



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:52 PM UTC

PDB ID : 8BCY / pdb_00008bcy
Title : HUMAN PI3KDELTA IN COMPLEX WITH COMPOUND 13
Authors : Pala, D.; Mazzucato, R.; Capelli, A.M.; Rancati, F.; Biagetti, M.
Deposited on : 2022-10-17
Resolution : 2.43 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

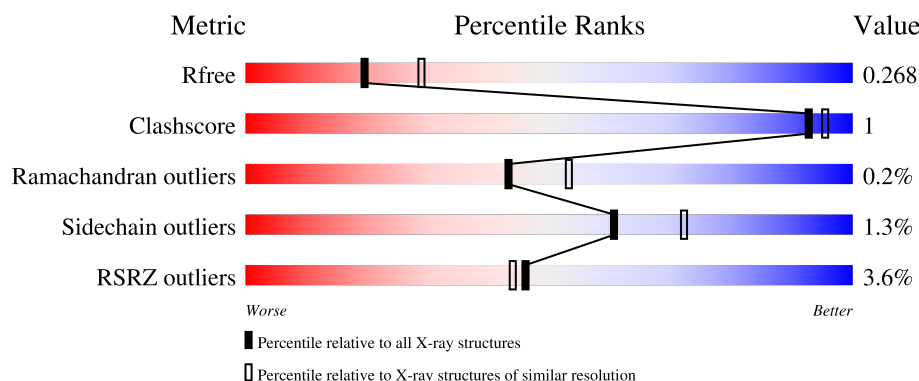
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

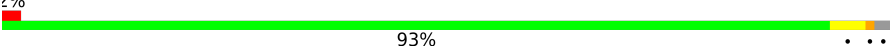
The reported resolution of this entry is 2.43 Å.

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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	1018	 3% 86% 5% 9%
2	B	169	 2% 93% ...

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8956 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.

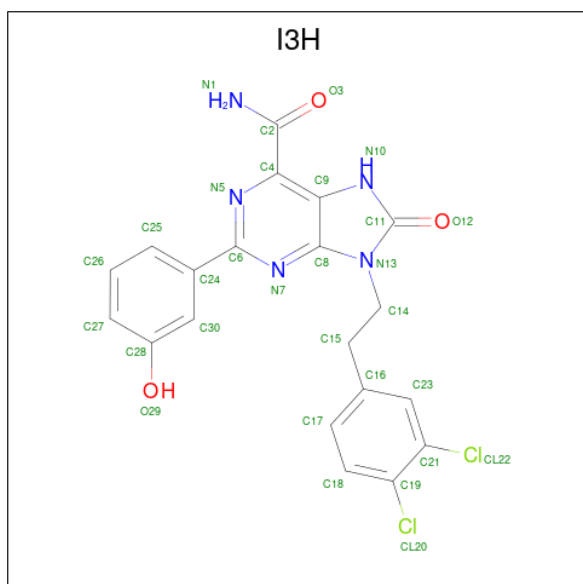
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit delta isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	922	7466	4778	1272	1363	53	220	2	0

- Molecule 2 is a protein called Phosphatidylinositol 3-kinase regulatory subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	165	1430	886	260	279	5	60	0	0

- Molecule 3 is 9-[2-(3,4-dichlorophenyl)ethyl]-2-(3-hydroxyphenyl)-8-oxidanylidene-7 {H}-purine-6-carboxamide (CCD ID: I3H) (formula: C₂₀H₁₅Cl₂N₅O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	N	O		
3	A	1	30	20	2	5	3	0	0

