



wwPDB X-ray Structure Validation Summary Report i

Feb 27, 2014 – 09:23 PM GMT

PDB ID : 3HS8
Title : Intersectin 1-peptide-AP2 alpha ear complex
Authors : Vahedi-Faridi, A.; Pechstein, A.; Schaefer, J.G.; Saenger, W.; Haucke, V.
Deposited on : 2009-06-10
Resolution : 1.90 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

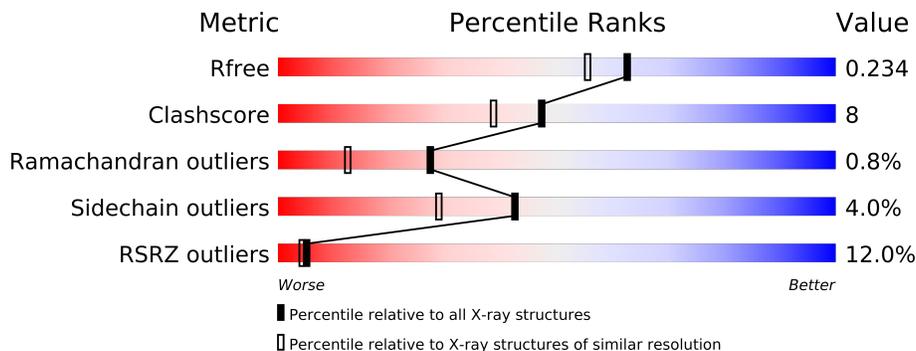
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.90 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}	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (1.90-1.90)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	273	
2	P	12	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 2171 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Adaptor protein complex AP-2, alpha 2 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	238	1910	1217	325	359	9	0	1	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	666	MET	-	EXPRESSION TAG	UNP Q6PEE6
A	667	GLY	-	EXPRESSION TAG	UNP Q6PEE6
A	668	SER	-	EXPRESSION TAG	UNP Q6PEE6
A	669	SER	-	EXPRESSION TAG	UNP Q6PEE6
A	670	HIS	-	EXPRESSION TAG	UNP Q6PEE6
A	671	HIS	-	EXPRESSION TAG	UNP Q6PEE6
A	672	HIS	-	EXPRESSION TAG	UNP Q6PEE6
A	673	HIS	-	EXPRESSION TAG	UNP Q6PEE6
A	674	HIS	-	EXPRESSION TAG	UNP Q6PEE6
A	675	HIS	-	EXPRESSION TAG	UNP Q6PEE6
A	676	SER	-	EXPRESSION TAG	UNP Q6PEE6
A	677	SER	-	EXPRESSION TAG	UNP Q6PEE6
A	678	GLY	-	EXPRESSION TAG	UNP Q6PEE6
A	679	LEU	-	EXPRESSION TAG	UNP Q6PEE6
A	680	VAL	-	EXPRESSION TAG	UNP Q6PEE6
A	681	PRO	-	EXPRESSION TAG	UNP Q6PEE6
A	682	ARG	-	EXPRESSION TAG	UNP Q6PEE6
A	683	GLY	-	EXPRESSION TAG	UNP Q6PEE6
A	684	SER	-	EXPRESSION TAG	UNP Q6PEE6
A	685	HIS	-	EXPRESSION TAG	UNP Q6PEE6
A	686	MET	-	EXPRESSION TAG	UNP Q6PEE6
A	687	ALA	-	EXPRESSION TAG	UNP Q6PEE6
A	688	SER	-	EXPRESSION TAG	UNP Q6PEE6
A	689	MET	-	EXPRESSION TAG	UNP Q6PEE6
A	690	THR	-	EXPRESSION TAG	UNP Q6PEE6
A	691	GLY	-	EXPRESSION TAG	UNP Q6PEE6
A	692	GLY	-	EXPRESSION TAG	UNP Q6PEE6

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	693	GLN	-	EXPRESSION TAG	UNP Q6PEE6
A	694	GLN	-	EXPRESSION TAG	UNP Q6PEE6
A	695	MET	-	EXPRESSION TAG	UNP Q6PEE6
A	696	GLY	-	EXPRESSION TAG	UNP Q6PEE6
A	697	ARG	-	EXPRESSION TAG	UNP Q6PEE6
A	698	GLY	-	EXPRESSION TAG	UNP Q6PEE6
A	699	SER	-	EXPRESSION TAG	UNP Q6PEE6
A	700	GLU	-	EXPRESSION TAG	UNP Q6PEE6
A	701	PHE	-	EXPRESSION TAG	UNP Q6PEE6

- Molecule 2 is a protein called peptide from Intersectin-1, residues 840-851.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	P	12	101	66	16	19	0	0	0

- Molecule 3 is water.

