



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:35 PM UTC

PDB ID : 5NCY / pdb_00005ncy
Title : mPI3Kd IN COMPLEX WITH inh1
Authors : Petersen, J.
Deposited on : 2017-03-06
Resolution : 1.90 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

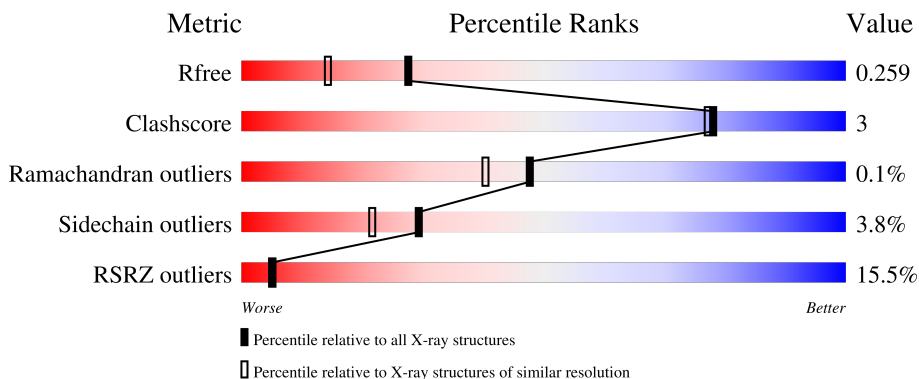
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	939	14% 79% 9% 12%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7081 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.

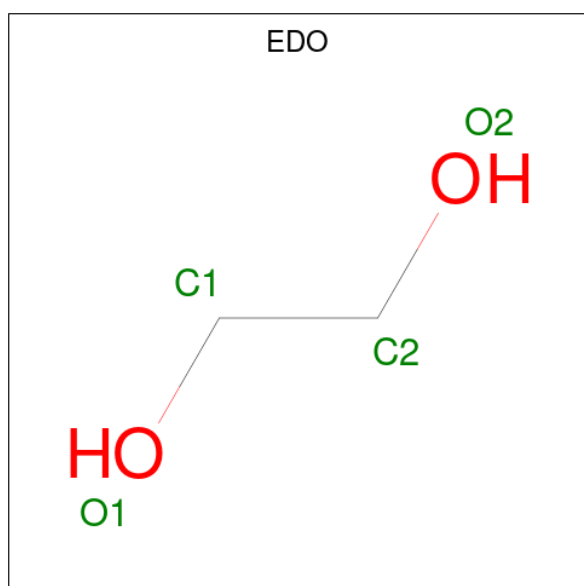
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit delta isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	827	6691	4290	1134	1212	55	7	4	0

There are 2 discrepancies between the modelled and reference sequences:

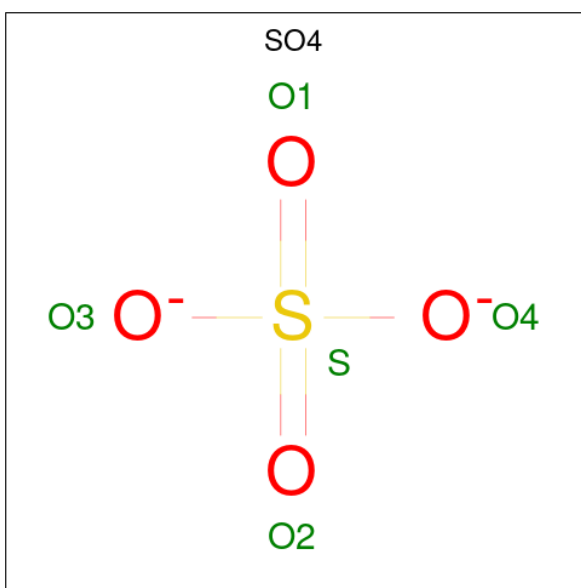
Chain	Residue	Modelled	Actual	Comment	Reference
A	497	ILE	HIS	conflict	UNP O35904
A	510A	GLN	-	insertion	UNP O35904

