



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:09 PM UTC

PDB ID : 6FTN / pdb_00006ftn
Title : mPI3Kd IN COMPLEX WITH AZ2
Authors : Petersen, J.
Deposited on : 2018-02-22
Resolution : 2.00 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

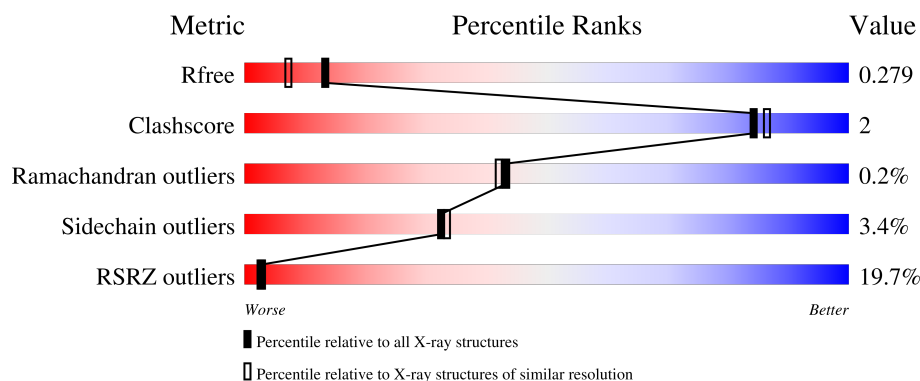
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	17% 82% 5% 12%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6899 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.

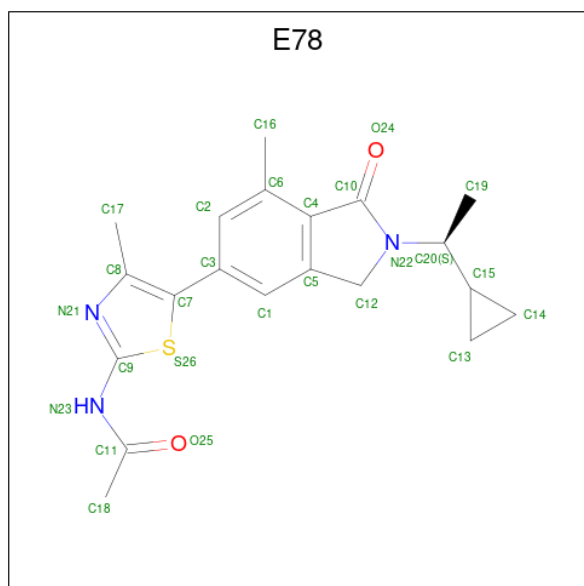
- Molecule 1 is a protein called Phosphor inositol 3 kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	827	6684	4285	1138	1206	55	0	2	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	508	GLN	-	insertion	UNP O35904

- Molecule 2 is {N}-[5-[2-[(1 {S})-1-cyclopropylethyl]-7-methyl-1-oxidanylidene-3 {H}-isindol-5-yl]-4-methyl-1,3-thiazol-2-yl]ethanamide (CCD ID: E78) (formula: C₂₀H₂₃N₃O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	26	20	3	2	1	0	0

