



Full wwPDB NMR Structure Validation Report ⓘ

Nov 23, 2017 – 01:24 AM EST

PDB ID : 2PNA
Title : STRUCTURE OF AN SH2 DOMAIN OF THE P85 ALPHA SUBUNIT OF PHOSPHATIDYLINOSITOL-3-OH KINASE
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Deposited on : unknown

This is a Full wwPDB NMR Structure Validation 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/NMRValidationReportHelp>

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:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : rb-20030345
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

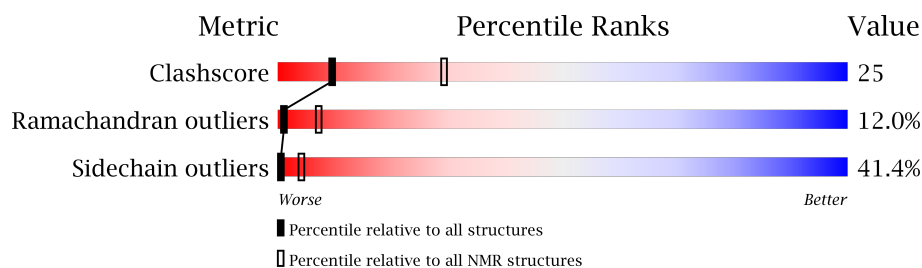
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Clashscore	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	104	

2 Ensemble composition and analysis

This entry contains 22 models. Model 7 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:17-A:49, A:56-A:102, A:112-A:118 (87)	0.32	7

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 3 clusters and 7 single-model clusters were found.

Cluster number	Models
1	1, 8, 9, 11, 12, 19, 21, 22
2	2, 6, 7, 15, 16
3	14, 17
Single-model clusters	3; 4; 5; 10; 13; 18; 20

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1699 atoms, of which 840 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PHOSPHATIDYLINOSITOL 3-KINASE P85-ALPHA SUB-UNIT N-TERMINAL SH2 DOMAIN.

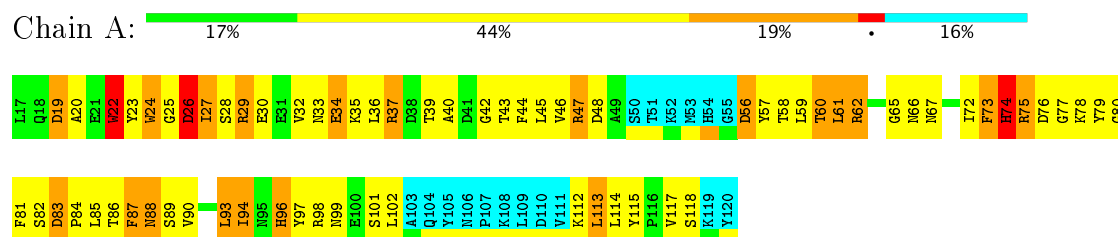
Mol	Chain	Residues	Atoms						Trace
1	A	104	Total	C	H	N	O	S	0
			1699	547	840	148	163	1	

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: PHOSPHATIDYLINOSITOL 3-KINASE P85-ALPHA SUBUNIT N-TERMINAL SH2 DOMAIN

