



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 5DXT / pdb_00005dxt
Title : p110alpha with GDC-0326
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Deposited on : 2015-09-23
Resolution : 2.25 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)

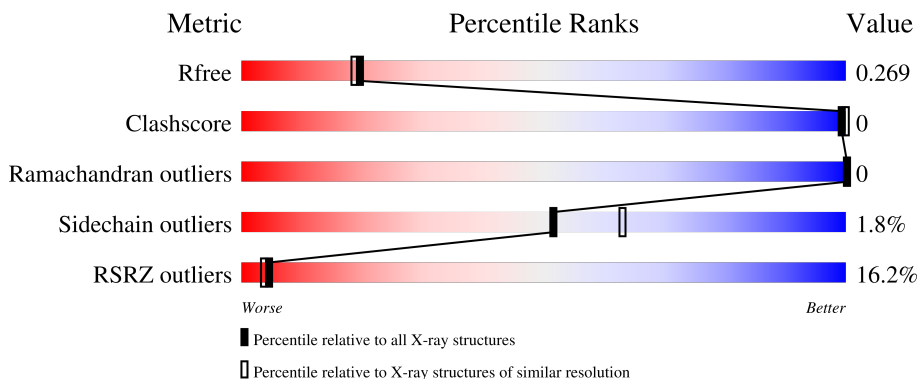
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	962	

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
 Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition [i](#)

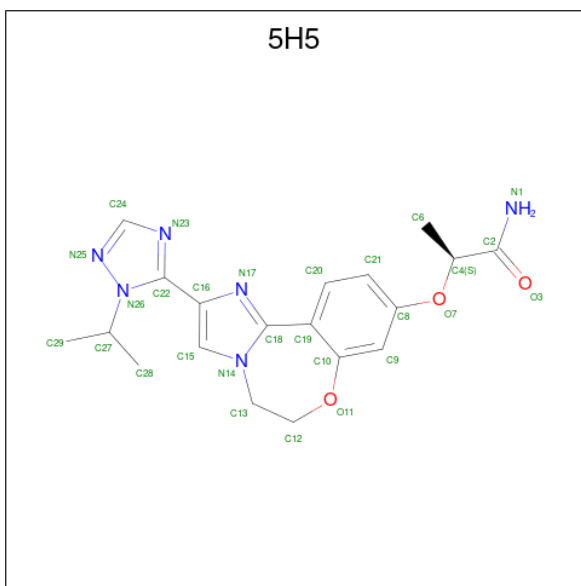
There are 4 unique types of molecules in this entry. The entry contains 7417 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	879	7187	4586	1235	1304	62	215	0	0

- Molecule 2 is (2S)-2-({2-[1-(propan-2-yl)-1H-1,2,4-triazol-5-yl]-5,6-dihydroimidazo[1,2-d][1,4]benzoxazepin-9-yl}oxy)propanamide (CCD ID: 5H5) (formula: C₁₉H₂₂N₆O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	28	19	6	3	0	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