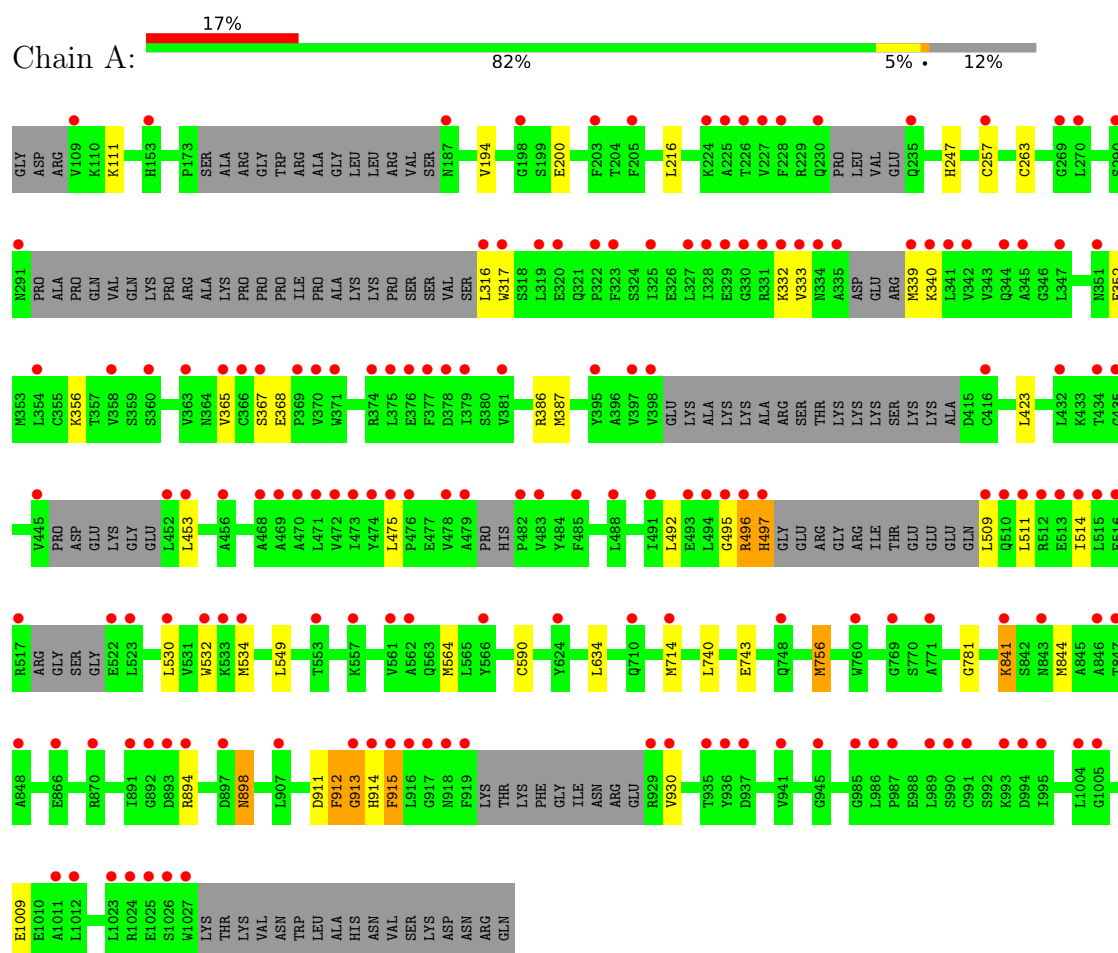
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	189	Total 189	O 189	0	0

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: Phosphor inositol 3 kinase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	141.23Å 65.01Å 116.34Å 90.00° 103.38° 90.00°	Depositor
Resolution (Å)	49.69 – 2.00 49.69 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.2 (49.69-2.00) 97.2 (49.69-2.00)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0027	Depositor
R, R_{free}	0.248 , 0.272 0.251 , 0.279	Depositor DCC
R_{free} test set	3450 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 24.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6899	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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: E78

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	0.39	1/6834 (0.0%)	0.66	0/9219

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	912	PHE	CA-C	6.47	1.55	1.52

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	6684	0	6670	30	1
2	A	26	0	0	1	0
3	A	189	0	0	0	0
All	All	6899	0	6670	31	1

