



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2026 – 01:57 AM UTC

PDB ID : 5NCZ / pdb_00005ncz
Title : mPI3Kd IN COMPLEX WITH inh1
Authors : Petersen, J.
Deposited on : 2017-03-06
Resolution : 1.94 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

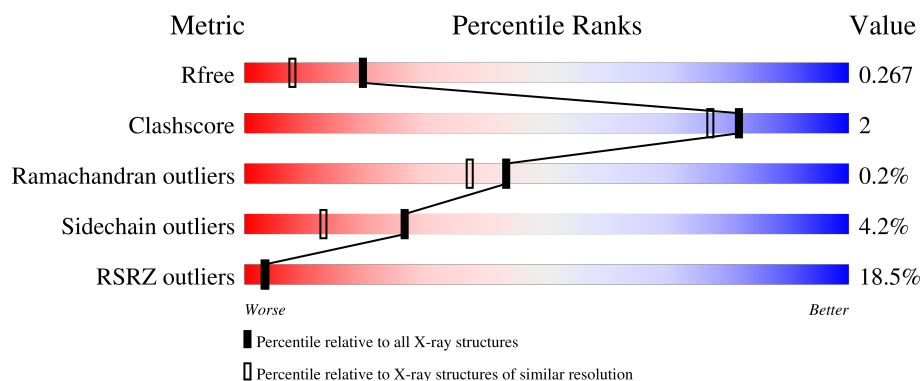
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	936	16% 80% 7% 12%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6993 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.

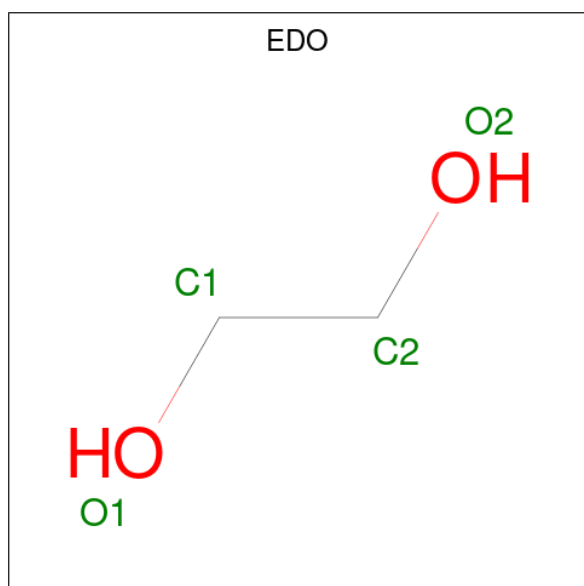
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit delta isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	827	6687	4287	1134	1211	55	3	3	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	497	ILE	HIS	conflict	UNP O35904
A	?	-	LEU	deletion	UNP O35904
A	?	-	GLN	deletion	UNP O35904

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



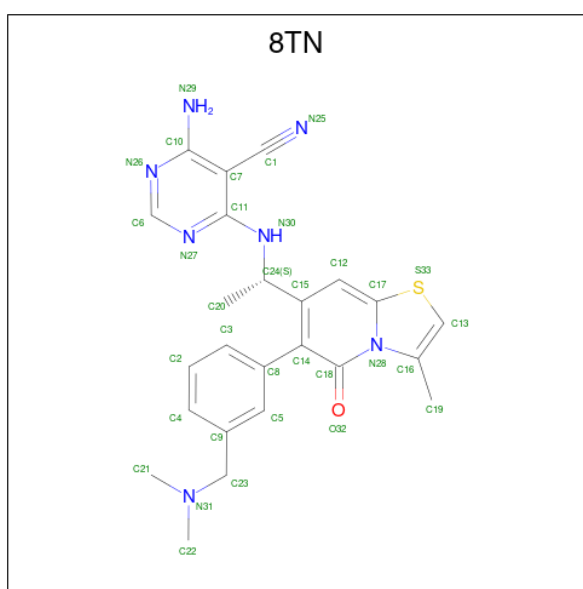
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	4	2	2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0

