wwPDB X-ray Structure Validation Summary Report (i)

May 13, 2020 – 01:27 pm BST

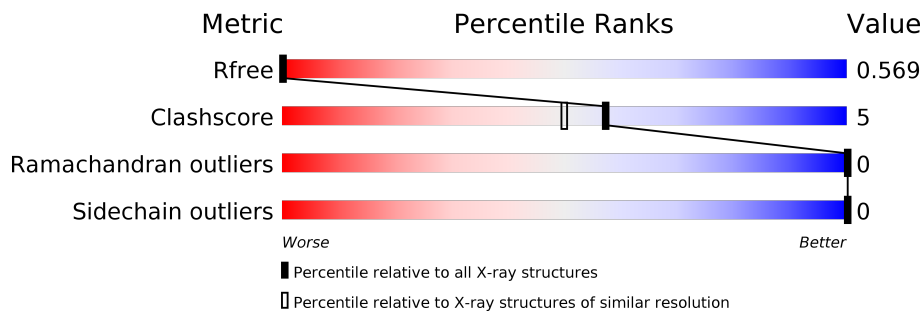|		
PDB ID	:	4Y3B
Title	:	Crystal structure of C-terminal modified Tau peptide-hybrid 201D with 14-3-3sigma
Authors	:	Bartel, M.; Milroy, L.G.; Brunsveld, L.; Ottmann, C.
Deposited on	:	2015-02-10
Resolution	:	1.80 Å(reported)

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 1.80 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	Percentile Ranks	Value
Rfree		0.569
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		0

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	236	89% 8% ·
1	B	236	91% 8% ·
2	C	7	71% 29%
2	D	7	71% 14% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	49F	C	301	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4572 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 14-3-3 protein sigma.

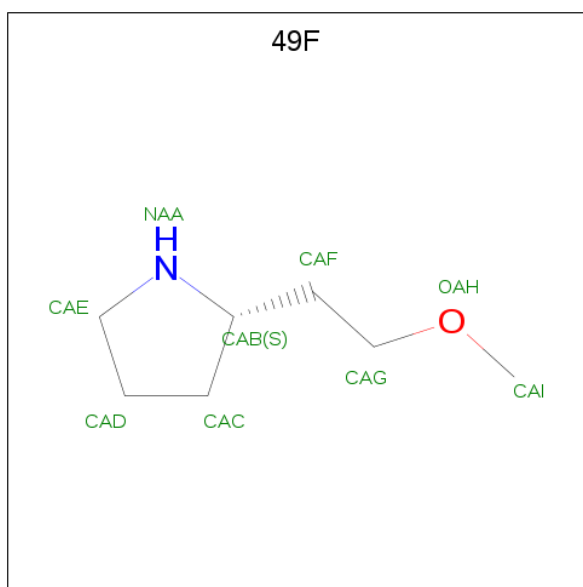| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	229	Total 1926	C 1220	N 316	O 378	S 12	0	26	0
1	B	234	Total 1847	C 1152	N 312	O 372	S 11	0	2	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P31947
A	-3	ALA	-	expression tag	UNP P31947
A	-2	MET	-	expression tag	UNP P31947
A	-1	GLY	-	expression tag	UNP P31947
A	0	SER	-	expression tag	UNP P31947
B	-4	GLY	-	expression tag	UNP P31947
B	-3	ALA	-	expression tag	UNP P31947
B	-2	MET	-	expression tag	UNP P31947
B	-1	GLY	-	expression tag	UNP P31947
B	0	SER	-	expression tag	UNP P31947

- Molecule 2 is a protein called ARG-THR-PRO-SEP-LEU-PRO-THR-[H][C@@]1(C(C2=CC=CC=C2)C3=CC=CC=C3)CCCN1C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	7	Total 57	C 33	N 10	O 13	P 1	0	0	0
2	D	6	Total 46	C 27	N 6	O 12	P 1	0	0	0

- Molecule 3 is (2S)-2-(2-methoxyethyl)pyrrolidine (three-letter code: 49F) (formula: $C_7H_{15}NO$).

49F

NAA

CAF

CAE

OAH

CAB(S)

CAG

CAI

CAD   CAC

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total 9	C 7	N 1	O 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	330	Total 330	O 330	0	0
4	B	334	Total 334	O 334	0	0
4	C	15	Total 15	O 15	0	0
4	D	8	Total 8	O 8	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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. 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. 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.
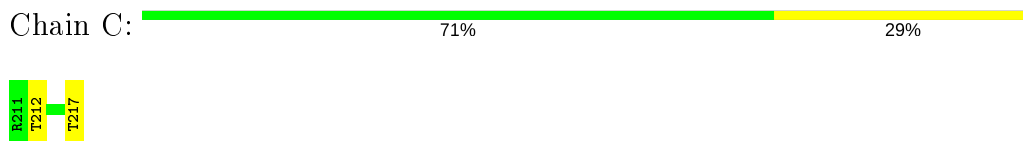
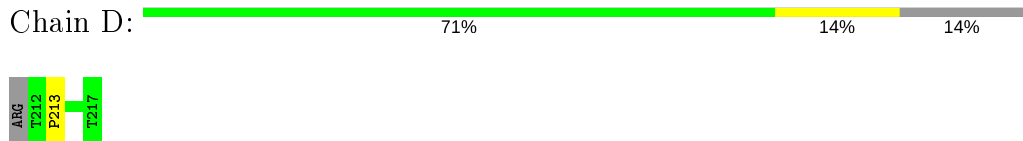- Molecule 1: 14-3-3 protein sigma
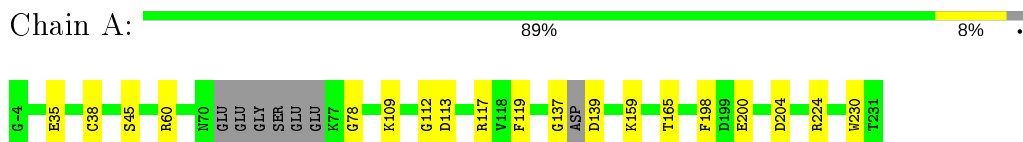
- Molecule 1: 14-3-3 protein sigma
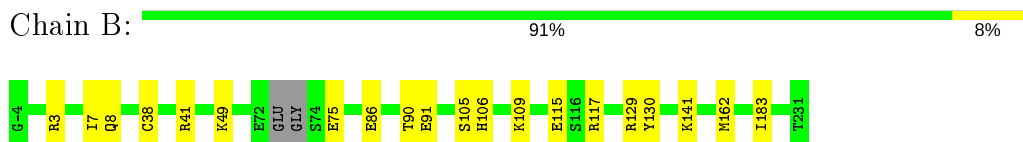
- Molecule 2: ARG-THR-PRO-SEP-LEU-PRO-THR-[H][C@@]1(C(C2=CC=CC=C2)C3=CC=CC=C3)CCCN1C