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



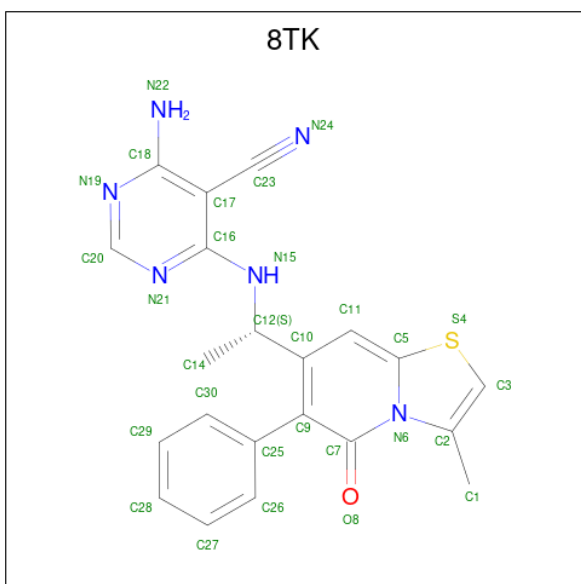
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	4	2	2	0	0
2	A	1	4	2	2	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 4-azanyl-6-[[[(1 {S})-1-(3-methyl-5-oxidanylidene-6-phenyl-[1,3]thiazolo[3,2-a]pyridin-7-yl)ethyl]amino]pyrimidine-5-carbonitrile (CCD ID: 8TK) (formula: C₂₁H₁₈N₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0
			29	21	6	1	1	

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	348	Total 348	O 348	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	140.99Å 64.55Å 116.01Å 90.00° 103.59° 90.00°	Depositor
Resolution (Å)	49.86 – 1.90 49.86 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.4 (49.86-1.90) 96.4 (49.86-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 1.90Å)	Xtriage
Refinement program	BUSTER 2.11.6	Depositor
R, R_{free}	0.222 , 0.264 0.220 , 0.259	Depositor DCC
R_{free} test set	3861 reflections (5.00%)	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)	0.32 , 38.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7081	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 5.14% 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: EDO, SO4, 8TK

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	0.82	1/6845 (0.0%)	1.21	9/9233 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	387	MET	SD-CE	-7.86	1.59	1.79

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	915	PHE	CA-CB-CG	6.96	120.76	113.80
1	A	332	LYS	CA-C-N	6.78	130.65	120.75
1	A	332	LYS	C-N-CA	6.78	130.65	120.75
1	A	433	LYS	CA-C-N	5.72	131.98	121.85
1	A	433	LYS	C-N-CA	5.72	131.98	121.85
1	A	643	ILE	CA-C-N	5.33	125.89	119.98
1	A	643	ILE	C-N-CA	5.33	125.89	119.98
1	A	203	PHE	CA-CB-CG	5.07	118.87	113.80
1	A	133	ASP	CA-CB-CG	5.05	117.65	112.60

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	6691	0	6678	37	0
2	A	8	0	12	0	0
3	A	5	0	0	0	0
4	A	29	0	0	0	0
5	A	348	0	0	1	0
All	All	7081	0	6690	37	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 3.