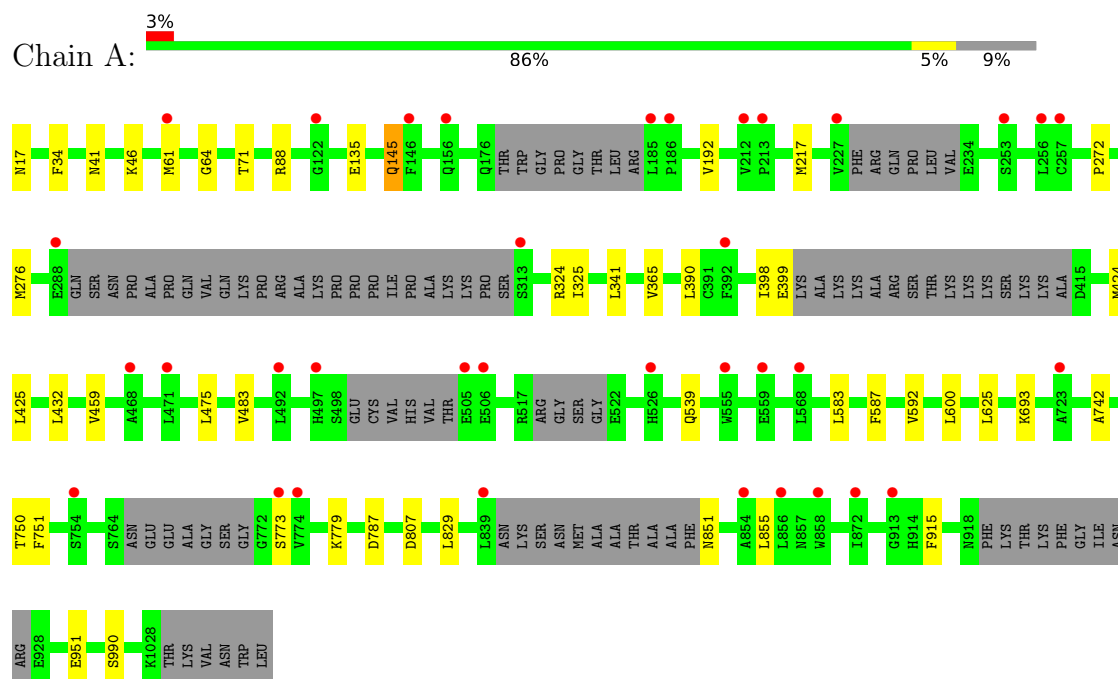
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	24	Total 24	O 24	0	0
4	B	6	Total 6	O 6	0	0

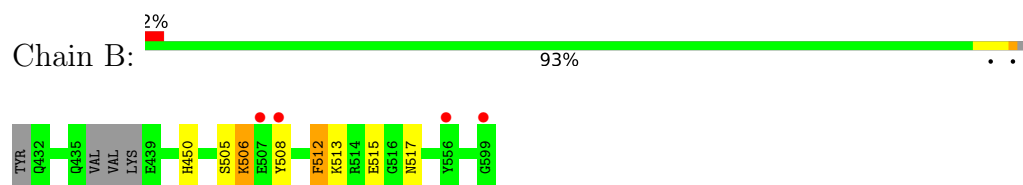
3 Residue-property plots [i](#)

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: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit delta isoform



- Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.60Å 108.81Å 142.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	86.51 – 2.43 86.51 – 2.43	Depositor EDS
% Data completeness (in resolution range)	95.3 (86.51-2.43) 95.3 (86.51-2.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.224 , 0.263 0.225 , 0.268	Depositor DCC
R_{free} test set	1049 reflections (1.95%)	wwPDB-VP
Wilson B-factor (Å ²)	63.0	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 43.7	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	0.95	EDS
Total number of atoms	8956	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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: I3H

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	2/7627 (0.0%)	0.88	4/10310 (0.0%)
2	B	0.66	0/1448	0.98	1/1929 (0.1%)
All	All	0.65	2/9075 (0.0%)	0.89	5/12239 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	807	ASP	C-N	-7.55	1.23	1.33
1	A	779	LYS	C-N	-5.72	1.26	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	PHE	N-CA-C	6.61	114.17	108.22
2	B	513	LYS	N-CA-C	-5.77	103.73	112.04
1	A	64	GLY	CA-C-N	5.25	124.70	119.24
1	A	64	GLY	C-N-CA	5.25	124.70	119.24
1	A	807	ASP	O-C-N	-5.23	116.21	123.01

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	7466	0	7449	18	0
2	B	1430	0	1415	8	0
3	A	30	0	0	0	0
4	A	24	0	0	1	0
4	B	6	0	0	1	0
All	All	8956	0	8864	25	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 1.