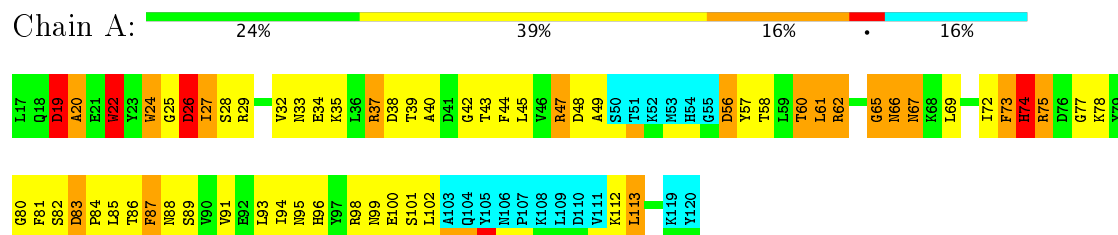


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

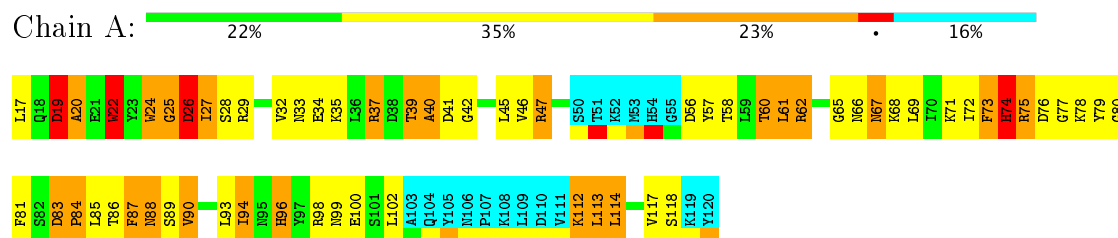
4.2.1 Score per residue for model 1

- Molecule 1: PHOSPHATIDYLINOSITOL 3-KINASE P85-ALPHA SUBUNIT N-TERMINAL SH2 DOMAIN



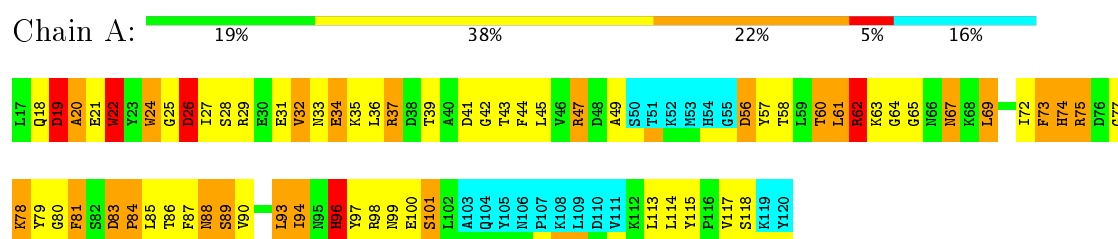
4.2.2 Score per residue for model 2

- Molecule 1: PHOSPHATIDYLINOSITOL 3-KINASE P85-ALPHA SUBUNIT N-TERMINAL SH2 DOMAIN



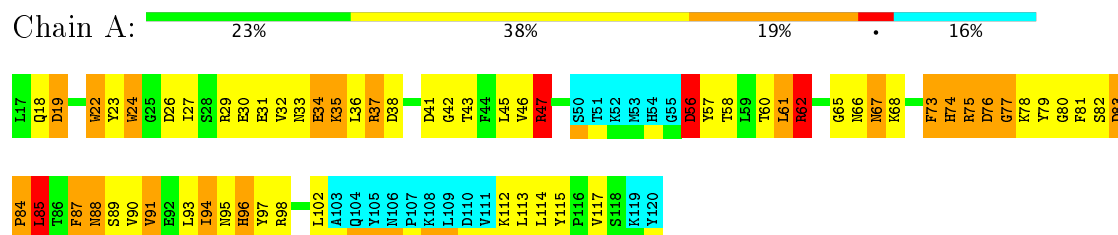
4.2.3 Score per residue for model 3

- Molecule 1: PHOSPHATIDYLINOSITOL 3-KINASE P85-ALPHA SUBUNIT N-TERMINAL SH2 DOMAIN



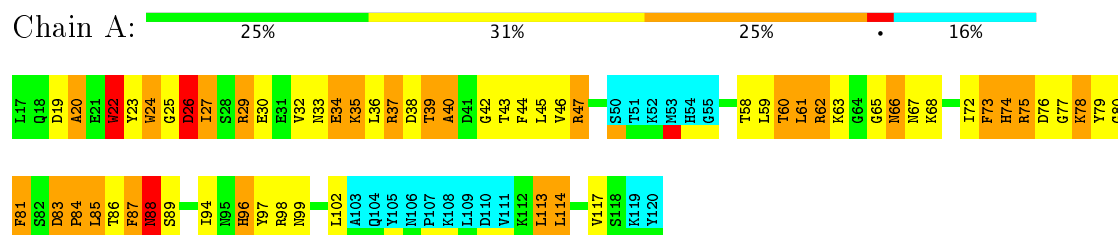
4.2.4 Score per residue for model 4

- Molecule 1: PHOSPHATIDYLINOSITOL 3-KINASE P85-ALPHA SUBUNIT N-TERMINAL SH2 DOMAIN



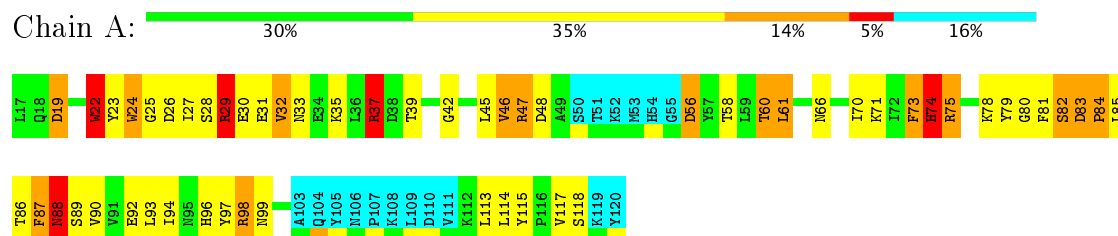
4.2.5 Score per residue for model 5

- Molecule 1: PHOSPHATIDYLINOSITOL 3-KINASE P85-ALPHA SUBUNIT N-TERMINAL SH2 DOMAIN



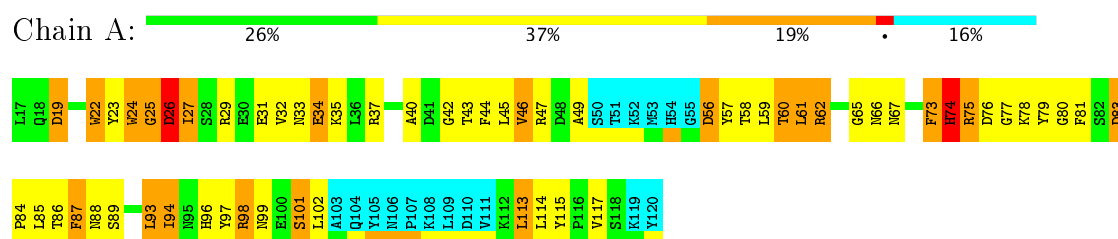
4.2.6 Score per residue for model 6

- Molecule 1: PHOSPHATIDYLINOSITOL 3-KINASE P85-ALPHA SUBUNIT N-TERMINAL SH2 DOMAIN



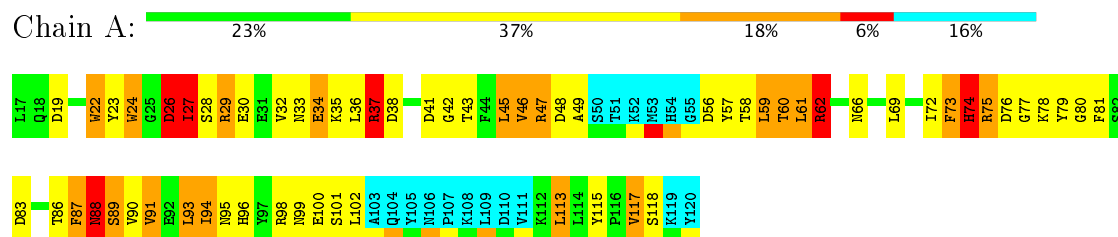
4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: PHOSPHATIDYLINOSITOL 3-KINASE P85-ALPHA SUBUNIT N-TERMINAL SH2 DOMAIN



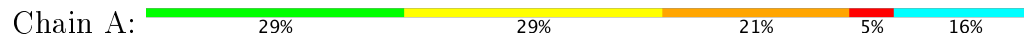
4.2.8 Score per residue for model 8

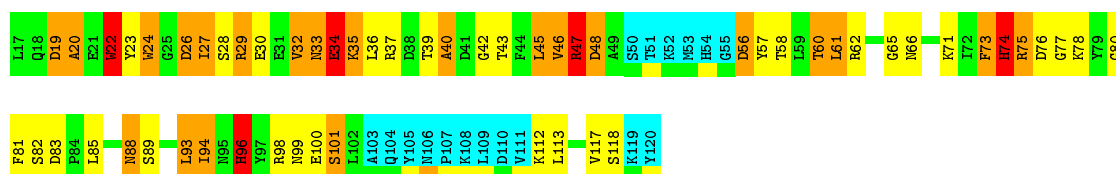
- Molecule 1: PHOSPHATIDYLINOSITOL 3-KINASE P85-ALPHA SUBUNIT N-TERMINAL SH2 DOMAIN



4.2.9 Score per residue for model 9

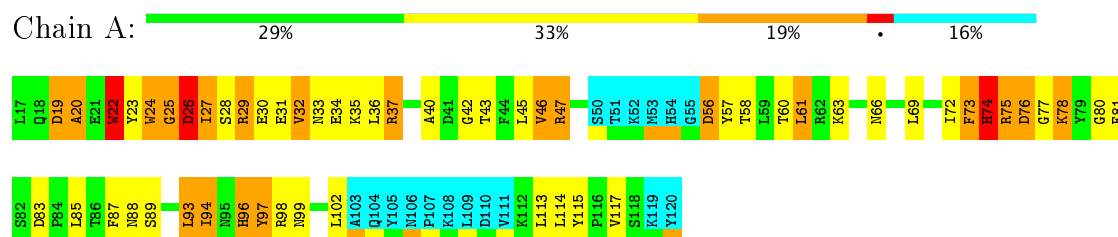
- Molecule 1: PHOSPHATIDYLINOSITOL 3-KINASE P85-ALPHA SUBUNIT N-TERMINAL SH2 DOMAIN