All (37) 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:386:ARG:HG3	1:A:387:MET:HE2	1.64	0.79
1:A:245:GLY:HA3	1:A:768:ALA:HB2	1.71	0.73
1:A:328:ILE:HB	1:A:472:VAL:HG23	1.70	0.72
1:A:756:MET:HE2	1:A:781:GLY:HA3	1.70	0.71
1:A:387:MET:HE3	1:A:590:CYS:HB3	1.84	0.59
1:A:859:LEU:HD21	1:A:905:GLY:HA2	1.88	0.55
1:A:194:VAL:HG21	1:A:216:LEU:HD21	1.90	0.54
1:A:617:GLN:HE21	1:A:984:ALA:HA	1.74	0.52
1:A:329:GLU:HG2	1:A:472:VAL:HG22	1.93	0.51
1:A:394:LEU:HD22	1:A:441:MET:HE1	1.93	0.50
1:A:432:LEU:HB3	1:A:483:VAL:HG23	1.94	0.50
1:A:637:ALA:HB1	1:A:644:GLY:HA2	1.96	0.48
1:A:247:HIS:CD2	1:A:740:LEU:HD21	2.48	0.48
1:A:895:HIS:H	1:A:898:ASN:HD21	1.60	0.48
1:A:841:LYS:HG3	1:A:844:MET:HE3	1.97	0.47
1:A:342:VAL:HG22	1:A:362:GLU:HG2	1.97	0.47
1:A:587:PHE:HB3	1:A:592:VAL:HG11	1.97	0.46
1:A:387:MET:HE3	1:A:590:CYS:SG	2.56	0.46
1:A:978:PHE:CD1	1:A:998:LEU:HD11	2.51	0.45
1:A:396:ALA:HB3	1:A:416:CYS:HB3	1.99	0.45
1:A:895:HIS:H	1:A:898:ASN:ND2	2.15	0.44
1:A:360:SER:HB3	5:A:1340:HOH:O	2.17	0.44
1:A:902:ARG:HD3	1:A:906:GLN:HB2	1.98	0.44
1:A:281:SER:O	1:A:285:MET:HG3	2.17	0.44
1:A:755:LYS:HB3	1:A:756:MET:H	1.68	0.43
1:A:784:LEU:HD12	1:A:823:GLY:HA3	2.01	0.42
1:A:886:THR:HA	1:A:891:ILE:HD12	2.02	0.42
1:A:491:ILE:HG21	1:A:565:LEU:HD23	2.00	0.42
1:A:205:PHE:HE1	1:A:223:LYS:HG3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:THR:HB	1:A:257:CYS:HB3	2.02	0.42
1:A:387:MET:HE3	1:A:590:CYS:CB	2.50	0.42
1:A:317:TRP:HZ2	1:A:491:ILE:HD13	1.85	0.41
1:A:325:ILE:HG22	1:A:475:LEU:HD13	2.03	0.41
1:A:341:LEU:HG	1:A:365:VAL:HG22	2.03	0.41
1:A:492:LEU:O	1:A:496:ARG:HB2	2.21	0.41
1:A:765:SER:HB3	1:A:772:GLY:HA3	2.03	0.41
1:A:317:TRP:HA	1:A:382:CYS:HB2	2.03	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	807/939 (86%)	788 (98%)	18 (2%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	332	LYS

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	736/827 (89%)	708 (96%)	28 (4%)	29	21

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	ARG
1	A	190	LEU
1	A	203	PHE
1	A	212	MET
1	A	270	LEU
1	A	332	LYS
1	A	333	VAL
1	A	340	LYS
1	A	352	GLU
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	514	ILE
1	A	530	LEU
1	A	565	LEU
1	A	634	LEU
1	A	743	GLU
1	A	755	LYS
1	A	757	LYS
1	A	841	LYS
1	A	847	THR
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 (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	GLN
1	A	187	ASN
1	A	193	ASN
1	A	247	HIS
1	A	253	ASN

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Mol	Chain	Res	Type
1	A	273	HIS
1	A	278	HIS
1	A	422	ASN
1	A	526	HIS
1	A	610	GLN
1	A	617	GLN
1	A	710	GLN
1	A	721	GLN
1	A	795	GLN
1	A	898	ASN
1	A	906	GLN
1	A	914	HIS
1	A	918	ASN
1	A	943	GLN
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](#)

4 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	0.24	0	2,2,2	0.24	0
2	EDO	A	1101	-	3,3,3	0.18	0	2,2,2	0.19	0
3	SO4	A	1103	-	4,4,4	0.28	0	6,6,6	0.10	0
4	8TK	A	1104	-	31,32,32	1.10	1 (3%)	30,46,46	2.20	8 (26%)

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	1101	-	-	0/1/1/1	-
4	8TK	A	1104	-	-	0/10/14/14	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1104	8TK	C5-S4	2.96	1.77	1.71

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1104	8TK	C3-C2-N6	5.35	119.05	111.30
4	A	1104	8TK	N21-C20-N19	-4.52	121.73	128.58
4	A	1104	8TK	C1-C2-C3	-4.18	118.43	127.33
4	A	1104	8TK	C9-C7-N6	3.89	121.59	115.81
4	A	1104	8TK	C2-C3-S4	-3.72	107.77	112.41
4	A	1104	8TK	O8-C7-C9	-3.51	117.19	124.73
4	A	1104	8TK	C17-C16-N21	-2.52	118.67	121.24
4	A	1104	8TK	C16-C17-C23	2.48	122.54	119.21

There are no chirality outliers.

