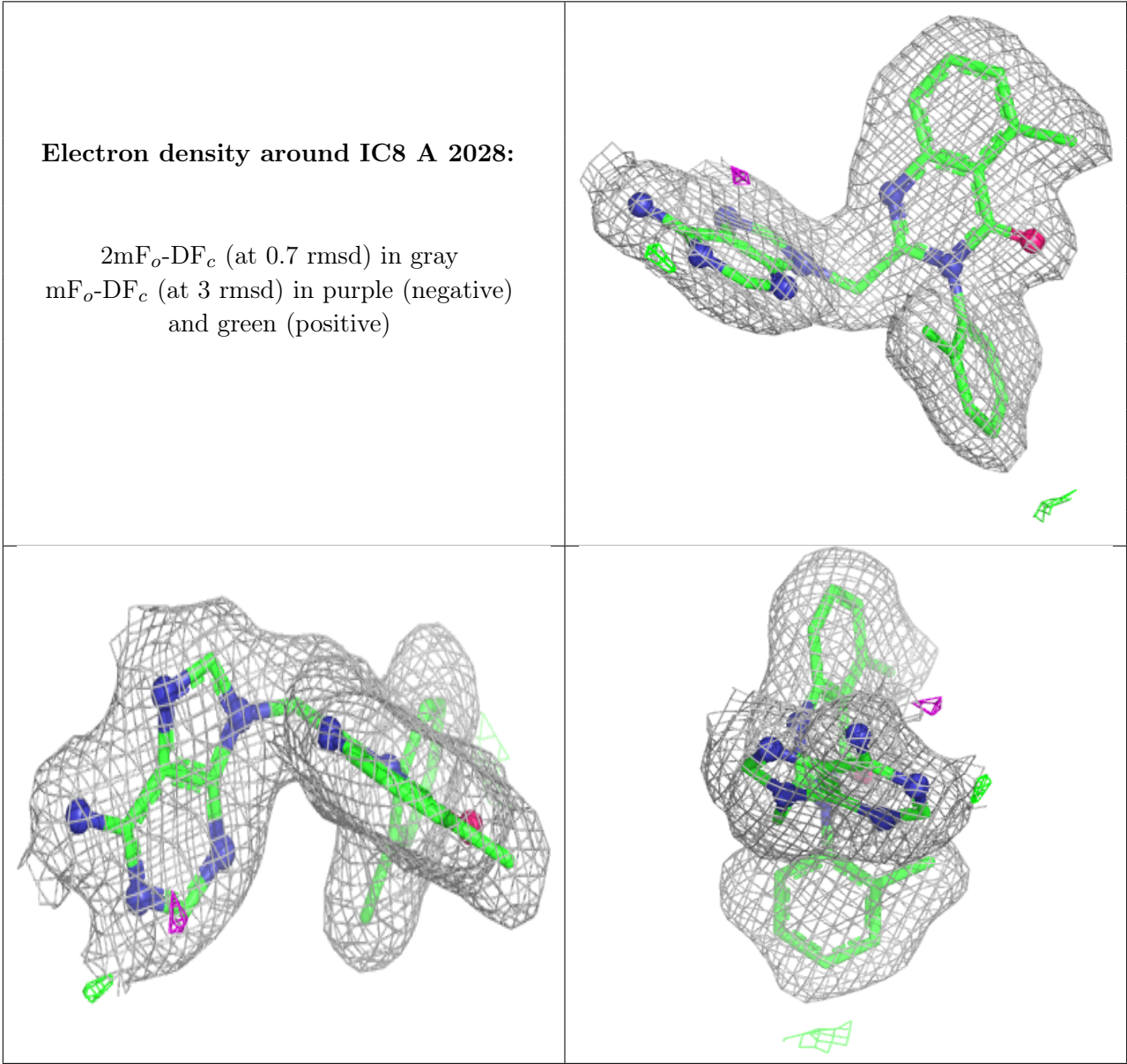
6.4 Ligands [i](#)

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
2	IC8	A	2028	30/30	0.94	0.07	23,27,32,34	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 ⓘ

There are no such residues in this entry.