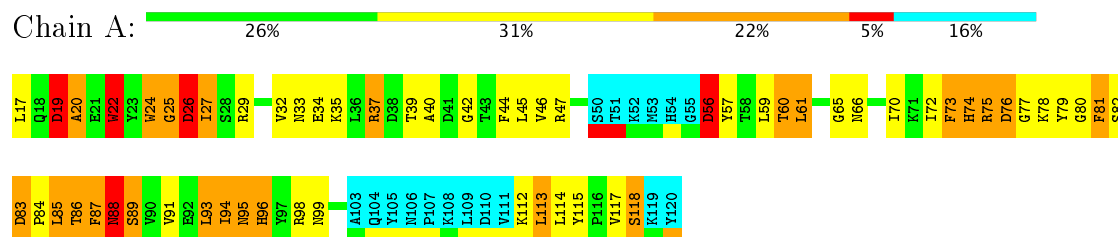
4.2.10 Score per residue for model 10

- Molecule 1: PHOSPHATIDYLINOSITOL 3-KINASE P85-ALPHA SUBUNIT N-TERMINAL SH2 DOMAIN



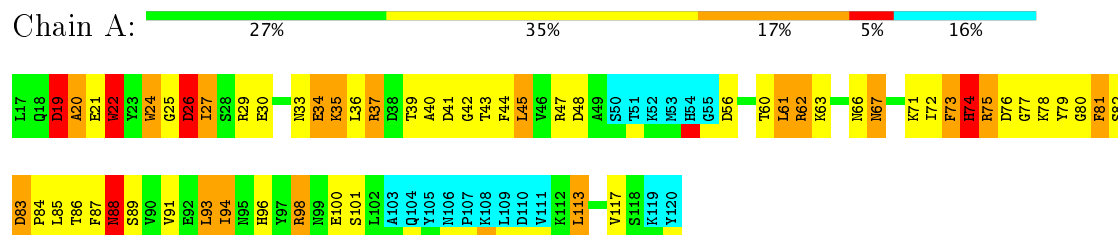
4.2.11 Score per residue for model 11

- Molecule 1: PHOSPHATIDYLINOSITOL 3-KINASE P85-ALPHA SUBUNIT N-TERMINAL SH2 DOMAIN



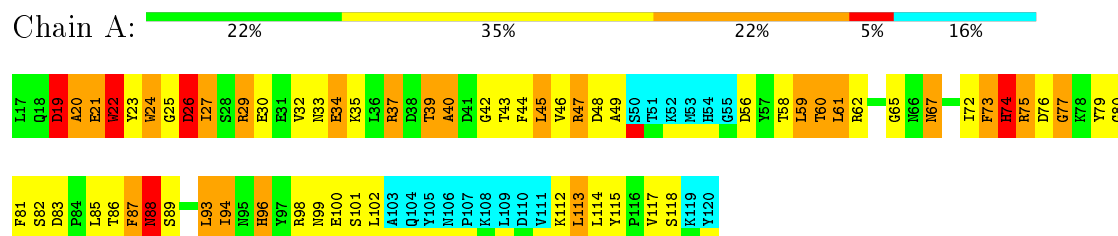
4.2.12 Score per residue for model 12

- Molecule 1: PHOSPHATIDYLINOSITOL 3-KINASE P85-ALPHA SUBUNIT N-TERMINAL SH2 DOMAIN



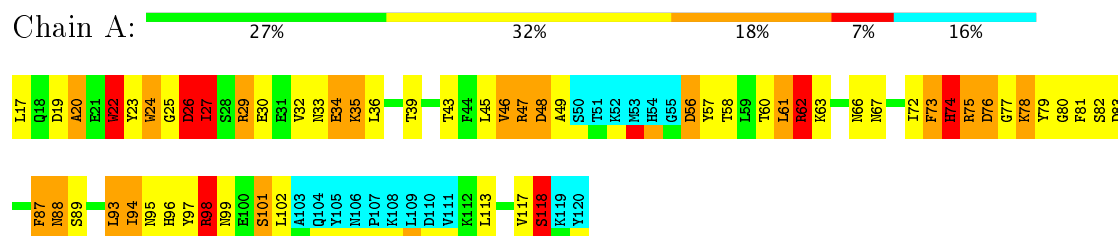
4.2.13 Score per residue for model 13

- Molecule 1: PHOSPHATIDYLINOSITOL 3-KINASE P85-ALPHA SUBUNIT N-TERMINAL SH2 DOMAIN



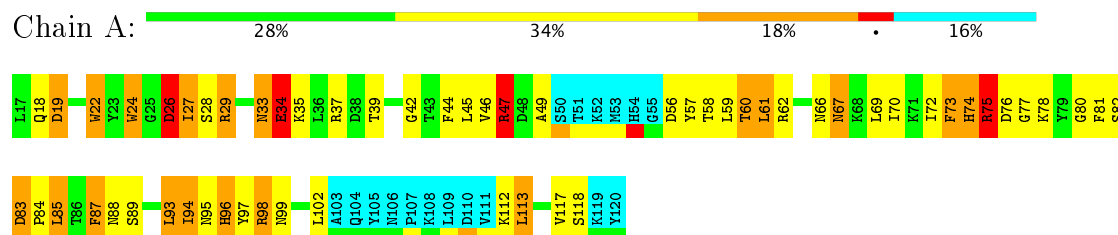
4.2.14 Score per residue for model 14

- Molecule 1: PHOSPHATIDYLINOSITOL 3-KINASE P85-ALPHA SUBUNIT N-TERMINAL SH2 DOMAIN



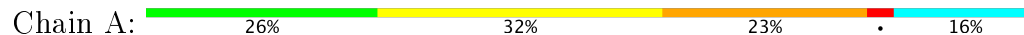
4.2.15 Score per residue for model 15

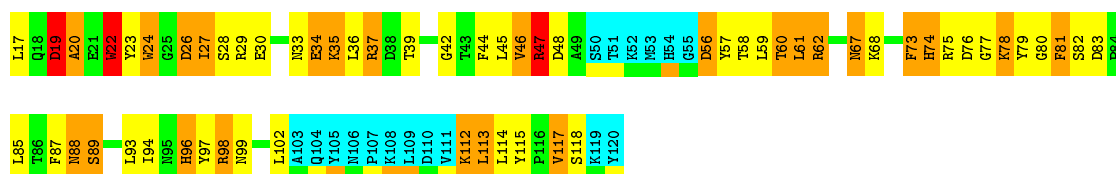
- Molecule 1: PHOSPHATIDYLINOSITOL 3-KINASE P85-ALPHA SUBUNIT N-TERMINAL SH2 DOMAIN