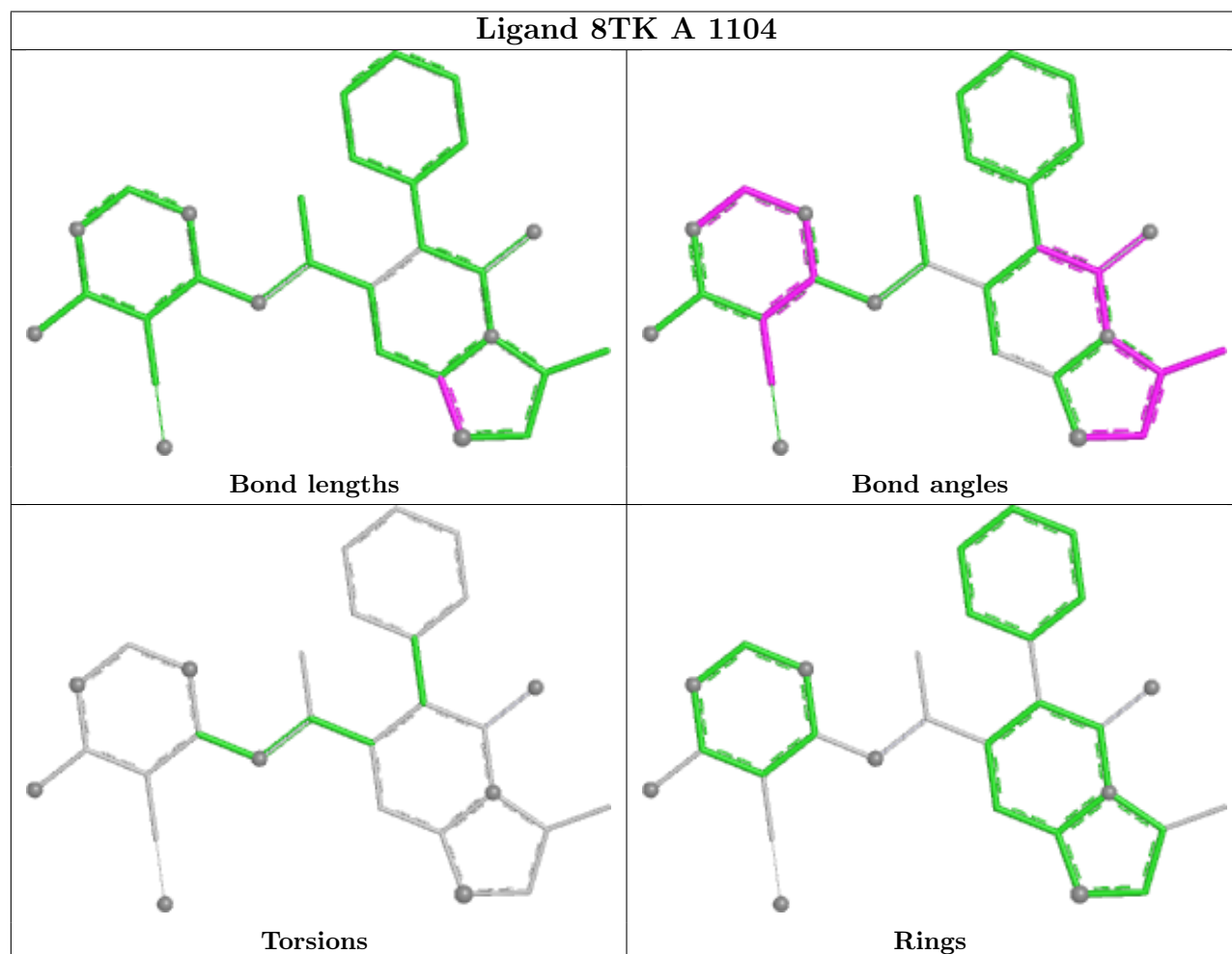
There are no torsion outliers.