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 (31) 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:912:PHE:HB2	1:A:913:GLY:HA3	1.55	0.86
1:A:549:LEU:HG	1:A:564:MET:HE1	1.66	0.77
1:A:495:GLY:O	1:A:497:HIS:N	2.22	0.72
1:A:492:LEU:O	1:A:496:ARG:HG3	1.90	0.71
1:A:387:MET:HE3	1:A:590:CYS:HB3	1.71	0.71
1:A:386:ARG:HG3	1:A:387:MET:HE2	1.74	0.69
1:A:495:GLY:C	1:A:497:HIS:N	2.47	0.69
1:A:495:GLY:C	1:A:497:HIS:H	1.99	0.69
1:A:367:SER:HB3	1:A:368:GLU:HB3	1.76	0.67
1:A:912:PHE:HB2	1:A:913:GLY:CA	2.29	0.62
1:A:912:PHE:CB	1:A:913:GLY:CA	2.82	0.57
1:A:912:PHE:CB	1:A:913:GLY:HA3	2.32	0.55
1:A:534:MET:HA	1:A:534:MET:HE2	1.89	0.54
1:A:367:SER:CB	1:A:368:GLU:C	2.83	0.52
1:A:549:LEU:CG	1:A:564:MET:HE1	2.40	0.48
1:A:894:ARG:NH1	1:A:911:ASP:O	2.39	0.48
1:A:756:MET:HE2	1:A:781:GLY:HA3	1.96	0.47
1:A:532:TRP:HZ3	1:A:564:MET:HE2	1.80	0.47
2:A:1101:E78:S26	2:A:1101:E78:O25	2.74	0.46
1:A:387:MET:HE3	1:A:590:CYS:CB	2.44	0.45
1:A:247:HIS:CD2	1:A:740:LEU:HD21	2.51	0.45
1:A:367:SER:HB2	1:A:368:GLU:C	2.43	0.44
1:A:894:ARG:NH2	1:A:912:PHE:O	2.51	0.44
1:A:898:ASN:HD22	1:A:898:ASN:C	2.26	0.43
1:A:367:SER:HB3	1:A:368:GLU:C	2.43	0.43
1:A:194:VAL:HG21	1:A:216:LEU:HD21	2.01	0.42
1:A:913:GLY:N	1:A:914:HIS:HB2	2.34	0.42
1:A:915:PHE:C	1:A:915:PHE:CD1	2.98	0.42
1:A:257:CYS:O	1:A:263:CYS:SG	2.78	0.42
1:A:841:LYS:HG2	1:A:844:MET:HG3	2.03	0.41
1:A:339:MET:O	1:A:365:VAL:HG23	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:MET:SD	1:A:714:MET:SD[2_555]	1.85	0.35

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	807/939 (86%)	778 (96%)	27 (3%)	2 (0%)	43	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	496	ARG
1	A	913	GLY

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	734/827 (89%)	709 (97%)	25 (3%)	32	33

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	LYS
1	A	200	GLU
1	A	316	LEU
1	A	317	TRP
1	A	332	LYS
1	A	333	VAL
1	A	340	LYS
1	A	352	GLU
1	A	356	LYS

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Mol	Chain	Res	Type
1	A	423	LEU
1	A	453	LEU
1	A	475	LEU
1	A	497	HIS
1	A	509	LEU
1	A	511	LEU
1	A	514	ILE
1	A	530	LEU
1	A	634	LEU
1	A	743	GLU
1	A	756	MET
1	A	841	LYS
1	A	898	ASN
1	A	915	PHE
1	A	930	VAL
1	A	1009	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	HIS
1	A	156	GLN
1	A	193	ASN
1	A	247	HIS
1	A	258	HIS
1	A	273	HIS
1	A	278	HIS
1	A	291	ASN
1	A	617	GLN
1	A	721	GLN
1	A	898	ASN
1	A	906	GLN
1	A	918	ASN
1	A	948	ASN
1	A	976	HIS

5.3.3 RNA ⓘ

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	E78	A	1101	-	27,29,29	1.08	1 (3%)	37,44,44	1.89	10 (27%)

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	E78	A	1101	-	-	0/16/30/30	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	E78	C10-N22	2.40	1.38	1.36

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	E78	O24-C10-N22	6.10	130.18	125.34
2	A	1101	E78	C5-C12-N22	-3.58	100.40	102.31
2	A	1101	E78	O25-C11-N23	3.57	127.51	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	E78	O24-C10-C4	-2.96	124.64	129.15
2	A	1101	E78	C18-C11-N23	-2.85	110.67	115.27
2	A	1101	E78	C12-C5-C4	2.60	111.85	109.96
2	A	1101	E78	C9-S26-C7	2.49	89.90	88.35
2	A	1101	E78	C12-N22-C10	2.47	114.19	113.15
2	A	1101	E78	C2-C6-C4	-2.18	116.38	118.75
2	A	1101	E78	S26-C9-N23	-2.10	120.91	123.72

There are no chirality outliers.