4.2.16 Score per residue for model 16

- Molecule 1: PHOSPHATIDYLINOSITOL 3-KINASE P85-ALPHA SUBUNIT N-TERMINAL SH2 DOMAIN

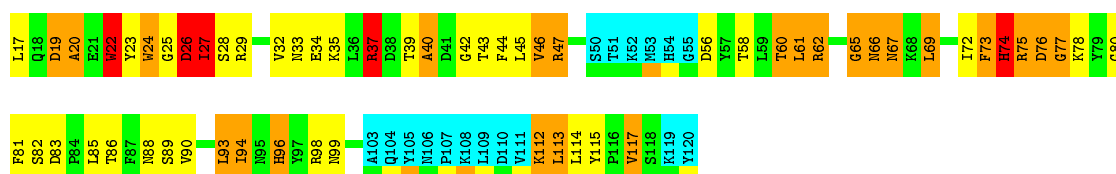




4.2.17 Score per residue for model 17

- Molecule 1: PHOSPHATIDYLINOSITOL 3-KINASE P85-ALPHA SUBUNIT N-TERMINAL SH2 DOMAIN

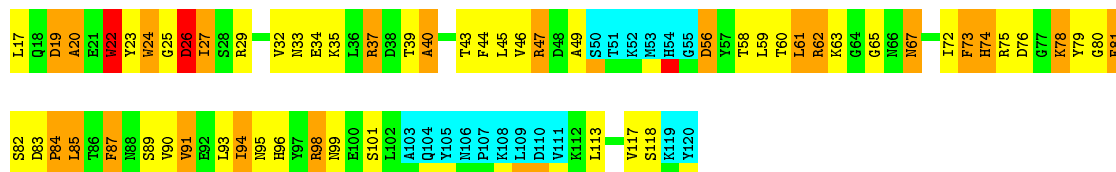
Chain A: 27% 30% 22% 5% 16%



4.2.18 Score per residue for model 18

- Molecule 1: PHOSPHATIDYLINOSITOL 3-KINASE P85-ALPHA SUBUNIT N-TERMINAL SH2 DOMAIN

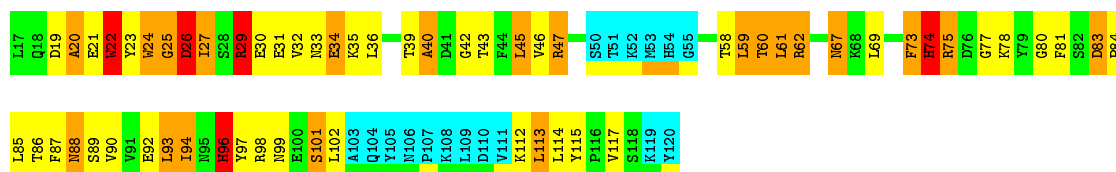
Chain A: 27% 35% 20% 5% 16%



4.2.19 Score per residue for model 19

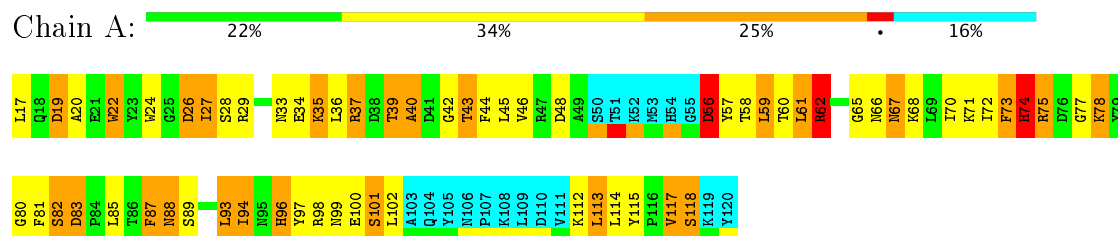
- Molecule 1: PHOSPHATIDYLINOSITOL 3-KINASE P85-ALPHA SUBUNIT N-TERMINAL SH2 DOMAIN

Chain A: 26% 33% 20% 5% 16%



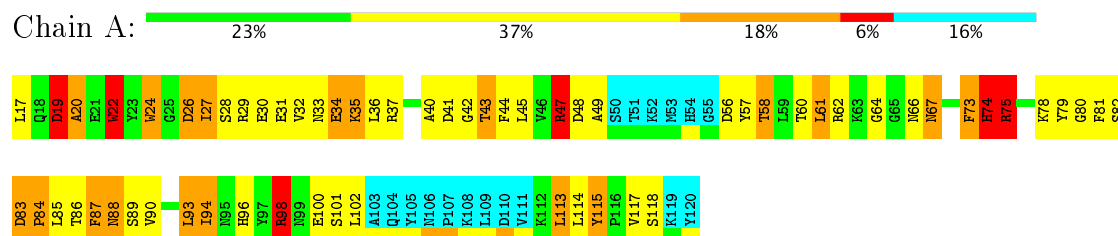
4.2.20 Score per residue for model 20

- Molecule 1: PHOSPHATIDYLINOSITOL 3-KINASE P85-ALPHA SUBUNIT N-TERMINAL SH2 DOMAIN



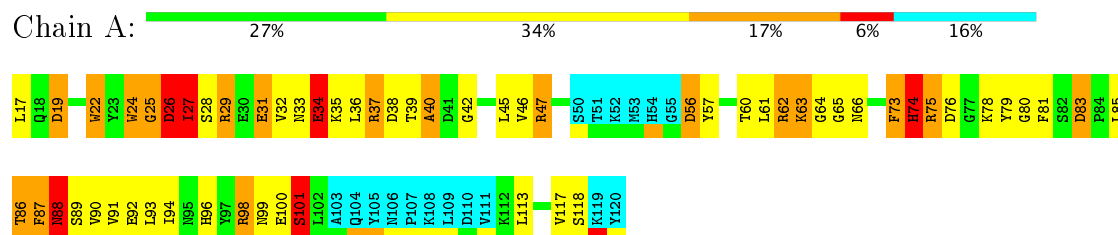
4.2.21 Score per residue for model 21

- Molecule 1: PHOSPHATIDYLINOSITOL 3-KINASE P85-ALPHA SUBUNIT N-TERMINAL SH2 DOMAIN



4.2.22 Score per residue for model 22

- Molecule 1: PHOSPHATIDYLINOSITOL 3-KINASE P85-ALPHA SUBUNIT N-TERMINAL SH2 DOMAIN



5 Refinement protocol and experimental data overview

Of the ? calculated structures, 22 were deposited, based on the following criterion: ?.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
X-PLOR	refinement	

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

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 (average) 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	1.15±0.01	4±0/737 (0.5±0.0%)	1.36±0.01	11±1/998 (1.1±0.1%)
All	All	1.15	88/16214 (0.5%)	1.36	250/21956 (1.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	5.6±0.5
All	All	0	124

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	24	TRP	CG-CD2	-8.04	1.29	1.43	5	22
1	A	22	TRP	CG-CD2	-7.28	1.31	1.43	5	22
1	A	74	HIS	CG-ND1	-6.26	1.25	1.38	3	22
1	A	96	HIS	CG-ND1	-6.22	1.25	1.38	9	22

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	24	TRP	NE1-CE2-CZ2	9.26	140.58	130.40	5	22
1	A	22	TRP	NE1-CE2-CZ2	9.09	140.40	130.40	20	22
1	A	22	TRP	NE1-CE2-CD2	-7.59	99.71	107.30	5	22
1	A	24	TRP	NE1-CE2-CD2	-7.51	99.79	107.30	5	22
1	A	24	TRP	CG-CD1-NE1	-6.94	103.16	110.10	17	22
1	A	24	TRP	CG-CD2-CE3	-6.92	127.67	133.90	5	15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	22	TRP	CG-CD1-NE1	-6.32	103.78	110.10	19	22
1	A	22	TRP	CD1-CG-CD2	6.29	111.33	106.30	5	22
1	A	24	TRP	CD1-NE1-CE2	6.26	114.64	109.00	4	22
1	A	24	TRP	CD1-CG-CD2	6.04	111.13	106.30	5	22
1	A	24	TRP	CE2-CD2-CG	5.82	111.96	107.30	9	14
1	A	22	TRP	CD1-NE1-CE2	5.80	114.22	109.00	16	22
1	A	22	TRP	CG-CD2-CE3	-5.16	129.26	133.90	19	1

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	98	ARG	Sidechain	22
1	A	29	ARG	Sidechain	21
1	A	47	ARG	Sidechain	21
1	A	75	ARG	Sidechain	21
1	A	37	ARG	Sidechain	20
1	A	62	ARG	Sidechain	19

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	720	702	699	36±4
All	All	15840	15444	15378	783

