



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 10:59 PM GMT

PDB ID : 5DXH
Title : p110alpha/p85alpha with compound 5
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Deposited on : 2015-09-23
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

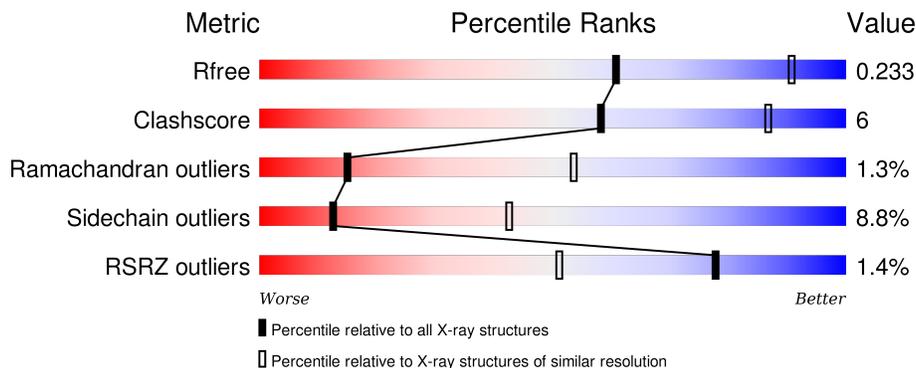
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	1067	 10% 73% 18% • 7%
1	D	1067	 10% 72% 18% • 8%
2	B	169	 10% 56% 14% • 28%
2	E	169	 10% 57% 14% • 26%

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 18333 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.

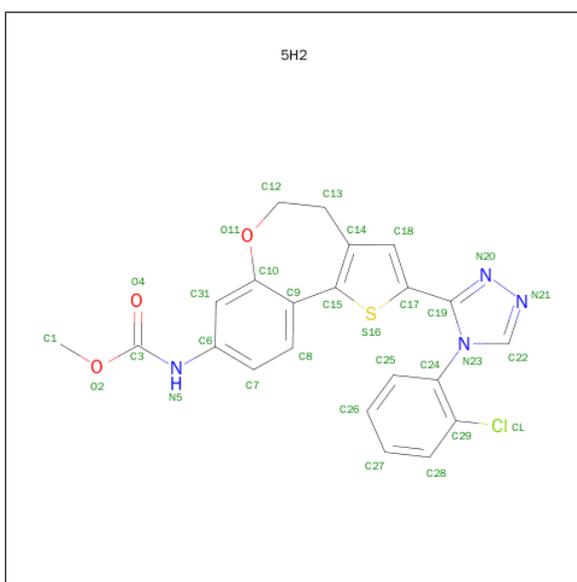
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit alpha isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	989	Total 8093	C 5185	N 1375	O 1464	S 69	0	0	0
1	D	981	Total 8033	C 5153	N 1361	O 1450	S 69	0	0	0

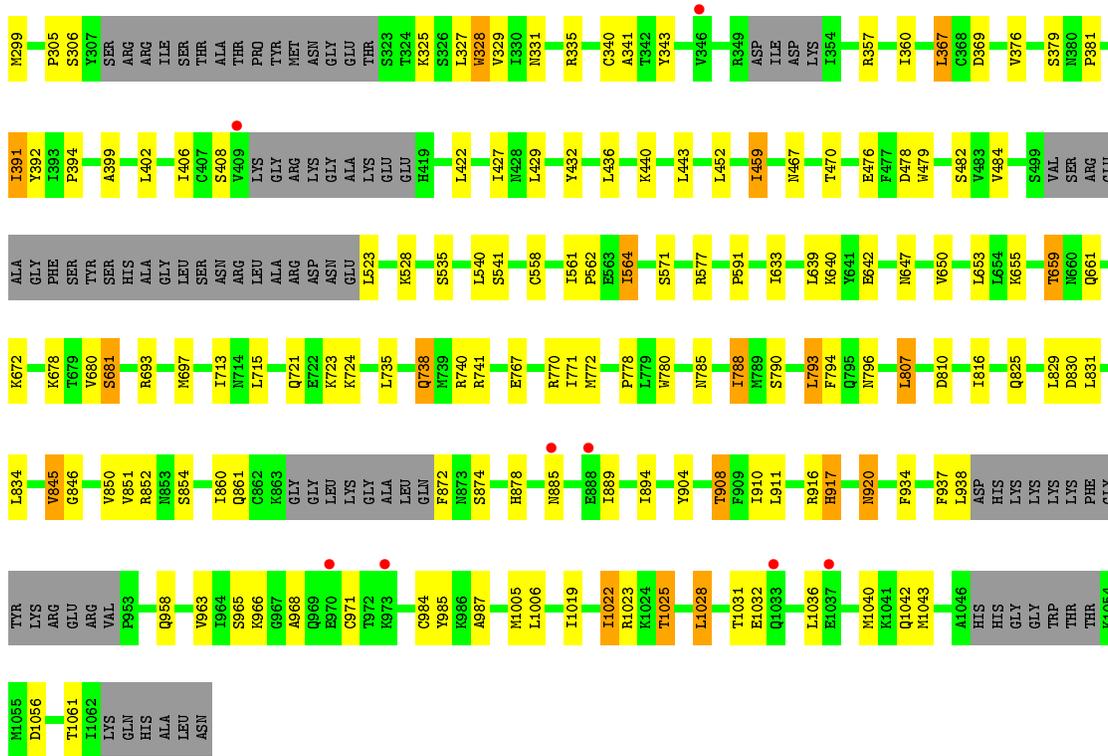
- Molecule 2 is a protein called Phosphatidylinositol 3-kinase regulatory subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	121	Total 1053	C 648	N 194	O 207	S 4	0	0	0
2	E	125	Total 1092	C 674	N 198	O 216	S 4	0	0	0

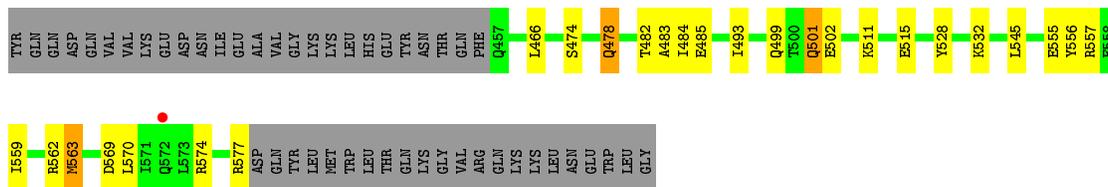
- Molecule 3 is methyl {2-[4-(2-chlorophenyl)-4H-1,2,4-triazol-3-yl]-4,5-dihydrothieno[3,2-d][1]benzoxepin-8-yl} carbamate (three-letter code: 5H2) (formula: C₂₂H₁₇ClN₄O₃S).



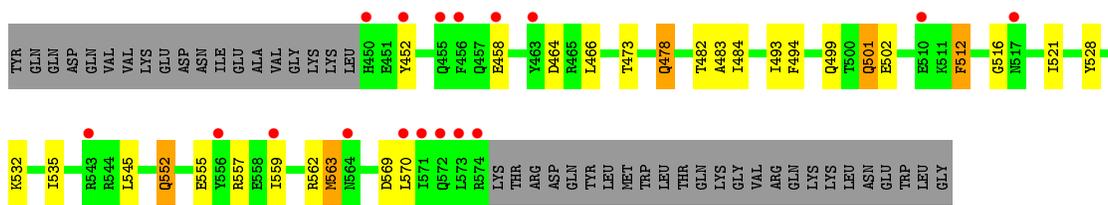
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
3	A	1	Total	C	Cl	N	O	S	0	0
			31	22	1	4	3	1		
3	D	1	Total	C	Cl	N	O	S	0	0
			31	22	1	4	3	1		



• Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit alpha



• Molecule 2: Phosphatidylinositol 3-kinase regulatory subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.66Å 121.83Å 166.36Å 90.00° 102.33° 90.00°	Depositor
Resolution (Å)	49.50 – 3.00 48.74 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.3 (49.50-3.00) 97.5 (48.74-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 3.01Å)	Xtrriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.181 , 0.218 0.198 , 0.233	Depositor DCC
R_{free} test set	3490 reflections (5.21%)	DCC
Wilson B-factor (Å ²)	88.8	Xtrriage
Anisotropy	0.438	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 73.1	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Outliers	0 of 70504 reflections	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18333	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 5H2

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	0.50	0/8273	0.71	2/11184 (0.0%)
1	D	0.49	0/8214	0.72	3/11104 (0.0%)
2	B	0.48	0/1064	0.66	0/1414
2	E	0.45	0/1106	0.63	0/1473
All	All	0.49	0/18657	0.71	5/25175 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	157	ASN	C-N-CA	5.81	136.22	121.70
1	A	328	TRP	CA-CB-CG	5.61	124.36	113.70
1	D	325	LYS	N-CA-C	-5.53	96.07	111.00
1	A	329	VAL	N-CA-C	-5.51	96.11	111.00
1	D	329	VAL	N-CA-C	-5.28	96.75	111.00

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	8093	0	8119	106	0
1	D	8033	0	8051	91	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1053	0	1053	13	0
2	E	1092	0	1072	13	0
3	A	31	0	17	4	0
3	D	31	0	17	0	0
All	All	18333	0	18329	217	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 6.

The worst 5 of 217 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:851:VAL:HG11	1:A:930:PHE:CZ	2.01	0.93
1:D:328:TRP:HB2	1:D:394:PRO:HB3	1.58	0.82
1:D:721:GLN:O	1:D:724:LYS:HG2	1.87	0.73
1:D:558:CYS:SG	1:D:564:ILE:HD11	2.28	0.73
1:A:558:CYS:SG	1:A:564:ILE:HD11	2.30	0.72

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	975/1067 (91%)	914 (94%)	49 (5%)	12 (1%)	16	56
1	D	965/1067 (90%)	903 (94%)	49 (5%)	13 (1%)	15	53
2	B	119/169 (70%)	116 (98%)	1 (1%)	2 (2%)	11	46
2	E	123/169 (73%)	119 (97%)	2 (2%)	2 (2%)	12	48
All	All	2182/2472 (88%)	2052 (94%)	101 (5%)	29 (1%)	15	53

5 of 29 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	298	PRO
1	A	299	MET
1	A	399	ALA
1	D	298	PRO
1	D	399	ALA

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	912/973 (94%)	842 (92%)	70 (8%)	16	50
1	D	905/973 (93%)	817 (90%)	88 (10%)	10	37
2	B	116/160 (72%)	106 (91%)	10 (9%)	13	44
2	E	120/160 (75%)	107 (89%)	13 (11%)	8	30
All	All	2053/2266 (91%)	1872 (91%)	181 (9%)	12	42

5 of 181 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	10	LEU
1	D	230	ARG
1	D	1061	THR
1	D	60	GLN
1	D	108	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	137	GLN
1	D	467	ASN
2	E	522	GLN
1	D	213	HIS
1	D	347	ASN

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 carbohydrates 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	5H2	A	1101	-	28,35,35	1.11	1 (3%)	30,50,50	2.58	10 (33%)
3	5H2	D	1101	-	28,35,35	1.06	1 (3%)	30,50,50	2.37	7 (23%)

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	5H2	A	1101	-	-	2/10/24/24	0/4/5/5
3	5H2	D	1101	-	-	2/10/24/24	0/4/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1101	5H2	N21-N20	-3.83	1.29	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	5H2	N21-N20	-3.75	1.29	1.37

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	5H2	O2-C3-O4	-4.17	118.75	124.61
3	D	1101	5H2	O2-C3-O4	-4.13	118.81	124.61
3	A	1101	5H2	C18-C17-S16	-2.55	108.02	110.75
3	A	1101	5H2	C24-C29-CL	-2.21	120.09	123.00
3	A	1101	5H2	C12-C13-C14	-2.20	108.94	114.66

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1101	5H2	C1-O2-C3-O4
3	D	1101	5H2	C1-O2-C3-N5
3	A	1101	5H2	C1-O2-C3-N5
3	A	1101	5H2	C1-O2-C3-O4

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1101	5H2	4	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	989/1067 (92%)	-0.06	6 (0%) 90 73	54, 93, 136, 186	0
1	D	981/1067 (91%)	-0.03	8 (0%) 87 67	59, 98, 139, 186	0
2	B	121/169 (71%)	-0.01	1 (0%) 87 67	70, 103, 153, 182	0
2	E	125/169 (73%)	0.89	17 (13%) 4 1	95, 145, 195, 210	0
All	All	2216/2472 (89%)	0.01	32 (1%) 78 51	54, 98, 148, 210	0

The worst 5 of 32 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	973	LYS	4.5
2	E	571	ILE	4.4
2	E	458	GLU	4.2
2	E	452	TYR	4.1
2	E	455	GLN	4.0

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	5H2	D	1101	31/31	0.97	0.25	0.52	70,85,96,99	0
3	5H2	A	1101	31/31	0.97	0.23	-0.29	60,68,76,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.