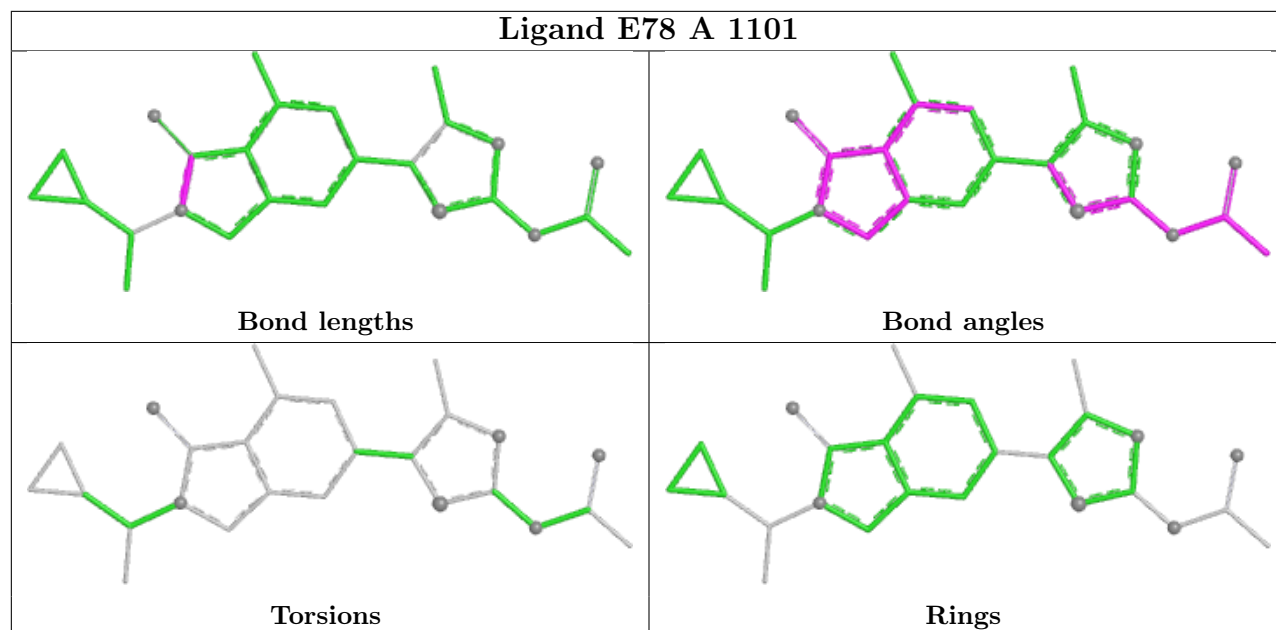
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	E78	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	827/939 (88%)	1.10	163 (19%) 3 3	16, 39, 64, 82	2 (0%)