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 25.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:27:ILE:H	1:A:27:ILE:HD13	0.79	1.36	8	1
1:A:114:LEU:HD23	1:A:114:LEU:N	0.78	1.93	2	1
1:A:27:ILE:N	1:A:27:ILE:HD13	0.77	1.93	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:LEU:N	1:A:114:LEU:HD23	0.77	1.96	5	1
1:A:36:LEU:HD11	1:A:45:LEU:HD21	0.77	1.56	9	1
1:A:60:THR:C	1:A:61:LEU:HD23	0.76	2.01	16	13
1:A:113:LEU:O	1:A:113:LEU:HD23	0.71	1.85	5	1
1:A:87:PHE:CG	1:A:88:ASN:N	0.70	2.59	20	9
1:A:73:PHE:N	1:A:73:PHE:CD1	0.70	2.58	18	11
1:A:113:LEU:HD23	1:A:113:LEU:O	0.70	1.86	8	5
1:A:73:PHE:CD1	1:A:73:PHE:N	0.69	2.59	6	11
1:A:27:ILE:HD13	1:A:27:ILE:H	0.69	1.48	14	1
1:A:74:HIS:CG	1:A:75:ARG:N	0.68	2.62	11	21
1:A:20:ALA:HB1	1:A:22:TRP:CZ3	0.68	2.23	13	15
1:A:113:LEU:C	1:A:114:LEU:HD23	0.66	2.10	2	1
1:A:23:TYR:OH	1:A:59:LEU:HD11	0.66	1.91	16	2
1:A:32:VAL:HG12	1:A:33:ASN:N	0.65	2.05	9	11
1:A:36:LEU:HD12	1:A:36:LEU:H	0.64	1.51	9	1
1:A:74:HIS:CD2	1:A:75:ARG:N	0.64	2.66	2	13
1:A:66:ASN:ND2	1:A:67:ASN:N	0.64	2.46	12	1
1:A:94:ILE:HD11	1:A:113:LEU:HD11	0.63	1.71	20	2
1:A:74:HIS:NE2	1:A:77:GLY:N	0.63	2.46	13	6
1:A:39:THR:HG22	1:A:40:ALA:N	0.62	2.09	17	1
1:A:88:ASN:N	1:A:88:ASN:ND2	0.61	2.44	9	2
1:A:74:HIS:ND1	1:A:75:ARG:N	0.61	2.49	3	2
1:A:74:HIS:CD2	1:A:77:GLY:H	0.61	2.14	1	1
1:A:37:ARG:NH1	1:A:67:ASN:ND2	0.61	2.48	4	1
1:A:29:ARG:CD	1:A:29:ARG:H	0.60	2.09	6	1
1:A:78:LYS:N	1:A:78:LYS:CD	0.60	2.64	20	3
1:A:24:TRP:CD1	1:A:24:TRP:N	0.60	2.66	17	12
1:A:73:PHE:CD2	1:A:80:GLY:O	0.59	2.56	1	22
1:A:78:LYS:CD	1:A:78:LYS:N	0.59	2.66	5	2
1:A:61:LEU:HD23	1:A:61:LEU:N	0.59	2.13	6	7
1:A:61:LEU:N	1:A:61:LEU:HD23	0.59	2.12	19	3
1:A:87:PHE:CD2	1:A:88:ASN:N	0.58	2.71	11	7
1:A:74:HIS:CD2	1:A:75:ARG:H	0.58	2.17	14	10
1:A:87:PHE:O	1:A:88:ASN:ND2	0.58	2.36	16	3
1:A:113:LEU:CD2	1:A:113:LEU:H	0.58	2.12	15	2
1:A:67:ASN:ND2	1:A:67:ASN:H	0.58	1.94	3	3
1:A:74:HIS:CD2	1:A:78:LYS:O	0.58	2.57	18	2
1:A:113:LEU:H	1:A:113:LEU:CD2	0.58	2.11	17	2
1:A:88:ASN:ND2	1:A:89:SER:H	0.58	1.97	11	1
1:A:29:ARG:CD	1:A:29:ARG:N	0.57	2.67	8	2
1:A:73:PHE:O	1:A:80:GLY:N	0.57	2.38	3	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:57:TYR:CD1	1:A:57:TYR:N	0.57	2.72	1	1
1:A:60:THR:OG1	1:A:69:LEU:HD12	0.57	1.98	3	4
1:A:36:LEU:HD12	1:A:36:LEU:N	0.57	2.14	9	1
1:A:56:ASP:O	1:A:57:TYR:CD1	0.57	2.58	9	6
1:A:66:ASN:ND2	1:A:67:ASN:H	0.57	1.98	12	1
1:A:27:ILE:HD11	1:A:46:VAL:O	0.56	2.00	8	1
1:A:44:PHE:CE1	1:A:113:LEU:O	0.56	2.58	11	8
1:A:83:ASP:O	1:A:85:LEU:N	0.56	2.38	4	13
1:A:113:LEU:O	1:A:113:LEU:CD2	0.56	2.53	5	5
1:A:44:PHE:CD2	1:A:113:LEU:HD12	0.56	2.36	7	2
1:A:17:LEU:CD1	1:A:20:ALA:HB2	0.56	2.31	16	3
1:A:24:TRP:N	1:A:24:TRP:CD1	0.56	2.74	6	8
1:A:37:ARG:NH1	1:A:67:ASN:HD21	0.55	2.00	4	1
1:A:33:ASN:O	1:A:35:LYS:N	0.55	2.39	11	20
1:A:22:TRP:HE1	1:A:98:ARG:HH11	0.55	1.43	14	2
1:A:27:ILE:CD1	1:A:27:ILE:N	0.55	2.69	8	2
1:A:29:ARG:H	1:A:29:ARG:CD	0.55	2.13	8	2
1:A:33:ASN:ND2	1:A:37:ARG:HE	0.54	2.00	17	3
1:A:39:THR:OG1	1:A:40:ALA:N	0.54	2.40	2	1
1:A:113:LEU:CD2	1:A:113:LEU:O	0.54	2.55	2	1
1:A:56:ASP:OD2	1:A:57:TYR:N	0.54	2.40	15	2
1:A:24:TRP:CE3	1:A:31:GLU:OE1	0.54	2.60	4	1
1:A:115:TYR:CD1	1:A:115:TYR:N	0.54	2.75	17	4
1:A:114:LEU:N	1:A:114:LEU:CD2	0.54	2.70	5	3
1:A:114:LEU:O	1:A:115:TYR:CD1	0.54	2.61	4	3
1:A:23:TYR:CE1	1:A:46:VAL:HG23	0.54	2.37	17	6
1:A:88:ASN:HD22	1:A:88:ASN:N	0.54	2.00	9	1
1:A:74:HIS:NE2	1:A:76:ASP:N	0.54	2.55	17	3
1:A:47:ARG:HH11	1:A:47:ARG:CG	0.54	2.16	22	1
1:A:79:TYR:O	1:A:87:PHE:CE1	0.53	2.61	13	10
1:A:66:ASN:HD22	1:A:67:ASN:N	0.53	2.02	12	3
1:A:41:ASP:OD2	1:A:65:GLY:N	0.53	2.41	2	1
1:A:36:LEU:O	1:A:62:ARG:NE	0.53	2.42	8	7
1:A:62:ARG:NH2	1:A:65:GLY:O	0.53	2.42	4	4
1:A:37:ARG:O	1:A:62:ARG:NH2	0.53	2.41	22	2
1:A:24:TRP:CE2	1:A:118:SER:O	0.53	2.61	11	1
1:A:26:ASP:N	1:A:26:ASP:OD1	0.53	2.42	22	2
1:A:37:ARG:CZ	1:A:67:ASN:HD21	0.53	2.17	4	1
1:A:56:ASP:OD1	1:A:57:TYR:CE2	0.52	2.62	2	3
1:A:62:ARG:NH1	1:A:65:GLY:O	0.52	2.43	3	1
1:A:26:ASP:OD1	1:A:57:TYR:CZ	0.52	2.63	2	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:THR:HG22	1:A:44:PHE:N	0.52	2.19	18	1
1:A:33:ASN:O	1:A:36:LEU:N	0.52	2.43	4	5
1:A:97:TYR:CG	1:A:102:LEU:CD2	0.52	2.92	10	2
1:A:94:ILE:O	1:A:98:ARG:N	0.52	2.43	15	3
1:A:63:LYS:O	1:A:65:GLY:N	0.52	2.43	22	1
1:A:43:THR:HG22	1:A:117:VAL:HG22	0.52	1.81	20	1
