Full wwPDB X-ray Structure Validation Report

Nov 6, 2023 – 09:51 pm GMT

PDB ID	:	6TCH
Title	:	Binary complex of 14-3-3 sigma and a high-affinity non-canonical 9-mer peptide binder
Authors	:	Somsen, B.A.; Ottmann, C.
Deposited on	:	2019-11-06
Resolution	:	1.80 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:

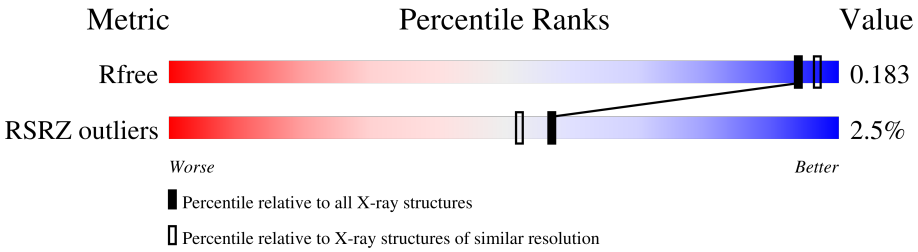
MolProbity	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	FAILED
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4315 atoms, of which 1940 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
			Total	C	H	N	O	S			
1	B	236	3809	1200	1879	325	393	12	0	13	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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 DLY-NVA-PPN-KCJ-SEP-PPN-B3S-BAL-PPN-LYS.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	H	N	O	P	S			
2	A	10	150	52	61	15	20	1	1	0	0	1

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
3	B	4	4	4	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
4	B	1	1	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	335	Total O 335 335	0	0
5	A	16	Total O 16 16	0	0

MolProbity failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

Xtriage (Phenix) failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	82.47Å 112.28Å 62.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.08 – 1.80 34.08 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.08-1.80) 96.2 (34.08-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.148 , 0.184 0.148 , 0.183	Depositor DCC
R_{free} test set	1377 reflections (5.04%)	wwPDB-VP
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 53.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4315	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains

8 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	PPN	A	5	2	12,14,15	2.91	1 (8%)	13,18,20	1.06	0
2	SEP	A	4	2	8,9,10	0.86	0	8,12,14	0.80	0
2	BAL	A	7	2	4,4,5	0.86	0	3,3,5	2.31	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	B3S	A	6	2	6,6,7	1.24	1 (16%)	4,6,8	2.84	2 (50%)
2	PPN	A	2	2	12,14,15	3.24	1 (8%)	13,18,20	1.74	2 (15%)
2	KCJ	A	3	2	5,10,11	0.85	0	3,12,14	2.01	1 (33%)
2	PPN	A	8	2	12,14,15	2.94	1 (8%)	13,18,20	2.07	6 (46%)
2	NVA	A	1	2	3,4,7	0.94	0	2,4,8	1.21	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	PPN	A	5	2	-	0/7/10/12	0/1/1/1
2	SEP	A	4	2	-	0/5/8/10	-
2	BAL	A	7	2	-	0/1/2/3	-
2	B3S	A	6	2	-	0/5/5/6	-
2	PPN	A	2	2	-	0/7/10/12	0/1/1/1
2	KCJ	A	3	2	-	2/5/6/8	0/1/1/1
2	PPN	A	8	2	-	0/7/10/12	0/1/1/1
2	NVA	A	1	2	-	0/0/2/7	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2	PPN	O1-N1	11.16	1.41	1.22
2	A	8	PPN	O1-N1	9.94	1.39	1.22
2	A	5	PPN	O1-N1	9.92	1.39	1.22
2	A	6	B3S	CG-CA	-2.61	1.48	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2	PPN	CG-CB-CA	-4.93	104.12	114.10
2	A	6	B3S	OD-CG-CA	-3.97	95.81	111.52
2	A	6	B3S	CA-CB-C	3.47	117.36	112.25
2	A	7	BAL	CB-CA-C	3.43	116.52	111.42
2	A	8	PPN	CG-CB-CA	-3.43	107.15	114.10
2	A	8	PPN	CB-CA-C	-3.32	105.25	111.47
2	A	8	PPN	CE1-CZ-N1	-3.13	117.02	119.38
2	A	8	PPN	CD2-CG-CD1	2.48	122.06	118.17
2	A	2	PPN	CE2-CZ-N1	2.47	121.24	119.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	3	KCJ	C13-S14-C15	2.34	97.13	92.37
2	A	8	PPN	CB-CG-CD1	-2.16	116.61	120.91
2	A	8	PPN	CE2-CZ-N1	2.08	120.94	119.38

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	3	KCJ	O-C-CA-C11
2	A	3	KCJ	C12-C11-CA-C

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates (i)

There are no monosaccharides in this entry.

4.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

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.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 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, 95^{th} 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	B	236/236 (100%)	-0.57	5 (2%) 63 59	5, 10, 33, 61	0
2	A	1/12 (8%)	2.43	1 (100%) 0 0	66, 66, 66, 66	0
All	All	237/248 (95%)	-0.56	6 (2%) 57 52	5, 10, 33, 66	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	74	SER	2.9
1	B	70	ASN	2.5
2	A	9	LYS	2.4
1	B	73	GLY	2.4
1	B	72	GLU	2.3
1	B	71	GLU	2.0

5.2 Non-standard residues in protein, DNA, RNA chains

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, 95^{th} 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(Å^2)	Q<0.9
2	PPN	A	2	14/15	0.78	0.30	31,53,63,76	0
2	NVA	A	1	5/8	0.79	0.37	55,60,82,83	0
2	BAL	A	7	5/6	0.81	0.18	18,37,45,45	0
2	KCJ	A	3	10/11	0.89	0.19	10,32,60,66	0
2	PPN	A	8	14/15	0.90	0.18	18,27,39,56	0
2	B3S	A	6	7/8	0.91	0.14	16,26,36,42	0
2	PPN	A	5	14/15	0.96	0.09	9,13,22,25	0
2	SEP	A	4	10/11	0.99	0.06	7,11,15,16	0

5.3 Carbohydrates (i)

There are no monosaccharides in this entry.

5.4 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, 95^{th} 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(Å^2)	Q<0.9
3	MG	B	301	1/1	0.95	0.11	29,29,29,29	0
3	MG	B	304	1/1	0.97	0.06	17,17,17,17	0
3	MG	B	303	1/1	0.99	0.07	6,6,6,6	0
3	MG	B	302	1/1	1.00	0.04	4,4,4,4	1
4	CL	B	305	1/1	1.00	0.05	11,11,11,11	0

5.5 Other polymers (i)

There are no such residues in this entry.