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	335	ALA	7.5
1	A	479	ALA	6.9
1	A	1027	TRP	6.7
1	A	919	PHE	6.5
1	A	317	TRP	6.4
1	A	316	LEU	6.1
1	A	366	CYS	5.7
1	A	333	VAL	5.7
1	A	367	SER	5.6
1	A	332	LYS	5.3
1	A	397	VAL	5.3
1	A	445	VAL	5.2
1	A	478	VAL	4.7
1	A	495	GLY	4.7
1	A	398	VAL	4.7
1	A	511	LEU	4.7
1	A	515	LEU	4.5
1	A	226	THR	4.3
1	A	228	PHE	4.2
1	A	509	LEU	4.2
1	A	482	PRO	4.2
1	A	562	ALA	4.2
1	A	514	ILE	4.1
1	A	510	GLN	4.1
1	A	517	ARG	4.1
1	A	395	TYR	4.1
1	A	523	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	892	GLY	4.1
1	A	516	GLU	3.8
1	A	936	TYR	3.7
1	A	847	THR	3.7
1	A	227	VAL	3.7
1	A	452	LEU	3.6
1	A	494	LEU	3.6
1	A	341	LEU	3.6
1	A	360	SER	3.5
1	A	471	LEU	3.4
1	A	914	HIS	3.4
1	A	496	ARG	3.4
1	A	472	VAL	3.4
1	A	205	PHE	3.4
1	A	377	PHE	3.4
1	A	937	ASP	3.3
1	A	109	VAL	3.3
1	A	769	GLY	3.3
1	A	918	ASN	3.3
1	A	1005	GLY	3.3
1	A	327	LEU	3.2
1	A	916	LEU	3.2
1	A	323	PHE	3.2
1	A	512	ARG	3.2
1	A	365	VAL	3.2
1	A	334	ASN	3.2
1	A	491	ILE	3.2
1	A	1023	LEU	3.2
1	A	497	HIS	3.1
1	A	771	ALA	3.1
1	A	203	PHE	3.0
1	A	841	LYS	3.0
1	A	1004	LEU	3.0
1	A	561	VAL	3.0
1	A	473	ILE	3.0
1	A	991	CYS	2.9
1	A	319	LEU	2.9
1	A	354	LEU	2.9
1	A	435	GLY	2.9
1	A	342	VAL	2.9
1	A	230	GLN	2.9
1	A	748	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	474	TYR	2.9
1	A	553	THR	2.8
1	A	566	TYR	2.8
1	A	269	GLY	2.8
1	A	345	ALA	2.8
1	A	331	ARG	2.8
1	A	375	LEU	2.8
1	A	371	TRP	2.8
1	A	470	ALA	2.7
1	A	846	ALA	2.7
1	A	894	ARG	2.7
1	A	1012	LEU	2.7
1	A	291	ASN	2.7
1	A	1025	GLU	2.7
1	A	522	GLU	2.6
1	A	929	ARG	2.6
1	A	913	GLY	2.6
1	A	488	LEU	2.6
1	A	363	VAL	2.6
1	A	339	MET	2.6
1	A	328	ILE	2.5
1	A	930	VAL	2.5
1	A	848	ALA	2.5
1	A	1011	ALA	2.5
1	A	530	LEU	2.5
1	A	897	ASP	2.5
1	A	935	THR	2.5
1	A	456	ALA	2.5
1	A	235	GLN	2.5
1	A	986	LEU	2.5
1	A	945	GLY	2.5
1	A	257	CYS	2.4
1	A	1026	SER	2.4
1	A	225	ALA	2.4
1	A	468	ALA	2.4
1	A	907	LEU	2.4
1	A	993	LYS	2.4
1	A	322	PRO	2.4
1	A	379	ILE	2.4
1	A	866	GLU	2.4
1	A	330	GLY	2.4
1	A	416	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	453	LEU	2.3
1	A	534	MET	2.3
1	A	381	VAL	2.3
1	A	378	ASP	2.3
1	A	290	SER	2.3
1	A	990	SER	2.3
1	A	153	HIS	2.3
1	A	376	GLU	2.3
1	A	270	LEU	2.3
1	A	347	LEU	2.3
1	A	485	PHE	2.3
1	A	493	GLU	2.3
1	A	915	PHE	2.3
1	A	187	ASN	2.3
1	A	870	ARG	2.3
1	A	989	LEU	2.3
1	A	374	ARG	2.2
1	A	369	PRO	2.2
1	A	476	PRO	2.2
1	A	891	ILE	2.2
1	A	995	ILE	2.2
1	A	198	GLY	2.2
1	A	432	LEU	2.2
1	A	557	LYS	2.2
1	A	483	VAL	2.2
1	A	344	GLN	2.2
1	A	469	ALA	2.2
1	A	1024	ARG	2.2
1	A	533	LYS	2.2
1	A	351	ASN	2.2
1	A	987	PRO	2.1
1	A	941	VAL	2.1
1	A	320	GLU	2.1
1	A	714	MET	2.1
1	A	843	ASN	2.1
1	A	893	ASP	2.1
1	A	917	GLY	2.1
1	A	760	TRP	2.1
1	A	358	VAL	2.1
1	A	329	GLU	2.1
1	A	513	GLU	2.1
1	A	994	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	532	TRP	2.1
1	A	475	LEU	2.0
1	A	710	GLN	2.0
1	A	224	LYS	2.0
1	A	340	LYS	2.0
1	A	325	ILE	2.0
1	A	370	VAL	2.0
1	A	434	THR	2.0
1	A	985	GLY	2.0
1	A	624	TYR	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](#)