1:A:79:TYR:O	1:A:87:PHE:CZ	0.52	2.63	16	4
1:A:39:THR:HG22	1:A:40:ALA:H	0.52	1.64	17	1
1:A:87:PHE:C	1:A:88:ASN:ND2	0.51	2.63	22	3
1:A:89:SER:OG	1:A:90:VAL:N	0.51	2.42	6	2
1:A:41:ASP:OD1	1:A:65:GLY:N	0.51	2.44	4	1
1:A:113:LEU:O	1:A:113:LEU:CG	0.51	2.59	12	5
1:A:115:TYR:N	1:A:115:TYR:CD1	0.51	2.78	21	3
1:A:114:LEU:C	1:A:115:TYR:CG	0.51	2.84	13	10
1:A:88:ASN:ND2	1:A:89:SER:OG	0.50	2.43	11	2
1:A:60:THR:HG23	1:A:67:ASN:ND2	0.50	2.21	15	1
1:A:74:HIS:NE2	1:A:76:ASP:CA	0.50	2.74	17	3
1:A:97:TYR:CD1	1:A:102:LEU:HD23	0.50	2.41	5	4
1:A:113:LEU:CD2	1:A:113:LEU:N	0.50	2.73	15	1
1:A:61:LEU:N	1:A:61:LEU:CD2	0.50	2.74	19	3
1:A:88:ASN:HD22	1:A:89:SER:N	0.50	2.05	8	1
1:A:74:HIS:CE1	1:A:76:ASP:N	0.50	2.80	11	1
1:A:39:THR:CG2	1:A:40:ALA:N	0.50	2.74	17	1
1:A:71:LYS:O	1:A:73:PHE:CE1	0.50	2.64	20	1
1:A:84:PRO:O	1:A:85:LEU:C	0.50	2.50	4	13
1:A:56:ASP:OD2	1:A:57:TYR:CD2	0.50	2.65	15	2
1:A:32:VAL:CG1	1:A:33:ASN:N	0.50	2.74	9	1
1:A:23:TYR:OH	1:A:59:LEU:CD1	0.50	2.60	5	5
1:A:113:LEU:CG	1:A:113:LEU:O	0.49	2.59	19	3
1:A:85:LEU:N	1:A:85:LEU:HD12	0.49	2.22	3	1
1:A:87:PHE:O	1:A:89:SER:OG	0.49	2.31	16	1
1:A:21:GLU:CG	1:A:22:TRP:N	0.49	2.75	19	1
1:A:33:ASN:HD21	1:A:37:ARG:HE	0.49	1.49	17	1
1:A:67:ASN:ND2	1:A:67:ASN:N	0.49	2.60	3	1
1:A:56:ASP:CG	1:A:57:TYR:N	0.49	2.64	2	2
1:A:30:GLU:O	1:A:34:GLU:CG	0.49	2.61	19	6
1:A:26:ASP:CG	1:A:57:TYR:CZ	0.49	2.86	22	2
1:A:113:LEU:N	1:A:113:LEU:CD2	0.49	2.76	17	3
1:A:84:PRO:O	1:A:86:THR:N	0.49	2.46	5	3
1:A:74:HIS:NE2	1:A:76:ASP:C	0.49	2.66	10	4
1:A:67:ASN:C	1:A:67:ASN:ND2	0.49	2.66	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:76:ASP:CG	1:A:77:GLY:N	0.49	2.66	4	1
1:A:62:ARG:NH1	1:A:65:GLY:C	0.49	2.65	17	1
1:A:87:PHE:C	1:A:87:PHE:CD1	0.49	2.87	20	1
1:A:25:GLY:O	1:A:26:ASP:O	0.48	2.32	11	8
1:A:62:ARG:CZ	1:A:65:GLY:O	0.48	2.61	22	1
1:A:87:PHE:CD1	1:A:87:PHE:N	0.48	2.76	7	3
1:A:34:GLU:N	1:A:34:GLU:CD	0.48	2.65	15	2
1:A:21:GLU:O	1:A:23:TYR:N	0.48	2.46	13	1
1:A:43:THR:O	1:A:61:LEU:CB	0.48	2.61	21	8
1:A:74:HIS:CE1	1:A:75:ARG:O	0.48	2.66	7	1
1:A:72:ILE:HD13	1:A:81:PHE:CE1	0.48	2.43	12	5
1:A:114:LEU:CD2	1:A:114:LEU:N	0.48	2.65	2	2
1:A:78:LYS:O	1:A:79:TYR:CD1	0.48	2.66	18	2
1:A:23:TYR:CD1	1:A:46:VAL:HG23	0.48	2.43	6	2
1:A:59:LEU:N	1:A:70:ILE:O	0.48	2.47	11	3
1:A:113:LEU:C	1:A:114:LEU:HD22	0.48	2.29	17	1
1:A:60:THR:HG23	1:A:67:ASN:OD1	0.48	2.09	13	1
1:A:87:PHE:N	1:A:87:PHE:CD1	0.47	2.81	15	4
1:A:26:ASP:CG	1:A:57:TYR:CE1	0.47	2.88	22	1
1:A:61:LEU:CD2	1:A:61:LEU:N	0.47	2.75	6	2
1:A:74:HIS:CG	1:A:75:ARG:H	0.47	2.28	11	2
1:A:78:LYS:H	1:A:78:LYS:CD	0.47	2.21	10	2
1:A:82:SER:OG	1:A:83:ASP:N	0.47	2.39	6	2
1:A:32:VAL:O	1:A:36:LEU:HD12	0.47	2.08	9	1
1:A:24:TRP:CZ2	1:A:118:SER:O	0.47	2.67	11	1
1:A:33:ASN:HD22	1:A:33:ASN:C	0.47	2.13	15	1
1:A:44:PHE:O	1:A:44:PHE:CG	0.47	2.67	5	1
1:A:63:LYS:C	1:A:65:GLY:N	0.47	2.68	22	1
1:A:114:LEU:N	1:A:114:LEU:HD22	0.47	2.25	17	1
1:A:56:ASP:OD1	1:A:57:TYR:CD2	0.47	2.68	2	1
1:A:112:LYS:CD	1:A:112:LYS:N	0.47	2.78	16	1
1:A:41:ASP:OD1	1:A:64:GLY:CA	0.46	2.62	21	1
1:A:100:GLU:O	1:A:101:SER:OG	0.46	2.30	12	6
1:A:24:TRP:NE1	1:A:117:VAL:O	0.46	2.47	17	4
1:A:74:HIS:CE1	1:A:79:TYR:CZ	0.46	3.04	18	1
1:A:67:ASN:N	1:A:67:ASN:OD1	0.46	2.47	2	1
1:A:36:LEU:O	1:A:62:ARG:NH2	0.46	2.48	20	1
1:A:19:ASP:O	1:A:20:ALA:O	0.46	2.34	11	11
1:A:100:GLU:O	1:A:101:SER:CB	0.46	2.63	22	4
1:A:63:LYS:C	1:A:65:GLY:H	0.46	2.14	22	2
1:A:46:VAL:CG1	1:A:47:ARG:N	0.46	2.79	16	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:TYR:O	1:A:100:GLU:N	0.46	2.48	20	1
1:A:26:ASP:O	1:A:26:ASP:CG	0.46	2.55	10	1
1:A:21:GLU:C	1:A:23:TYR:N	0.46	2.69	13	1
1:A:96:HIS:O	1:A:96:HIS:ND1	0.46	2.48	4	1
1:A:39:THR:O	1:A:40:ALA:O	0.46	2.34	5	7
1:A:25:GLY:O	1:A:26:ASP:OD2	0.46	2.34	13	7
1:A:49:ALA:HB3	1:A:56:ASP:O	0.46	2.10	1	1
1:A:112:LYS:O	1:A:112:LYS:CG	0.46	2.63	4	1
1:A:96:HIS:CE1	1:A:100:GLU:OE1	0.45	2.68	2	1
1:A:18:GLN:H	1:A:18:GLN:CD	0.45	2.14	3	1
1:A:113:LEU:HD23	1:A:113:LEU:H	0.45	1.72	15	1
1:A:47:ARG:NH1	1:A:47:ARG:CG	0.45	2.79	22	1
1:A:62:ARG:HH11	1:A:65:GLY:C	0.45	2.14	17	1
1:A:93:LEU:O	1:A:96:HIS:N	0.45	2.49	10	5
1:A:56:ASP:N	1:A:56:ASP:OD1	0.45	2.49	3	1
1:A:114:LEU:C	1:A:115:TYR:CD1	0.45	2.90	20	4
1:A:49:ALA:HB2	1:A:57:TYR:CA	0.45	2.42	21	2
1:A:117:VAL:O	1:A:118:SER:O	0.45	2.35	20	1
1:A:30:GLU:O	1:A:34:GLU:OE1	0.45	2.34	9	2