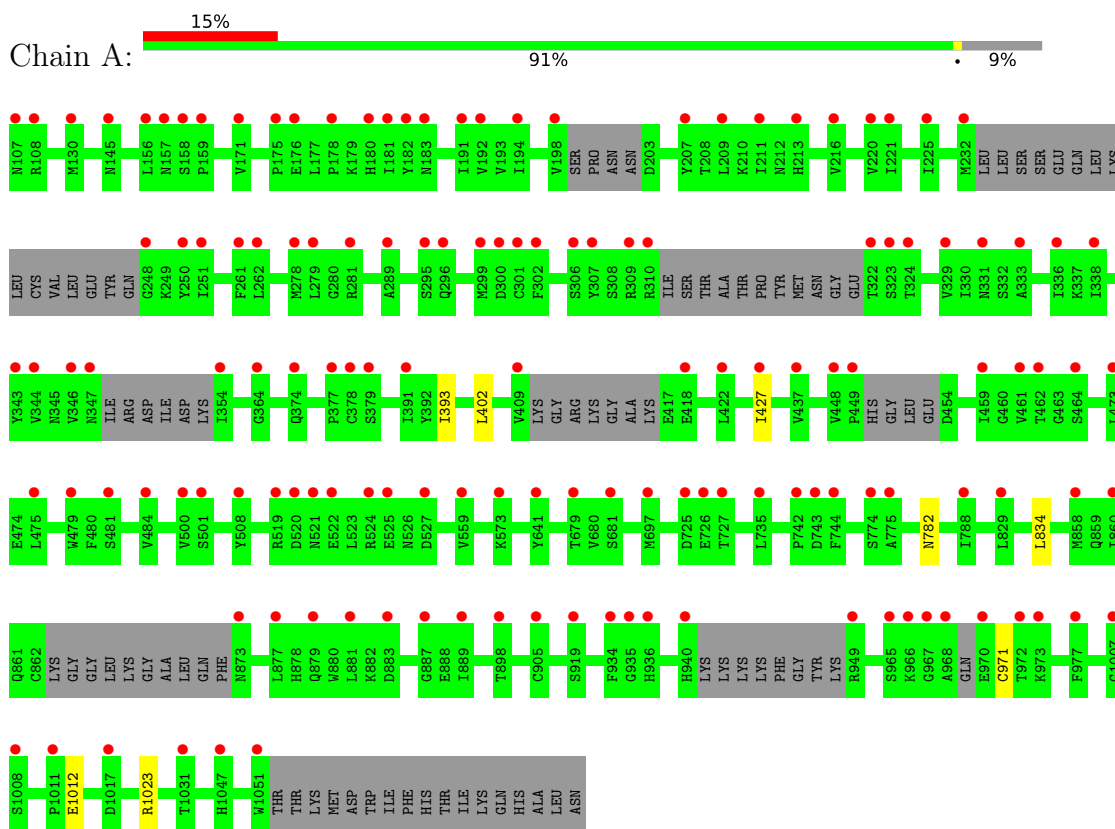
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	198	Total	O	0	0
			198	198		

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 alpha isoform



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.51Å 133.67Å 141.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	97.12 – 2.25 97.12 – 2.25	Depositor EDS
% Data completeness (in resolution range)	97.0 (97.12-2.25) 97.0 (97.12-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.24Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.227 , 0.262 (Not available) , 0.269	Depositor DCC
R_{free} test set	1388 reflections (2.60%)	wwPDB-VP
Wilson B-factor (Å ²)	46.0	Xtrriage
Anisotropy	0.414	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7417	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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: 5H5, EDO

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	0.59	1/7344 (0.0%)	0.79	0/9919

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	393	ILE	CA-CB	7.78	1.58	1.54

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	7187	0	7151	2	0
2	A	28	0	22	0	0
3	A	4	0	6	0	0
4	A	198	0	0	0	0
All	All	7417	0	7179	2	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 0.

All (2) 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:782:ASN:HD22	1:A:782:ASN:C	2.20	0.49
1:A:402:LEU:HD23	1:A:427:ILE:HD12	2.01	0.43

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	859/962 (89%)	837 (97%)	22 (3%)	0	100 100

There are no Ramachandran outliers to report.

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	220/875 (25%)	216 (98%)	4 (2%)	51 63

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	834	LEU
1	A	971	CYS
1	A	1012	GLU

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Mol	Chain	Res	Type
1	A	1023	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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](#)

2 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	$\# Z > 2$
3	EDO	A	1102	-	3,3,3	0.46	0	2,2,2	0.20	0
2	5H5	A	1101	-	31,31,31	1.21	3 (9%)	36,45,45	3.35	13 (36%)

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	EDO	A	1102	-	-	1/1/1/1	-
2	5H5	A	1101	-	-	0/16/26/26	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	5H5	C18-N14	3.69	1.39	1.36
2	A	1101	5H5	N26-N25	2.07	1.40	1.37
2	A	1101	5H5	C16-N17	-2.03	1.34	1.38