- Molecule 3 is 4-azanyl-6-[[[(1 {S})-1-[6-[3-[(dimethylamino)methyl]phenyl]-3-methyl-5-oxido-1H-1,3,4-thiazolo[3,2-a]pyridin-7-yl]ethyl]amino]pyrimidine-5-carbonitrile (CCD ID: 8TN) (formula: C₂₄H₂₅N₇OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			33	24	7	1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	257	Total O 257 257	0	0

- 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	141.65Å 64.84Å 116.60Å 90.00° 103.63° 90.00°	Depositor
Resolution (Å)	42.97 – 1.94 42.97 – 1.94	Depositor EDS
% Data completeness (in resolution range)	96.9 (42.97-1.94) 96.9 (42.97-1.94)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 1.94Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.225 , 0.259 0.232 , 0.267	Depositor DCC
R_{free} test set	3715 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6993	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% 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: EDO, 8TN

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	0.80	2/6838 (0.0%)	1.25	10/9223 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	564	MET	SD-CE	-5.93	1.64	1.79
1	A	387	MET	SD-CE	-5.81	1.65	1.79

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	915	PHE	CA-CB-CG	8.19	121.99	113.80
1	A	898	ASN	CA-CB-CG	5.50	118.10	112.60
1	A	332	LYS	CA-C-N	5.38	129.87	121.85
1	A	332	LYS	C-N-CA	5.38	129.87	121.85
1	A	243	VAL	N-CA-C	-5.22	102.00	108.89
1	A	745[A]	CYS	CA-C-N	5.18	127.28	120.60
1	A	745[A]	CYS	C-N-CA	5.18	127.28	120.60
1	A	745[B]	CYS	CA-C-N	5.18	127.28	120.60
1	A	745[B]	CYS	C-N-CA	5.18	127.28	120.60
1	A	203	PHE	CA-CB-CG	5.08	118.88	113.80

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	6687	0	6671	33	0
2	A	16	0	24	1	0
3	A	33	0	0	0	0
4	A	257	0	0	0	0
All	All	6993	0	6695	33	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 2.

All (33) 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:549:LEU:HG	1:A:564:MET:HE1	1.37	1.05
1:A:245:GLY:HA3	1:A:768:ALA:HB2	1.50	0.93
1:A:328:ILE:HB	1:A:472:VAL:HG23	1.74	0.68
1:A:386:ARG:HG3	1:A:387:MET:HE2	1.77	0.65
1:A:756:MET:HE2	1:A:781:GLY:HA3	1.82	0.61
1:A:387:MET:HE3	1:A:590:CYS:HB3	1.83	0.59
1:A:642:LYS:HG2	2:A:1103:EDO:H21	1.85	0.58
1:A:784:LEU:HD12	1:A:823:GLY:HA3	1.84	0.58
1:A:512:ARG:HG2	1:A:530:LEU:HD12	1.86	0.57
1:A:194:VAL:HG21	1:A:216:LEU:HD21	1.87	0.56
1:A:271:THR:O	1:A:273:HIS:HD2	1.90	0.55
1:A:331:ARG:HD2	1:A:470:ALA:HB3	1.89	0.53
1:A:859:LEU:HD21	1:A:905:GLY:HA2	1.90	0.53
1:A:247:HIS:CD2	1:A:740:LEU:HD21	2.45	0.52
1:A:549:LEU:CG	1:A:564:MET:HE1	2.26	0.50
1:A:515:LEU:HD12	1:A:516:GLU:HG3	1.95	0.48
1:A:532:TRP:HZ3	1:A:564:MET:HE2	1.79	0.47
1:A:549:LEU:HG	1:A:564:MET:CE	2.28	0.47
1:A:329:GLU:HB2	1:A:369:PRO:O	2.15	0.46
1:A:213:PRO:O	1:A:217:MET:HG3	2.17	0.45
1:A:192:VAL:HG11	1:A:216:LEU:HD11	1.99	0.44
1:A:902:ARG:HD3	1:A:906:GLN:HB2	1.98	0.44
1:A:324:SER:HB3	1:A:376:GLU:HG3	1.99	0.44
1:A:971:GLY:HA3	1:A:1004:LEU:HD21	2.00	0.44
1:A:157:LEU:HD22	1:A:161:GLU:HB3	2.00	0.43
1:A:329:GLU:HG2	1:A:472:VAL:HG22	2.01	0.43
1:A:209:THR:HB	1:A:257:CYS:HB3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:637:ALA:HB1	1:A:644:GLY:HA2	2.02	0.41
1:A:617:GLN:HE21	1:A:984:ALA:HA	1.85	0.41
1:A:859:LEU:HD23	1:A:859:LEU:HA	1.94	0.40
1:A:342:VAL:HG22	1:A:362:GLU:HG2	2.02	0.40
1:A:394:LEU:HD22	1:A:441:MET:HE1	2.02	0.40
1:A:507:THR:C	1:A:509:GLU:H	2.29	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	806/936 (86%)	787 (98%)	17 (2%)	2 (0%)	43 37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	LEU
1	A	328	ILE