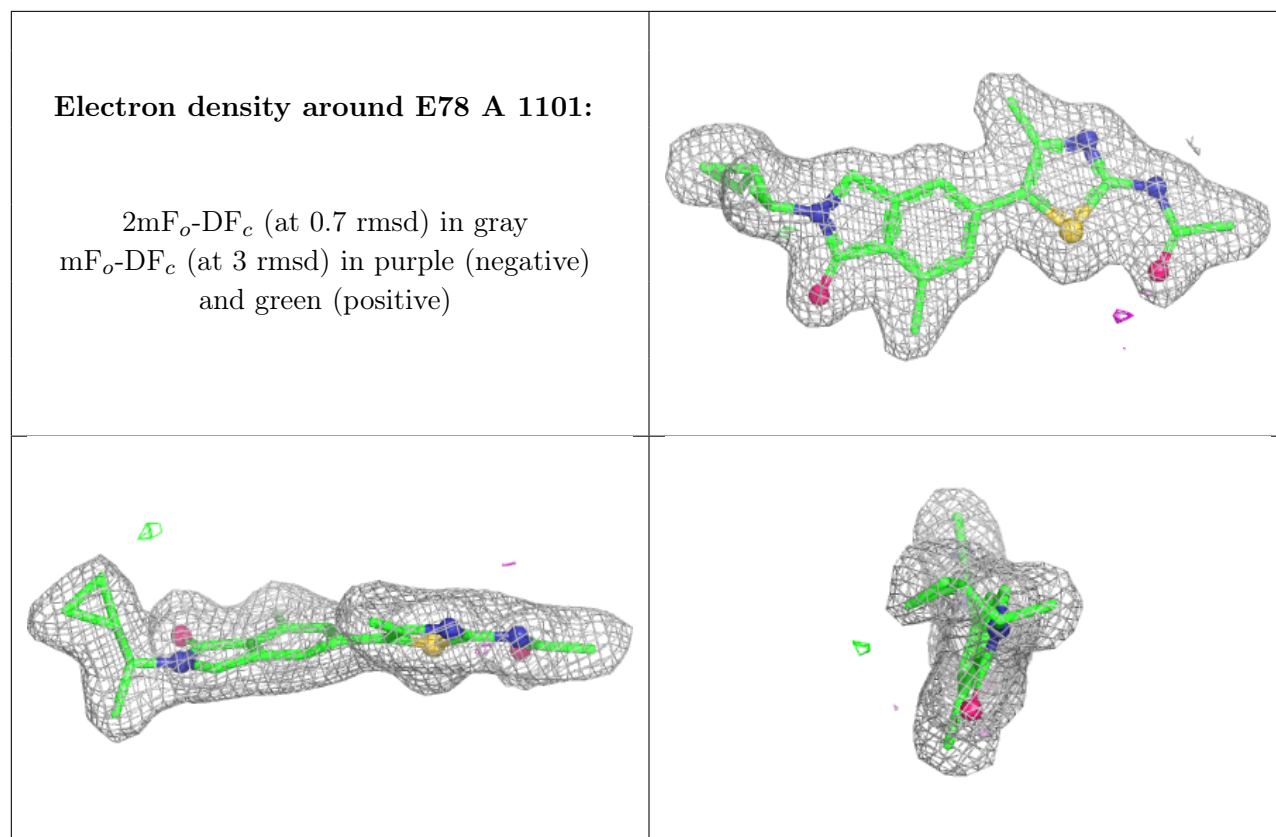
There are no oligosaccharides in this entry.

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	E78	A	1101	26/26	0.94	0.08	27,29,32,33	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.