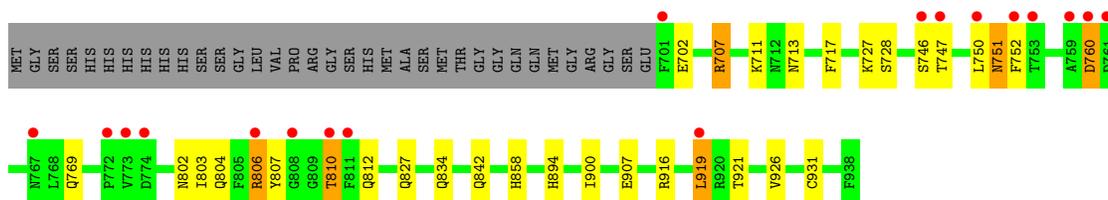
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	158	158	158	0	0
3	P	2	2	2	0	0

3 Residue-property plots i

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Adaptor protein complex AP-2, alpha 2 subunit

Chain A: 



- Molecule 2: peptide from Intersectin-1, residues 840-851

Chain P: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	64.48Å 120.41Å 32.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.10 – 1.90 28.41 – 1.90	Depositor EDS
% Data completeness (in resolution range)	93.4 (30.10-1.90) 93.4 (28.41-1.90)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.12 (at 1.91Å)	Xtrriage
Refinement program	REFMAC 5.3.0040	Depositor
R, R_{free}	0.189 , 0.235 0.193 , 0.234	Depositor DCC
R_{free} test set	1000 reflections (5.50%)	DCC
Wilson B-factor (Å ²)	23.0	Xtrriage
Anisotropy	0.158	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.7	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtrriage
Outliers	0 of 19174 reflections	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2171	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.79	2/1950 (0.1%)	0.73	0/2639
2	P	0.81	0/107	1.07	2/148 (1.4%)
All	All	0.79	2/2057 (0.1%)	0.75	2/2787 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	746	SER	CB-OG	5.77	1.49	1.42
1	A	806	ARG	C-O	5.76	1.34	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	851	PRO	N-CA-C	5.43	126.21	112.10
2	P	850	TRP	C-N-CD	-5.39	108.73	120.60

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1910	0	1904	30	0
2	P	101	0	81	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	158	0	0	4	0
3	P	2	0	0	0	0
All	All	2171	0	1985	32	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

The worst 5 of 32 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:769:GLN:HB2	3:A:110:HOH:O	1.66	0.94
1:A:750:LEU:HD23	1:A:751:ASN:N	1.87	0.89
1:A:810:THR:CG2	1:A:812:GLN:HE21	1.89	0.86
1:A:713:ASN:HD22	1:A:727:LYS:HA	1.52	0.74
1:A:810:THR:HG21	1:A:812:GLN:HE21	1.52	0.73

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 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 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	237/273 (87%)	232 (98%)	4 (2%)	1 (0%)	43	29
2	P	10/12 (83%)	7 (70%)	2 (20%)	1 (10%)	1	0
All	All	247/285 (87%)	239 (97%)	6 (2%)	2 (1%)	27	12

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	760	ASP
2	P	841	ASN

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	215/241 (89%)	208 (97%)	7 (3%)	50	37
2	P	11/11 (100%)	9 (82%)	2 (18%)	2	0
All	All	226/252 (90%)	217 (96%)	9 (4%)	42	29

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	842	GLN
2	P	851	PRO
1	A	921	THR
1	A	760	ASP
1	A	919	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	765	ASN
1	A	858	HIS
1	A	802	ASN
1	A	713	ASN
1	A	812	GLN

5.3.3 RNA [i](#)

There are no RNA chains 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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	238/273 (87%)	0.40	18 (7%) 14 13	20, 26, 36, 48	1 (0%)
2	P	12/12 (100%)	6.70	12 (100%) 0 0	22, 25, 32, 32	0
All	All	250/285 (87%)	0.70	30 (12%) 5 4	20, 26, 35, 48	1 (0%)

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	840	PRO	11.3
2	P	841	ASN	9.8
2	P	842	ASN	8.4
2	P	843	TRP	8.0
2	P	851	PRO	7.4

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.