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	735/824 (89%)	704 (96%)	31 (4%)	26 13

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	VAL
1	A	190	LEU
1	A	203	PHE
1	A	270	LEU
1	A	316	LEU
1	A	317	TRP
1	A	325	ILE
1	A	331	ARG
1	A	332	LYS
1	A	333	VAL
1	A	340	LYS
1	A	356	LYS
1	A	423	LEU
1	A	437	ARG
1	A	453	LEU
1	A	507	THR
1	A	511	LEU
1	A	512	ARG
1	A	530	LEU
1	A	553	THR
1	A	565	LEU
1	A	634	LEU
1	A	642	LYS
1	A	743	GLU
1	A	755	LYS
1	A	766	GLU
1	A	841	LYS
1	A	855	LEU
1	A	898	ASN
1	A	915	PHE
1	A	1004	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	ASN
1	A	247	HIS
1	A	273	HIS
1	A	278	HIS
1	A	291	ASN
1	A	344	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	422	ASN
1	A	610	GLN
1	A	617	GLN
1	A	721	GLN
1	A	773	ASN
1	A	780	ASN
1	A	792	GLN
1	A	836	ASN
1	A	898	ASN
1	A	906	GLN
1	A	914	HIS
1	A	918	ASN
1	A	976	HIS

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](#)

5 ligands are 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	EDO	A	1102	-	3,3,3	0.25	0	2,2,2	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	A	1103	-	3,3,3	0.15	0	2,2,2	0.17	0
3	8TN	A	1105	-	35,36,36	1.20	4 (11%)	36,52,52	1.71	9 (25%)
2	EDO	A	1101	-	3,3,3	0.17	0	2,2,2	0.15	0
2	EDO	A	1104	-	3,3,3	0.21	0	2,2,2	0.17	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
2	EDO	A	1102	-	-	0/1/1/1	-
2	EDO	A	1103	-	-	0/1/1/1	-
3	8TN	A	1105	-	-	0/14/18/18	0/4/4/4
2	EDO	A	1101	-	-	0/1/1/1	-
2	EDO	A	1104	-	-	0/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1105	8TN	C11-N30	3.64	1.40	1.35
3	A	1105	8TN	C7-C10	-2.96	1.38	1.42
3	A	1105	8TN	C7-C11	-2.38	1.39	1.42
3	A	1105	8TN	C10-N29	2.37	1.40	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1105	8TN	C7-C11-N30	-5.14	117.73	120.94
3	A	1105	8TN	O32-C18-N28	4.03	125.62	119.87
3	A	1105	8TN	S33-C17-N28	3.05	114.54	111.02
3	A	1105	8TN	O32-C18-C14	-2.82	118.66	124.73
3	A	1105	8TN	N30-C11-N27	2.66	121.77	118.00
3	A	1105	8TN	C13-C16-N28	2.64	115.12	111.30
3	A	1105	8TN	C12-C15-C14	2.41	121.11	115.93
3	A	1105	8TN	C11-C7-C1	2.40	122.44	119.21
3	A	1105	8TN	C19-C16-C13	-2.16	122.73	127.33

There are no chirality outliers.