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	5H5	C24-N23-C22	9.63	110.43	101.80
2	A	1101	5H5	C16-N17-C18	8.74	111.76	106.23
2	A	1101	5H5	C24-N25-N26	8.19	107.53	101.28
2	A	1101	5H5	C4-C2-N1	5.18	120.40	117.31
2	A	1101	5H5	N25-C24-N23	-4.96	108.92	116.78
2	A	1101	5H5	C27-N26-N25	4.28	124.04	119.62
2	A	1101	5H5	N14-C18-N17	-3.96	106.61	111.67
2	A	1101	5H5	C22-C16-N17	3.81	127.53	121.46
2	A	1101	5H5	C16-C22-N26	3.35	129.34	124.89
2	A	1101	5H5	C15-C16-N17	-3.22	106.58	111.12
2	A	1101	5H5	C8-O7-C4	3.12	123.48	118.40
2	A	1101	5H5	C12-O11-C10	3.05	121.19	116.13
2	A	1101	5H5	C16-C15-N14	2.14	108.02	106.61

There are no chirality outliers.

All (1) torsion outliers are listed below:

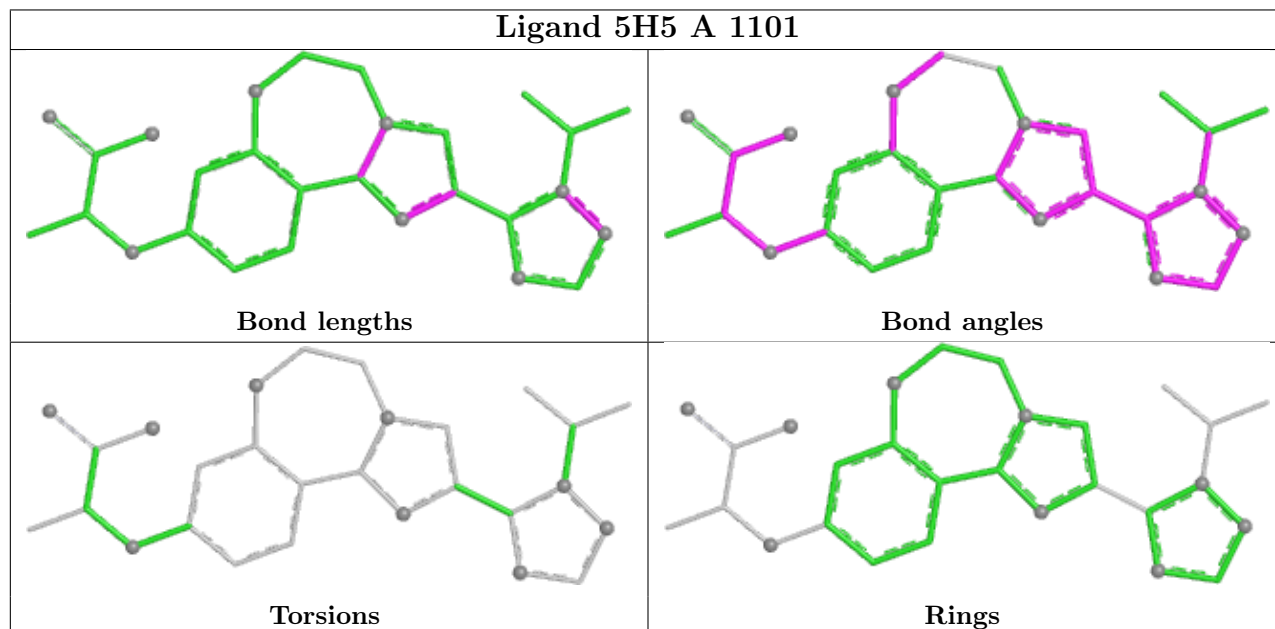
Mol	Chain	Res	Type	Atoms
3	A	1102	EDO	O1-C1-C2-O2

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	879/962 (91%)	1.10	142 (16%) 4 4	30, 66, 96, 122	59 (6%)