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	827/939 (88%)	0.80	128 (15%) 5 5	9, 33, 68, 116	7 (0%)

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	919	PHE	8.8
1	A	335	ALA	8.7
1	A	479	ALA	8.2
1	A	1027	TRP	7.6
1	A	445	VAL	7.1
1	A	333	VAL	6.9
1	A	316	LEU	6.7
1	A	514	ILE	6.3
1	A	398	VAL	6.2
1	A	365	VAL	6.1
1	A	497	ILE	6.0
1	A	517	ARG	5.9
1	A	228	PHE	5.8
1	A	334	ASN	5.3
1	A	846	ALA	5.1
1	A	515	LEU	5.1
1	A	511	LEU	4.8
1	A	523	LEU	4.7
1	A	109	VAL	4.5
1	A	1023	LEU	4.3
1	A	416	CYS	4.3
1	A	474	TYR	4.1
1	A	341	LEU	4.1
1	A	507	THR	4.0
1	A	317	TRP	4.0
1	A	478	VAL	3.9
1	A	930	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	510	GLU	3.7
1	A	323	PHE	3.7
1	A	270	LEU	3.7
1	A	524	TYR	3.7
1	A	332	LYS	3.7
1	A	394	LEU	3.7
1	A	291	ASN	3.7
1	A	360	SER	3.6
1	A	191	LEU	3.6
1	A	331	ARG	3.6
1	A	318	SER	3.5
1	A	377	PHE	3.5
1	A	226	THR	3.4
1	A	395	TYR	3.3
1	A	847	THR	3.3
1	A	227	VAL	3.2
1	A	230	GLN	3.2
1	A	359	SER	3.2
1	A	1004	LEU	3.1
1	A	374	ARG	3.1
1	A	516	GLU	3.1
1	A	482	PRO	3.1
1	A	330	GLY	3.1
1	A	358	VAL	3.1
1	A	471	LEU	3.1
1	A	257	CYS	3.1
1	A	936	TYR	3.1
1	A	397	VAL	3.0
1	A	513	GLU	3.0
1	A	483	VAL	3.0
1	A	512	ARG	3.0
1	A	845	ALA	3.0
1	A	769	GLY	2.9
1	A	962	ARG	2.9
1	A	931	PRO	2.9
1	A	1022	ALA	2.8
1	A	319	LEU	2.8
1	A	187	ASN	2.8
1	A	435	GLY	2.8
1	A	363	VAL	2.8
1	A	203	PHE	2.7
1	A	434	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	119	LEU	2.7
1	A	173	PRO	2.7
1	A	755	LYS	2.7
1	A	1014	HIS	2.7
1	A	370	VAL	2.7
1	A	373	GLN	2.6
1	A	841	LYS	2.6
1	A	491	ILE	2.6
1	A	475	LEU	2.6
1	A	328	ILE	2.6
1	A	327	LEU	2.6
1	A	488	LEU	2.6
1	A	929	ARG	2.6
1	A	418	ILE	2.6
1	A	396	ALA	2.6
1	A	990	SER	2.6
1	A	225	ALA	2.5
1	A	205	PHE	2.5
1	A	1012	LEU	2.5
1	A	417	PRO	2.5
1	A	325	ILE	2.5
1	A	339	MET	2.5
1	A	345	ALA	2.5
1	A	472	VAL	2.5
1	A	494	LEU	2.4
1	A	493	GLU	2.4
1	A	534	MET	2.4
1	A	342	VAL	2.4
1	A	452	LEU	2.4
1	A	484	TYR	2.4
1	A	1017	VAL	2.4
1	A	492	LEU	2.3
1	A	705	LYS	2.3
1	A	485	PHE	2.3
1	A	369	PRO	2.3
1	A	453	LEU	2.3
1	A	843	ASN	2.3
1	A	324	SER	2.3
1	A	918	ASN	2.3
1	A	223	LYS	2.3
1	A	372	LYS	2.3
1	A	1024	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	393	ALA	2.2
1	A	771	ALA	2.2
1	A	378	ASP	2.2
1	A	382	CYS	2.2
1	A	196	PHE	2.2
1	A	995	ILE	2.2
1	A	340	LYS	2.2
1	A	375	LEU	2.2
1	A	253	ASN	2.2
1	A	219	CYS	2.2
1	A	198	GLY	2.2
1	A	153	HIS	2.1
1	A	508	GLU	2.1
1	A	269	GLY	2.1
1	A	937	ASP	2.1
1	A	495	GLY	2.0
1	A	229	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.