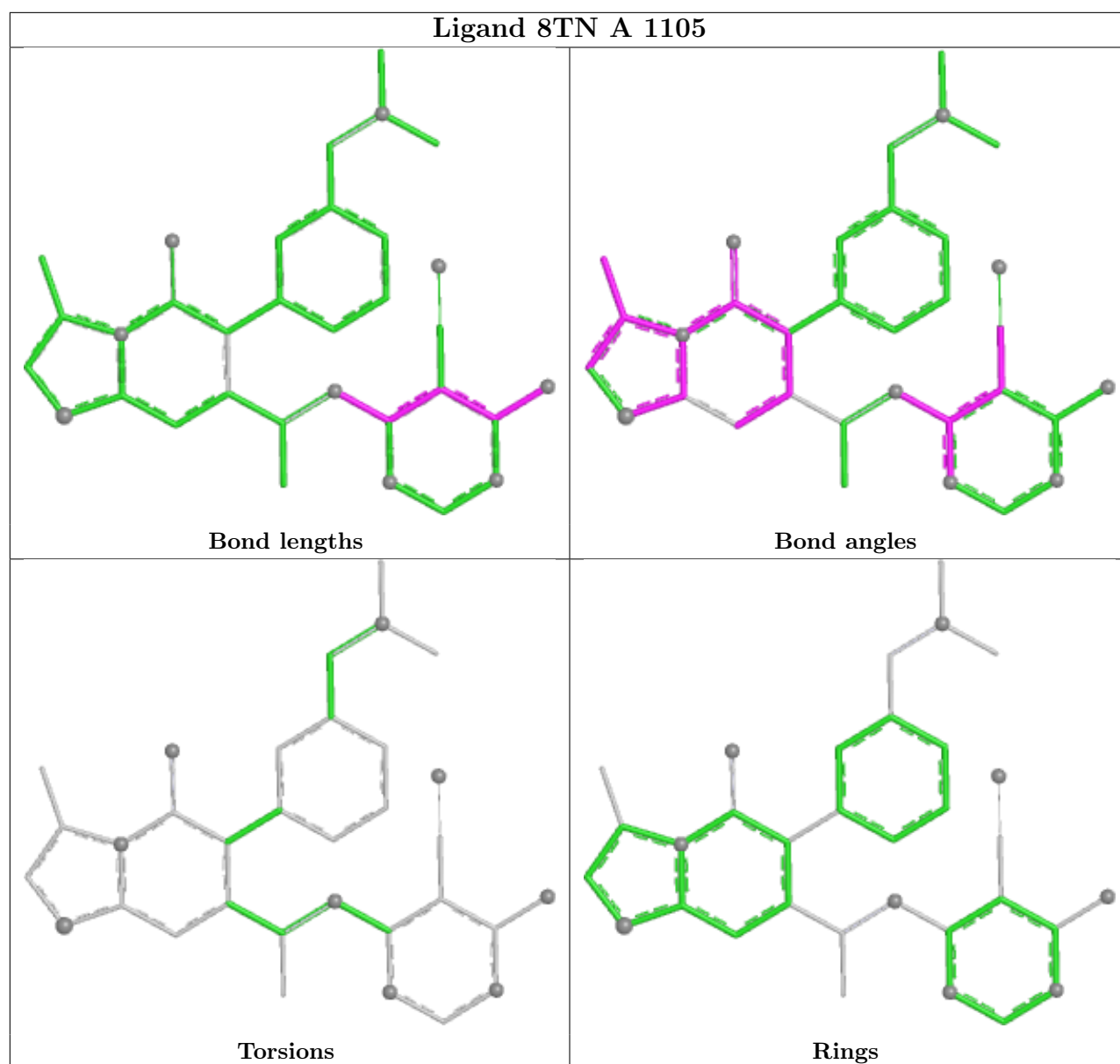
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1103	EDO	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	827/936 (88%)	0.94	153 (18%) 3 3	10, 34, 69, 112	6 (0%)