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	347	ASN	5.3
1	A	970	GLU	5.1
1	A	301	CYS	4.5
1	A	725	ASP	4.4
1	A	949	ARG	4.4
1	A	968	ALA	4.3
1	A	427	ILE	4.2
1	A	940	HIS	4.1
1	A	198	VAL	4.1
1	A	159	PRO	3.8
1	A	378	CYS	3.8
1	A	521	ASN	3.7
1	A	461	VAL	3.7
1	A	967	GLY	3.6
1	A	459	ILE	3.6
1	A	520	ASP	3.6
1	A	107	ASN	3.5
1	A	449	PRO	3.5
1	A	479	TRP	3.5
1	A	158	SER	3.4
1	A	527	ASP	3.4
1	A	250	TYR	3.3
1	A	295	SER	3.3
1	A	344	VAL	3.3
1	A	248	GLY	3.3
1	A	157	ASN	3.3
1	A	473	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	883	ASP	3.3
1	A	309	ARG	3.3
1	A	973	LYS	3.3
1	A	329	VAL	3.2
1	A	889	ILE	3.2
1	A	232	MET	3.2
1	A	935	GLY	3.2
1	A	225	ILE	3.1
1	A	364	GLY	3.1
1	A	788	ILE	3.1
1	A	1051	TRP	3.1
1	A	641	TYR	3.0
1	A	322	THR	3.0
1	A	501	SER	3.0
1	A	697	MET	3.0
1	A	354	ILE	3.0
1	A	829	LEU	3.0
1	A	346	VAL	2.9
1	A	194	ILE	2.9
1	A	966	LYS	2.9
1	A	181	ILE	2.9
1	A	209	LEU	2.9
1	A	448	VAL	2.9
1	A	130	MET	2.8
1	A	145	ASN	2.8
1	A	183	ASN	2.8
1	A	742	PRO	2.8
1	A	278	MET	2.8
1	A	211	ILE	2.8
1	A	418	GLU	2.8
1	A	379	SER	2.8
1	A	681	SER	2.8
1	A	176	GLU	2.8
1	A	775	ALA	2.8
1	A	744	PHE	2.8
1	A	216	VAL	2.8
1	A	391	ILE	2.7
1	A	323	SER	2.7
1	A	262	LEU	2.7
1	A	422	LEU	2.7
1	A	296	GLN	2.7
1	A	873	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	299	MET	2.7
1	A	374	GLN	2.6
1	A	182	TYR	2.6
1	A	175	PRO	2.6
1	A	300	ASP	2.6
1	A	409	VAL	2.6
1	A	377	PRO	2.6
1	A	879	GLN	2.6
1	A	192	VAL	2.6
1	A	213	HIS	2.6
1	A	261	PHE	2.6
1	A	977	PHE	2.6
1	A	484	VAL	2.6
1	A	462	THR	2.5
1	A	1031	THR	2.5
1	A	331	ASN	2.5
1	A	898	THR	2.5
1	A	251	ILE	2.5
1	A	220	VAL	2.5
1	A	310	ARG	2.5
1	A	156	LEU	2.5
1	A	735	LEU	2.5
1	A	289	ALA	2.5
1	A	936	HIS	2.5
1	A	1047	HIS	2.5
1	A	965	SER	2.4
1	A	333	ALA	2.4
1	A	679	THR	2.4
1	A	306	SER	2.4
1	A	178	PRO	2.4
1	A	727	THR	2.4
1	A	221	ILE	2.4
1	A	180	HIS	2.4
1	A	281	ARG	2.4
1	A	108	ARG	2.3
1	A	972	THR	2.3
1	A	464	SER	2.3
1	A	524	ARG	2.3
1	A	774	SER	2.3
1	A	500	VAL	2.3
1	A	519	ARG	2.2
1	A	207	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	525	GLU	2.2
1	A	336	ILE	2.2
1	A	338	ILE	2.2
1	A	437	VAL	2.2
1	A	475	LEU	2.2
1	A	881	LEU	2.2
1	A	191	ILE	2.2
1	A	905	CYS	2.2
1	A	573	LYS	2.2
1	A	481	SER	2.2
1	A	1008	SER	2.2
1	A	887	GLY	2.2
1	A	307	TYR	2.1
1	A	302	PHE	2.1
1	A	1007	GLY	2.1
1	A	324	THR	2.1
1	A	858	MET	2.1
1	A	860	ILE	2.1
1	A	934	PHE	2.1
1	A	522	GLU	2.1
1	A	726	GLU	2.1
1	A	343	TYR	2.1
1	A	743	ASP	2.1
1	A	1011	PRO	2.1
1	A	171	VAL	2.1
1	A	919	SER	2.0
1	A	279	LEU	2.0
1	A	508	TYR	2.0
1	A	559	VAL	2.0
1	A	877	LEU	2.0
1	A	1017	ASP	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](#)

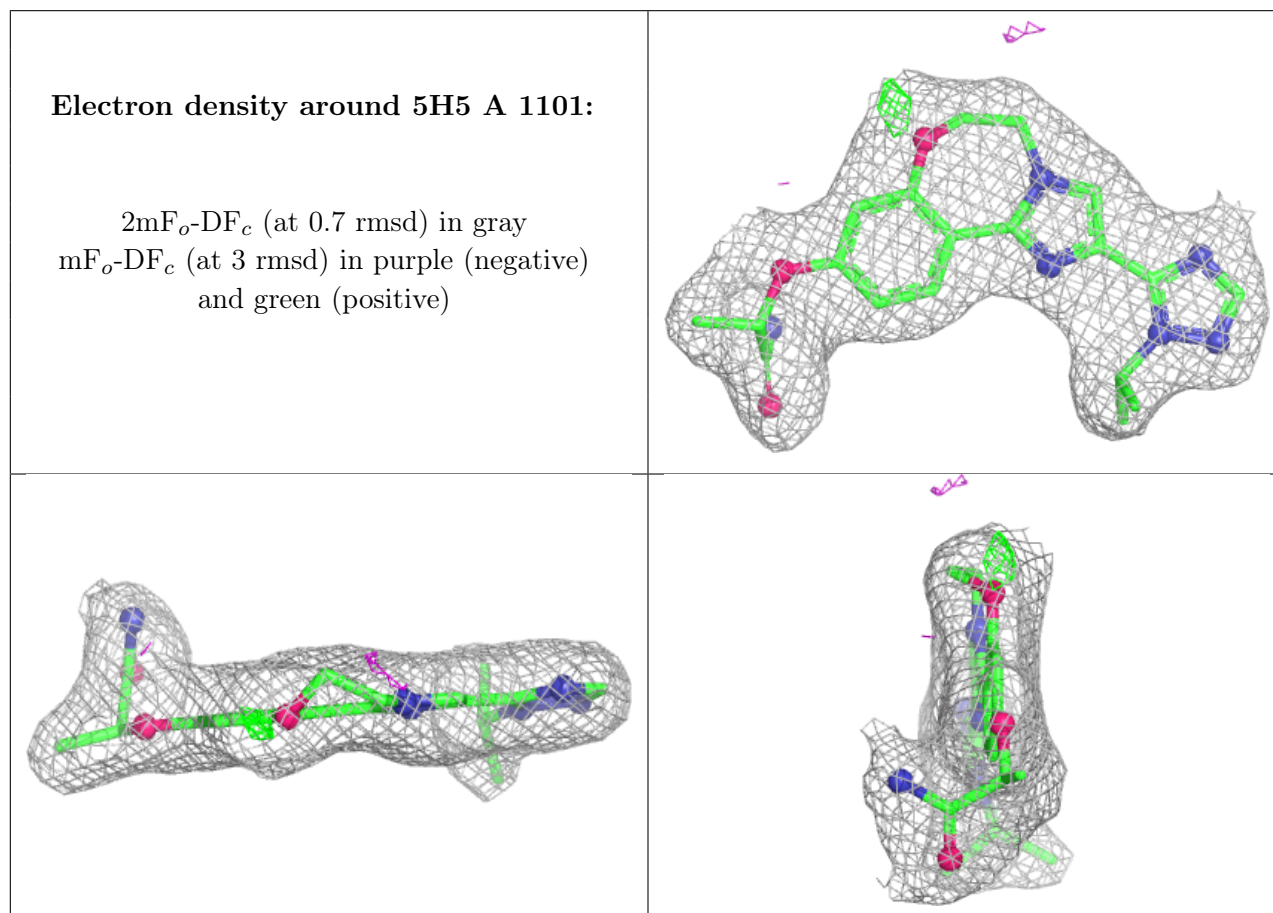
There are no oligosaccharides in this entry.

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(\AA^2)	Q<0.9
3	EDO	A	1102	4/4	0.91	0.17	71,72,73,75	0
2	5H5	A	1101	28/28	0.95	0.10	53,55,60,61	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.