1:A:46:VAL:HG13	1:A:47:ARG:N	0.45	2.27	15	2
1:A:97:TYR:CD1	1:A:102:LEU:CD2	0.45	3.00	5	1
1:A:49:ALA:HB2	1:A:56:ASP:O	0.45	2.12	18	1
1:A:90:VAL:O	1:A:94:ILE:N	0.44	2.50	2	5
1:A:39:THR:HG23	1:A:40:ALA:N	0.44	2.28	19	1
1:A:56:ASP:CG	1:A:57:TYR:CD2	0.44	2.91	2	2
1:A:91:VAL:O	1:A:95:ASN:CB	0.44	2.65	4	4
1:A:31:GLU:O	1:A:32:VAL:C	0.44	2.56	22	7
1:A:39:THR:CG2	1:A:40:ALA:H	0.44	2.25	17	1
1:A:33:ASN:C	1:A:35:LYS:N	0.44	2.71	20	9
1:A:44:PHE:CG	1:A:113:LEU:HD12	0.44	2.48	7	1
1:A:28:SER:C	1:A:30:GLU:N	0.44	2.71	8	1
1:A:39:THR:HG21	1:A:43:THR:OG1	0.44	2.12	14	1
1:A:83:ASP:C	1:A:85:LEU:H	0.44	2.15	20	2
1:A:44:PHE:CD2	1:A:113:LEU:CD1	0.44	3.01	7	1
1:A:86:THR:O	1:A:87:PHE:O	0.44	2.35	22	3
1:A:45:LEU:HD12	1:A:45:LEU:C	0.44	2.33	12	2
1:A:36:LEU:HD22	1:A:62:ARG:HB2	0.43	1.90	5	1
1:A:41:ASP:O	1:A:41:ASP:OD1	0.43	2.35	12	1
1:A:21:GLU:CG	1:A:22:TRP:H	0.43	2.26	19	1
1:A:57:TYR:N	1:A:57:TYR:CD1	0.43	2.86	4	1
1:A:26:ASP:CG	1:A:26:ASP:O	0.43	2.56	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:22:TRP:HE1	1:A:98:ARG:CZ	0.43	2.26	6	1
1:A:56:ASP:OD1	1:A:72:ILE:O	0.43	2.36	18	3
1:A:67:ASN:CG	1:A:67:ASN:O	0.43	2.56	16	1
1:A:113:LEU:HD23	1:A:113:LEU:C	0.43	2.34	12	1
1:A:26:ASP:OD1	1:A:48:ASP:CB	0.43	2.67	16	1
1:A:34:GLU:OE1	1:A:34:GLU:O	0.43	2.37	22	1
1:A:26:ASP:OD1	1:A:26:ASP:O	0.43	2.36	15	1
1:A:113:LEU:HG	1:A:113:LEU:O	0.43	2.14	1	2
1:A:95:ASN:ND2	1:A:95:ASN:C	0.43	2.71	11	1
1:A:33:ASN:O	1:A:34:GLU:C	0.42	2.57	3	7
1:A:49:ALA:HB3	1:A:57:TYR:HA	0.42	1.90	3	1
1:A:94:ILE:CG2	1:A:95:ASN:N	0.42	2.82	14	2
1:A:79:TYR:CD2	1:A:90:VAL:CG2	0.42	3.03	3	1
1:A:78:LYS:CD	1:A:78:LYS:H	0.42	2.25	16	1
1:A:39:THR:CG2	1:A:39:THR:O	0.42	2.67	1	1
1:A:56:ASP:O	1:A:56:ASP:OD2	0.42	2.36	18	2
1:A:35:LYS:O	1:A:39:THR:CG2	0.42	2.67	5	1
1:A:113:LEU:H	1:A:113:LEU:HD23	0.42	1.74	21	1
1:A:36:LEU:O	1:A:37:ARG:C	0.42	2.58	22	1
1:A:39:THR:O	1:A:39:THR:HG23	0.42	2.15	1	1
1:A:93:LEU:O	1:A:94:ILE:C	0.42	2.58	14	13
1:A:37:ARG:CZ	1:A:67:ASN:ND2	0.42	2.81	4	1
1:A:93:LEU:HD23	1:A:94:ILE:N	0.42	2.29	4	1
1:A:47:ARG:O	1:A:48:ASP:C	0.42	2.58	9	3
1:A:97:TYR:CG	1:A:102:LEU:HD23	0.42	2.49	15	1
1:A:60:THR:O	1:A:61:LEU:HD23	0.42	2.15	5	1
1:A:39:THR:O	1:A:43:THR:OG1	0.42	2.37	9	1
1:A:39:THR:O	1:A:40:ALA:HB3	0.42	2.15	22	1
1:A:35:LYS:O	1:A:39:THR:OG1	0.41	2.33	17	1
1:A:79:TYR:CG	1:A:90:VAL:HG22	0.41	2.50	4	1
1:A:43:THR:CG2	1:A:44:PHE:N	0.41	2.83	18	1
1:A:47:ARG:O	1:A:58:THR:N	0.41	2.53	21	1
1:A:26:ASP:OD1	1:A:26:ASP:N	0.41	2.52	8	1
1:A:56:ASP:OD1	1:A:57:TYR:N	0.41	2.53	10	1
1:A:56:ASP:OD2	1:A:79:TYR:CZ	0.41	2.74	14	1
1:A:90:VAL:C	1:A:92:GLU:N	0.41	2.73	22	1
1:A:41:ASP:OD1	1:A:41:ASP:O	0.41	2.37	3	1
1:A:66:ASN:HD22	1:A:66:ASN:C	0.41	2.19	5	1
1:A:88:ASN:ND2	1:A:88:ASN:N	0.41	2.69	15	2
1:A:76:ASP:OD1	1:A:77:GLY:N	0.41	2.53	4	1
1:A:115:TYR:N	1:A:115:TYR:CD2	0.41	2.87	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:113:LEU:HD23	1:A:113:LEU:N	0.41	2.31	17	1
1:A:102:LEU:N	1:A:102:LEU:HD23	0.41	2.31	5	2
1:A:48:ASP:OD1	1:A:49:ALA:N	0.41	2.54	8	1
1:A:56:ASP:C	1:A:57:TYR:CG	0.41	2.93	20	2
1:A:27:ILE:CG1	1:A:28:SER:H	0.41	2.29	17	1
1:A:66:ASN:O	1:A:68:LYS:N	0.41	2.53	5	1
1:A:115:TYR:CD2	1:A:115:TYR:N	0.41	2.85	10	1
1:A:88:ASN:ND2	1:A:92:GLU:OE1	0.41	2.52	6	1
1:A:45:LEU:C	1:A:45:LEU:HD12	0.41	2.36	13	2
1:A:74:HIS:NE2	1:A:78:LYS:O	0.41	2.54	18	1
1:A:44:PHE:CG	1:A:113:LEU:HD11	0.41	2.51	3	1
1:A:32:VAL:O	1:A:36:LEU:CD1	0.41	2.69	9	1
1:A:56:ASP:C	1:A:57:TYR:CD1	0.41	2.94	15	1
1:A:60:THR:HG23	1:A:67:ASN:HD22	0.41	1.76	15	1
1:A:67:ASN:O	1:A:67:ASN:CG	0.41	2.59	20	1
1:A:98:ARG:O	1:A:114:LEU:HD22	0.41	2.16	21	1
1:A:56:ASP:O	1:A:56:ASP:CG	0.41	2.60	11	1
1:A:27:ILE:CG1	1:A:28:SER:N	0.41	2.84	22	1
1:A:28:SER:O	1:A:30:GLU:N	0.40	2.54	10	1
1:A:84:PRO:C	1:A:86:THR:N	0.40	2.75	5	2
1:A:41:ASP:OD1	1:A:64:GLY:N	0.40	2.53	3	1
1:A:74:HIS:NE2	1:A:75:ARG:C	0.40	2.73	10	1
1:A:62:ARG:NH1	1:A:67:ASN:ND2	0.40	2.69	18	1
1:A:74:HIS:CD2	1:A:77:GLY:N	0.40	2.89	20	1
1:A:28:SER:O	1:A:29:ARG:C	0.40	2.60	22	1
1:A:36:LEU:O	1:A:62:ARG:CZ	0.40	2.69	20	1
1:A:56:ASP:C	1:A:57:TYR:CD2	0.40	2.94	20	1
1:A:67:ASN:OD1	1:A:67:ASN:N	0.40	2.53	21	1
1:A:87:PHE:O	1:A:88:ASN:CG	0.40	2.59	1	1
1:A:36:LEU:CD1	1:A:36:LEU:N	0.40	2.84	19	1
1:A:17:LEU:O	1:A:17:LEU:HD23	0.40	2.17	14	1
1:A:26:ASP:OD1	1:A:26:ASP:C	0.40	2.60	18	1