- Molecule 2: ARG-THR-PRO-SEP-LEU-PRO-THR-[H][C@@]1(C(C2=CC=CC=C2)C3=CC=CC=C3)CCCN1C

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	63.06Å 70.28Å 128.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.49 – 1.80 64.39 – 1.14	Depositor EDS
% Data completeness (in resolution range)	98.8 (45.49-1.80) 12.3 (64.39-1.14)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.34 (at 1.14Å)	Xtriage
Refinement program	PHENIX 1.9	Depositor
R, R_{free}	0.165 , 0.193 0.575 , 0.569	Depositor DCC
R_{free} test set	2000 reflections (7.43%)	wwPDB-VP
Wilson B-factor (Å^2)	0.1	Xtriage
Anisotropy	2.773	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.48 , 601.8	EDS
L-test for twinning[2]	$<|L|> = 0.50$, $<L^2> = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.19	EDS
Total number of atoms	4572	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 97.60 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2630e-10. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $<|L|>$, $<L^2>$ 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: 49F, SEP

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	0.35	0/2029	0.49	0/2722
1	B	0.32	0/1881	0.46	0/2527
2	C	0.39	0/47	0.69	0/63
2	D	0.34	0/36	0.90	0/49
All	All	0.34	0/3993	0.49	0/5361

There are no bond length outliers.

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	1926	0	1990	18	0
1	B	1847	0	1827	15	0
2	C	57	0	54	5	0
2	D	46	0	41	1	0
3	C	9	0	12	6	0
4	A	330	0	0	10	7
4	B	334	0	0	9	5
4	C	15	0	0	0	0
4	D	8	0	0	1	0
All	All	4572	0	3924	38	7

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 5.

The worst 5 of 38 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)
3:C:301:49F:CAD	3:C:301:49F:CAC	1.81	1.37
1:A:38:CYS:SG	4:A:546:HOH:O	2.24	0.94
1:A:139:ASP:N	4:A:302:HOH:O	2.01	0.92
1:A:198:PHE:HZ	1:A:224:ARG:HH21	1.25	0.83
1:B:38:CYS:SG	4:B:544:HOH:O	2.38	0.81

The worst 5 of 7 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)
4:A:472:HOH:O	4:B:301:HOH:O[1_565]	1.90	0.30
4:A:573:HOH:O	4:A:597:HOH:O[4_555]	2.05	0.15
4:A:556:HOH:O	4:B:302:HOH:O[4_445]	2.06	0.14
4:A:355:HOH:O	4:B:611:HOH:O[2_555]	2.11	0.09
4:A:408:HOH:O	4:A:536:HOH:O[4_555]	2.16	0.04

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	248/236 (105%)	246 (99%)	2 (1%)	0	100	100
1	B	231/236 (98%)	228 (99%)	3 (1%)	0	100	100
2	C	4/7 (57%)	4 (100%)	0	0	100	100
2	D	3/7 (43%)	3 (100%)	0	0	100	100
All	All	486/486 (100%)	481 (99%)	5 (1%)	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	217/198 (110%)	217 (100%)	0	100	100
1	B	199/198 (100%)	199 (100%)	0	100	100
2	C	6/6 (100%)	6 (100%)	0	100	100
2	D	5/6 (83%)	5 (100%)	0	100	100
All	All	427/408 (105%)	427 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some 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)

2 non-standard protein/DNA/RNA residues 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	SEP	D	214	2	8,9,10	1.53	1 (12%)	8,12,14	0.98	0
2	SEP	C	214	2	8,9,10	1.38	1 (12%)	8,12,14	1.10	0

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	SEP	D	214	2	-	0/5/8/10	-
2	SEP	C	214	2	-	0/5/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	214	SEP	P-O1P	3.32	1.61	1.50
2	C	214	SEP	P-O1P	2.95	1.60	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates 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	#$|Z| > 2$
3	49F	C	301	-	8,9,9	3.37	2 (25%)	5,10,10	2.82	3 (60%)

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	49F	C	301	-	-	1/4/11/11	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	49F	CAD-CAC	7.03	1.81	1.51
3	C	301	49F	CAD-CAE	-5.83	1.22	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	301	49F	CAC-CAD-CAE	-5.08	80.05	103.64
3	C	301	49F	CAC-CAB-NAA	-2.83	97.05	103.54
3	C	301	49F	CAD-CAE-NAA	2.08	111.78	105.69

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	301	49F	CAF-CAG-OAH-CAI

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	301	49F	6	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Continued from previous page...

Mol	Chain	Number of breaks

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	70:ASN	C	72:GLU	N	4.38

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.