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	316	LEU	8.8
1	A	479	ALA	8.7
1	A	335	ALA	8.5
1	A	1027	TRP	8.4
1	A	445	VAL	8.0
1	A	317	TRP	7.6
1	A	919	PHE	7.3
1	A	333	VAL	6.9
1	A	497	ILE	6.6
1	A	523	LEU	5.4
1	A	323	PHE	5.4
1	A	377	PHE	5.3
1	A	398	VAL	5.2
1	A	365	VAL	5.0
1	A	334	ASN	4.7
1	A	514	ILE	4.7
1	A	332	LYS	4.6
1	A	471	LEU	4.6
1	A	291	ASN	4.5
1	A	511	LEU	4.5
1	A	319	LEU	4.4
1	A	517	ARG	4.3
1	A	395	TYR	4.1
1	A	226	THR	4.1
1	A	507	THR	4.1
1	A	228	PHE	4.1
1	A	930	VAL	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	515	LEU	4.0
1	A	488	LEU	4.0
1	A	270	LEU	3.9
1	A	341	LEU	3.9
1	A	474	TYR	3.9
1	A	492	LEU	3.8
1	A	434	THR	3.8
1	A	318	SER	3.8
1	A	330	GLY	3.7
1	A	846	ALA	3.6
1	A	109	VAL	3.6
1	A	356	LYS	3.5
1	A	363	VAL	3.5
1	A	841	LYS	3.5
1	A	331	ARG	3.4
1	A	227	VAL	3.4
1	A	397	VAL	3.3
1	A	769	GLY	3.3
1	A	1023	LEU	3.3
1	A	512	ARG	3.3
1	A	203	PHE	3.3
1	A	360	SER	3.3
1	A	936	TYR	3.2
1	A	1017	VAL	3.2
1	A	358	VAL	3.2
1	A	524	TYR	3.1
1	A	435	GLY	3.1
1	A	381	VAL	3.1
1	A	230	GLN	3.1
1	A	416	CYS	3.1
1	A	847	THR	3.1
1	A	962	ARG	3.0
1	A	1004	LEU	2.9
1	A	342	VAL	2.9
1	A	508	GLU	2.9
1	A	553	THR	2.9
1	A	173	PRO	2.8
1	A	370	VAL	2.8
1	A	929	ARG	2.8
1	A	993	LYS	2.8
1	A	1003	ALA	2.8
1	A	205	PHE	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	483	VAL	2.8
1	A	322	PRO	2.8
1	A	495	GLY	2.7
1	A	557	LYS	2.7
1	A	1014	HIS	2.7
1	A	601	ARG	2.7
1	A	934	LEU	2.6
1	A	1012	LEU	2.6
1	A	472	VAL	2.6
1	A	755	LYS	2.6
1	A	995	ILE	2.6
1	A	340	LYS	2.6
1	A	1013	LYS	2.6
1	A	559	GLU	2.5
1	A	191	LEU	2.5
1	A	530	LEU	2.5
1	A	937	ASP	2.5
1	A	490	LYS	2.5
1	A	533	LYS	2.5
1	A	345	ALA	2.5
1	A	478	VAL	2.5
1	A	321	GLN	2.5
1	A	546	LEU	2.5
1	A	510	GLU	2.5
1	A	269	GLY	2.5
1	A	327	LEU	2.5
1	A	325	ILE	2.5
1	A	493	GLU	2.5
1	A	257	CYS	2.4
1	A	843	ASN	2.4
1	A	453	LEU	2.4
1	A	1026	SER	2.4
1	A	470	ALA	2.4
1	A	1022	ALA	2.4
1	A	482	PRO	2.4
1	A	591	TYR	2.4
1	A	1024	ARG	2.4
1	A	382	CYS	2.4
1	A	418	ILE	2.4
1	A	351	ASN	2.4
1	A	419	ALA	2.3
1	A	473	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	913	GLY	2.3
1	A	359	SER	2.3
1	A	509	GLU	2.3
1	A	375	LEU	2.3
1	A	549	LEU	2.3
1	A	534	MET	2.3
1	A	396	ALA	2.3
1	A	417	PRO	2.3
1	A	415	ASP	2.3
1	A	373	GLN	2.2
1	A	552	VAL	2.2
1	A	374	ARG	2.2
1	A	354	LEU	2.2
1	A	452	LEU	2.2
1	A	516	GLU	2.2
1	A	134	PRO	2.2
1	A	328	ILE	2.2
1	A	119	LEU	2.2
1	A	475	LEU	2.2
1	A	494	LEU	2.2
1	A	1002	LEU	2.2
1	A	199	SER	2.2
1	A	1011	ALA	2.2
1	A	484	TYR	2.1
1	A	357	THR	2.1
1	A	219	CYS	2.1
1	A	476	PRO	2.1
1	A	393	ALA	2.1
1	A	491	ILE	2.1
1	A	223	LYS	2.1
1	A	362	GLU	2.1
1	A	189	ALA	2.1
1	A	196	PHE	2.1
1	A	258	HIS	2.1
1	A	371	TRP	2.1
1	A	394	LEU	2.1
1	A	432	LEU	2.1
1	A	433	LYS	2.0
1	A	347	LEU	2.0
1	A	771	ALA	2.0
1	A	324	SER	2.0
1	A	496	ARG	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](#)

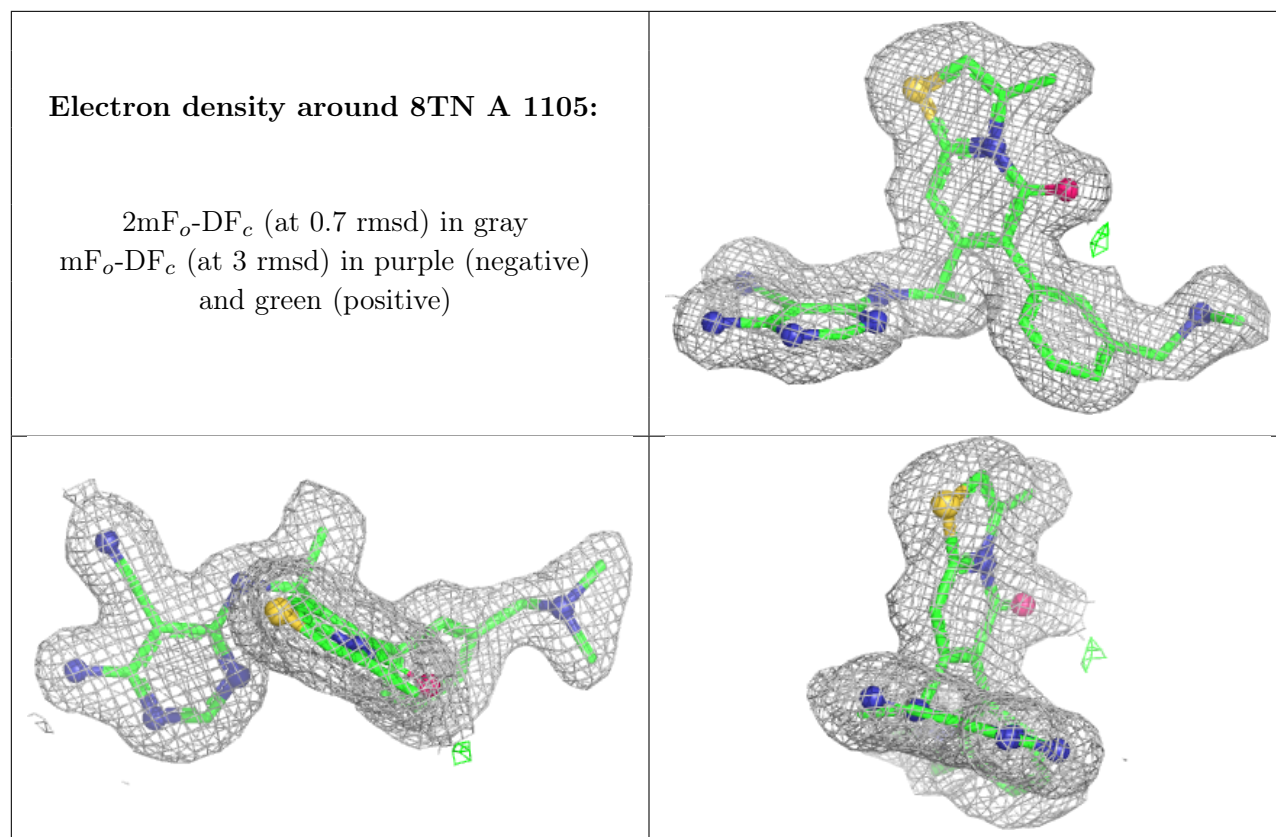
There are no oligosaccharides in this entry.

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
2	EDO	A	1101	4/4	0.94	0.08	23,28,29,30	0
2	EDO	A	1104	4/4	0.94	0.10	21,23,24,24	0
2	EDO	A	1102	4/4	0.95	0.08	26,30,32,35	0
2	EDO	A	1103	4/4	0.96	0.07	22,25,28,30	0
3	8TN	A	1105	33/33	0.96	0.07	14,19,34,35	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.