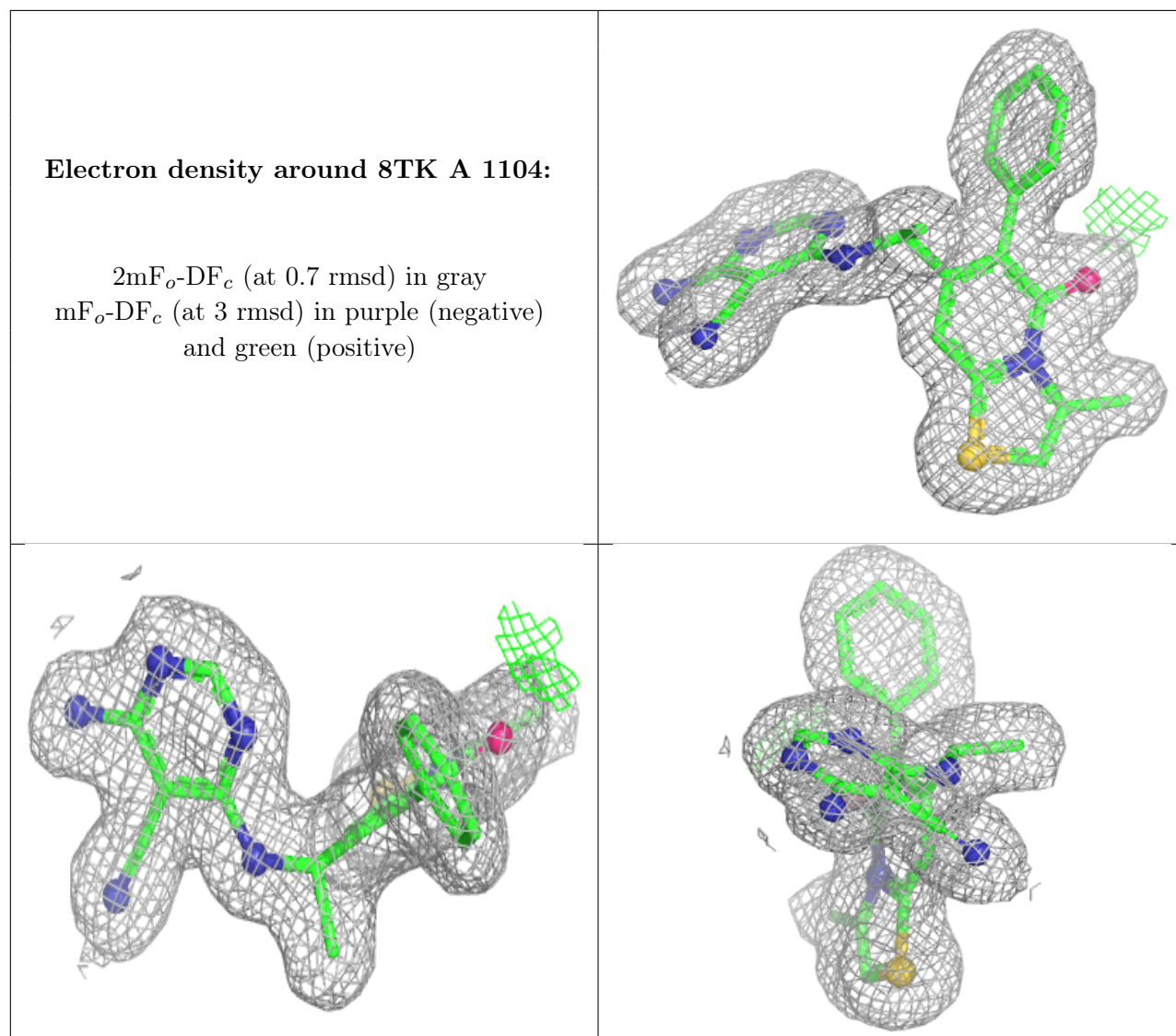
6.4 Ligands [i](#)

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
3	SO4	A	1103	5/5	0.83	0.14	56,61,62,64	0
2	EDO	A	1102	4/4	0.95	0.09	24,28,31,33	0
2	EDO	A	1101	4/4	0.97	0.06	24,25,26,28	0
4	8TK	A	1104	29/29	0.98	0.04	15,18,22,25	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.