All (25) 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:512:PHE:HB2	2:B:517:ASN:HB3	1.29	1.06
2:B:512:PHE:CB	2:B:517:ASN:HB3	1.94	0.97
1:A:145[A]:GLN:HE21	1:A:145[A]:GLN:C	1.87	0.81
2:B:508:TYR:O	2:B:512:PHE:CE1	2.54	0.61
1:A:424:MET:HG2	1:A:459:VAL:HG11	1.89	0.55
1:A:587:PHE:HB3	1:A:592:VAL:HG11	1.91	0.53
2:B:512:PHE:HB3	2:B:517:ASN:HB3	1.88	0.52
2:B:450:HIS:HE1	4:B:803:HOH:O	1.92	0.51
1:A:61:MET:HE3	2:B:508:TYR:OH	2.11	0.51
2:B:505:SER:O	2:B:506:LYS:C	2.57	0.48
1:A:693:LYS:HD3	4:A:1208:HOH:O	2.15	0.46
1:A:583:LEU:HD11	1:A:600:LEU:HD11	1.98	0.46
1:A:773:SER:O	1:A:829:LEU:HD11	2.15	0.46
1:A:341:LEU:HG	1:A:365:VAL:HG22	1.98	0.45
1:A:325:ILE:HG22	1:A:475:LEU:HD23	1.99	0.45
1:A:390:LEU:HB2	1:A:425:LEU:HD21	1.98	0.45
1:A:41:ASN:HA	1:A:88:ARG:HA	1.98	0.44
1:A:398:ILE:HG23	1:A:398:ILE:O	2.18	0.44
1:A:217:MET:HB3	1:A:276:MET:HE1	2.00	0.43
1:A:398:ILE:O	1:A:399:GLU:C	2.60	0.43
1:A:135:GLU:HG2	1:A:625:LEU:HD12	2.00	0.43
1:A:192:VAL:HG12	1:A:272:PRO:HG2	2.03	0.41
1:A:432:LEU:HB3	1:A:483:VAL:HG13	2.03	0.40
1:A:750:THR:OG1	1:A:751:PHE:N	2.54	0.40
2:B:512:PHE:HA	2:B:515:GLU:HB3	2.03	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	904/1018 (89%)	874 (97%)	29 (3%)	1 (0%)	48	60
2	B	161/169 (95%)	153 (95%)	7 (4%)	1 (1%)	21	25
All	All	1065/1187 (90%)	1027 (96%)	36 (3%)	2 (0%)	43	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	742	ALA
2	B	506	LYS

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	827/903 (92%)	814 (98%)	13 (2%)	55	68
2	B	156/160 (98%)	155 (99%)	1 (1%)	78	85
All	All	983/1063 (92%)	969 (99%)	14 (1%)	61	70

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	46	LYS
1	A	71	THR
1	A	145[A]	GLN

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Mol	Chain	Res	Type
1	A	145[B]	GLN
1	A	324	ARG
1	A	539	GLN
1	A	787	ASP
1	A	851	ASN
1	A	855	LEU
1	A	915	PHE
1	A	951	GLU
1	A	990	SER
2	B	512	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	GLN
1	A	187	ASN
1	A	244	ASN
1	A	247	HIS
1	A	422	ASN
1	A	526	HIS
1	A	536	HIS
1	A	539	GLN
1	A	656	HIS
1	A	696	ASN
1	A	851	ASN
1	A	1014	HIS
2	B	455	GLN
2	B	475	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

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
3	I3H	A	1101	-	32,33,33	0.86	1 (3%)	41,48,48	2.55	10 (24%)

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	I3H	A	1101	-	-	3/13/13/13	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	I3H	C11-N13	-3.64	1.35	1.38

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	I3H	N10-C11-N13	9.66	111.16	106.76
3	A	1101	I3H	C4-N5-C6	6.34	123.28	116.19
3	A	1101	I3H	C14-N13-C11	5.04	127.59	123.50
3	A	1101	I3H	C9-N10-C11	-4.71	107.28	109.82
3	A	1101	I3H	N7-C8-N13	4.17	132.68	125.67
3	A	1101	I3H	O12-C11-N10	-3.88	124.14	127.49
3	A	1101	I3H	C4-C9-N10	3.73	134.55	130.82
3	A	1101	I3H	O3-C2-N1	-2.66	118.78	122.62
3	A	1101	I3H	C15-C16-C23	-2.37	116.56	120.54
3	A	1101	I3H	N7-C6-N5	-2.02	121.81	125.13

There are no chirality outliers.

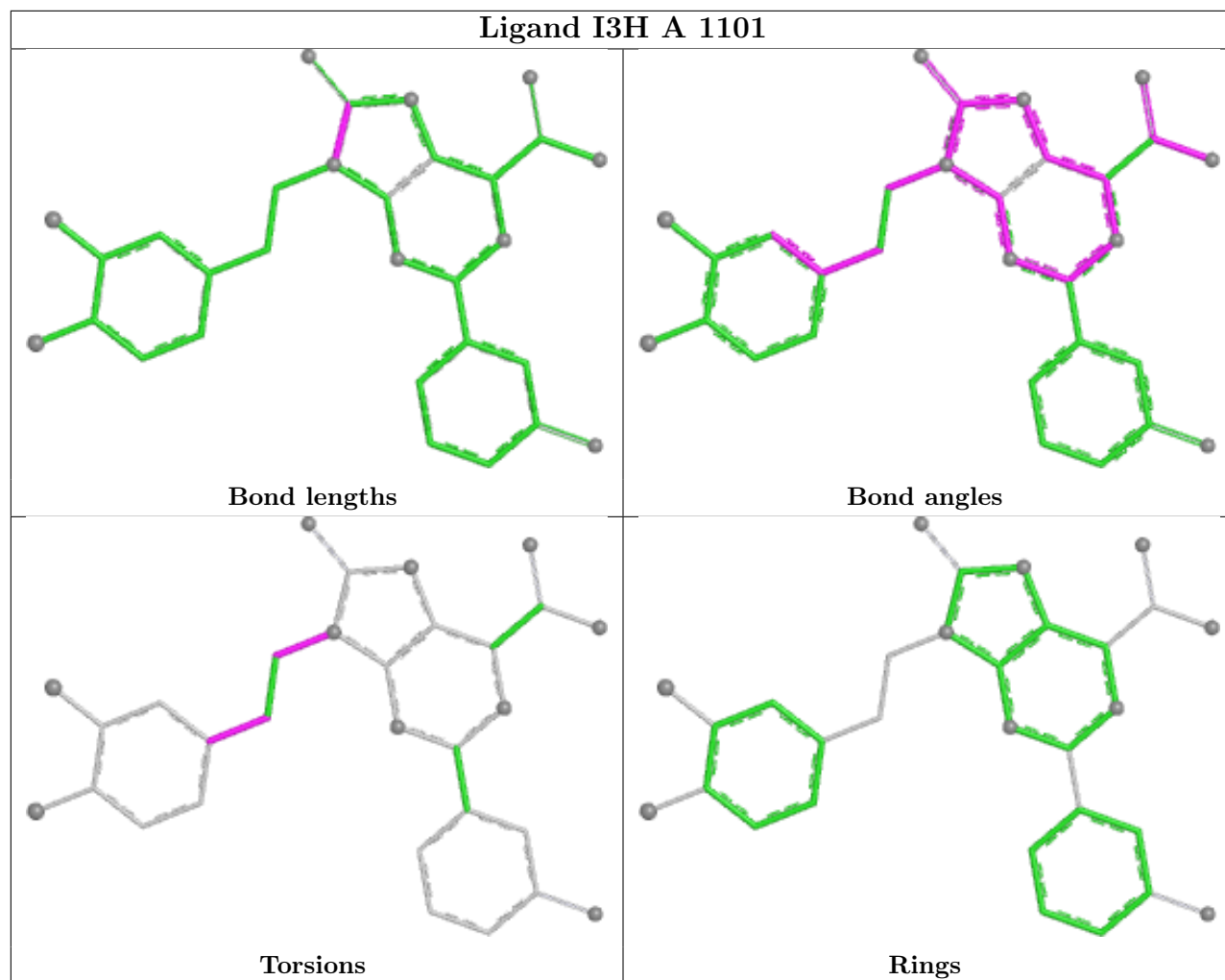
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1101	I3H	C15-C14-N13-C8
3	A	1101	I3H	C14-C15-C16-C17
3	A	1101	I3H	C14-C15-C16-C23

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	922/1018 (90%)	0.42	35 (3%) 44 42	27, 72, 113, 172	64 (6%)
2	B	165/169 (97%)	0.27	4 (2%) 59 60	41, 70, 100, 117	21 (12%)
All	All	1087/1187 (91%)	0.39	39 (3%) 46 44	27, 72, 111, 172	85 (7%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	508	TYR	4.9
1	A	506	GLU	4.2
1	A	61	MET	4.0
1	A	227	VAL	3.9
1	A	185	LEU	3.7
1	A	555	TRP	3.2
1	A	186	PRO	3.2
1	A	212	VAL	3.2
1	A	257	CYS	3.1
1	A	253	SER	3.0
1	A	156	GLN	3.0
1	A	839	LEU	2.9
1	A	313	SER	2.9
2	B	599	GLY	2.8
1	A	568	LEU	2.8
1	A	256	LEU	2.7
1	A	913	GLY	2.6
1	A	526	HIS	2.6
1	A	856	LEU	2.5
1	A	505	GLU	2.5
1	A	471	LEU	2.5
1	A	854	ALA	2.5
1	A	754	SER	2.4
1	A	773	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	146	PHE	2.3
1	A	213	PRO	2.2
1	A	392	PHE	2.2
1	A	288	GLU	2.2
1	A	559	GLU	2.2
1	A	122	GLY	2.2
1	A	872	ILE	2.2
1	A	723	ALA	2.1
2	B	556	TYR	2.1
1	A	492	LEU	2.1
1	A	497	HIS	2.1
2	B	507	GLU	2.1
1	A	858	TRP	2.1
1	A	774	VAL	2.0
1	A	468	ALA	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](#)

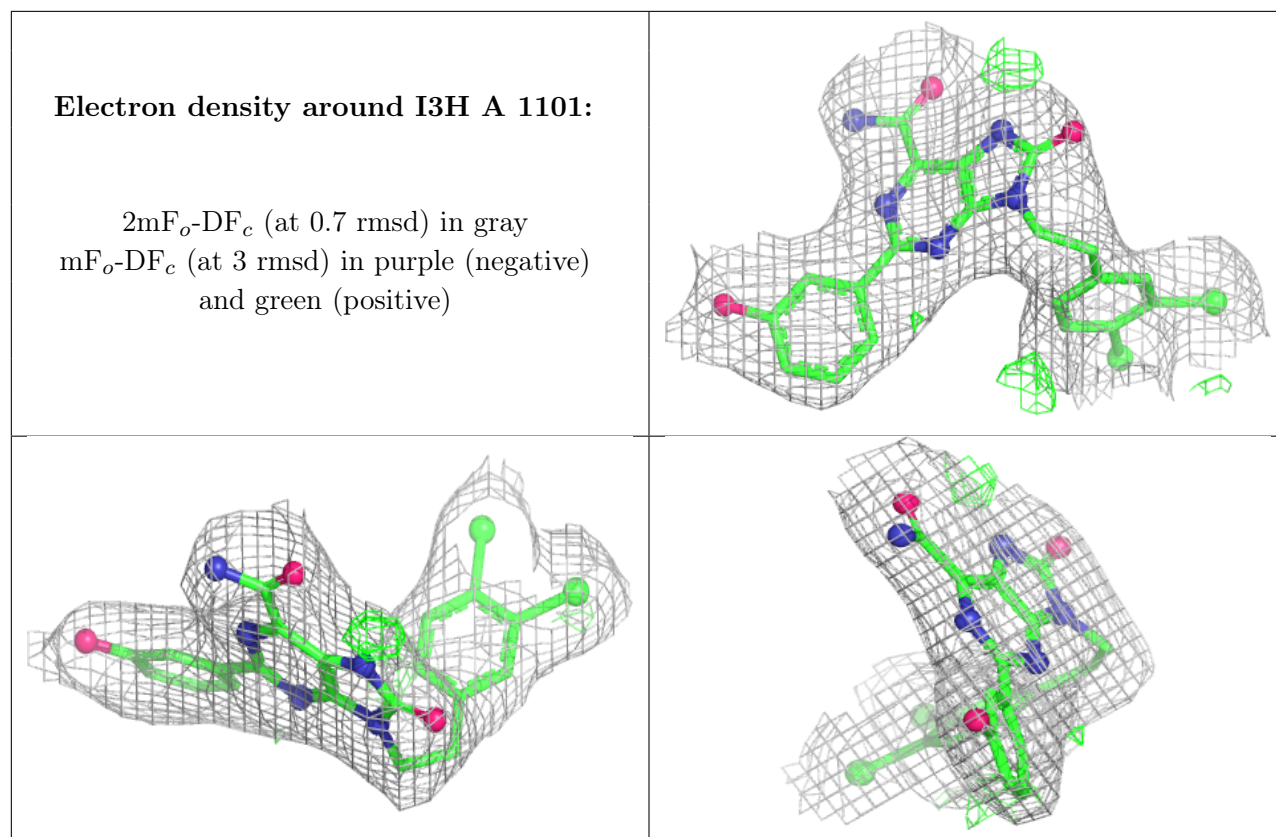
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
3	I3H	A	1101	30/30	0.92	0.10	51,61,91,100	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.