6.3 Torsion angles ⓘ

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	86/104 (83%)	52±3 (61±3%)	24±3 (27±3%)	10±2 (12±3%)	1	7
All	All	1892/2288 (83%)	1146 (61%)	519 (27%)	227 (12%)	1	7

All 25 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	27	ILE	21
1	A	42	GLY	20
1	A	34	GLU	20
1	A	26	ASP	19
1	A	20	ALA	15
1	A	40	ALA	15
1	A	19	ASP	15
1	A	77	GLY	14
1	A	88	ASN	14
1	A	87	PHE	12
1	A	65	GLY	7
1	A	101	SER	7
1	A	56	ASP	7
1	A	84	PRO	7
1	A	37	ARG	7
1	A	25	GLY	6
1	A	32	VAL	5
1	A	38	ASP	4
1	A	85	LEU	3
1	A	118	SER	3
1	A	75	ARG	2
1	A	82	SER	1
1	A	22	TRP	1
1	A	67	ASN	1
1	A	64	GLY	1

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	78/93 (84%)	46±3 (59±4%)	32±3 (41±4%)	0	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1716/2046 (84%)	1006 (59%)	710 (41%)	0 4

All 68 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	81	PHE	22
1	A	73	PHE	22
1	A	22	TRP	22
1	A	60	THR	22
1	A	45	LEU	22
1	A	19	ASP	22
1	A	61	LEU	22
1	A	94	ILE	22
1	A	113	LEU	21
1	A	83	ASP	21
1	A	117	VAL	20
1	A	26	ASP	20
1	A	78	LYS	20
1	A	89	SER	20
1	A	27	ILE	20
1	A	93	LEU	20
1	A	58	THR	19
1	A	99	ASN	19
1	A	66	ASN	16
1	A	46	VAL	16
1	A	76	ASP	15
1	A	67	ASN	15
1	A	47	ARG	15
1	A	74	HIS	15
1	A	56	ASP	14
1	A	88	ASN	14
1	A	82	SER	13
1	A	118	SER	11
1	A	35	LYS	10
1	A	86	THR	10
1	A	39	THR	10
1	A	28	SER	9
1	A	112	LYS	9
1	A	29	ARG	9
1	A	43	THR	9
1	A	96	HIS	9

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Mol	Chain	Res	Type	Models (Total)
1	A	85	LEU	8
1	A	72	ILE	8
1	A	48	ASP	7
1	A	37	ARG	7
1	A	91	VAL	6
1	A	63	LYS	6
1	A	69	LEU	6
1	A	62	ARG	6
1	A	101	SER	5
1	A	17	LEU	5
1	A	98	ARG	5
1	A	59	LEU	4
1	A	34	GLU	4
1	A	68	LYS	4
1	A	87	PHE	4
1	A	21	GLU	3
1	A	71	LYS	3
1	A	97	TYR	3
1	A	102	LEU	3
1	A	33	ASN	2
1	A	30	GLU	2
1	A	18	GLN	2
1	A	90	VAL	2
1	A	114	LEU	2
1	A	92	GLU	1
1	A	95	ASN	1
1	A	38	ASP	1
1	A	75	ARG	1
1	A	115	TYR	1
1	A	31	GLU	1
1	A	70	ILE	1
1	A	41	ASP	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided