wwPDB X-ray Structure Validation Summary Report (i)

Mar 9, 2024 – 08:42 PM EST

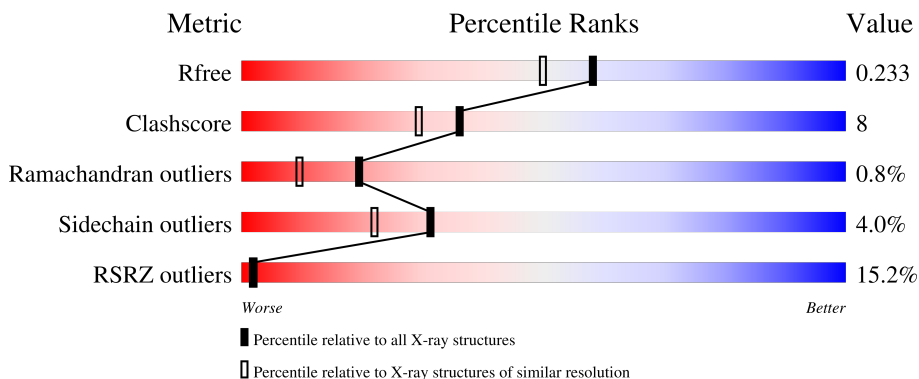|		
PDB ID	:	3HS8
Title	:	Intersectin 1-peptide-AP2 alpha ear complex
Authors	:	Vahedi-Faridi, A.; Pechstein, A.; Schaefer, J.G.; Saenger, W.; Haucke, V.
Deposited on	:	2009-06-10
Resolution	:	1.90 Å(reported)

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 1.90 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	Percentile Ranks	Value
Rfree		0.233
Clashscore		8
Ramachandran outliers		0.8%
Sidechain outliers		4.0%
RSRZ outliers		15.2%

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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 of 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% 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	273	10% / 75% 10% • 13%
2	P	12	83% / 58% 17% 17% 8%

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2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 2171 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 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

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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
2	P	12	Total 101	C 66	N 16	O 19	0	0	0

- Molecule 3 is water.

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

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 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:
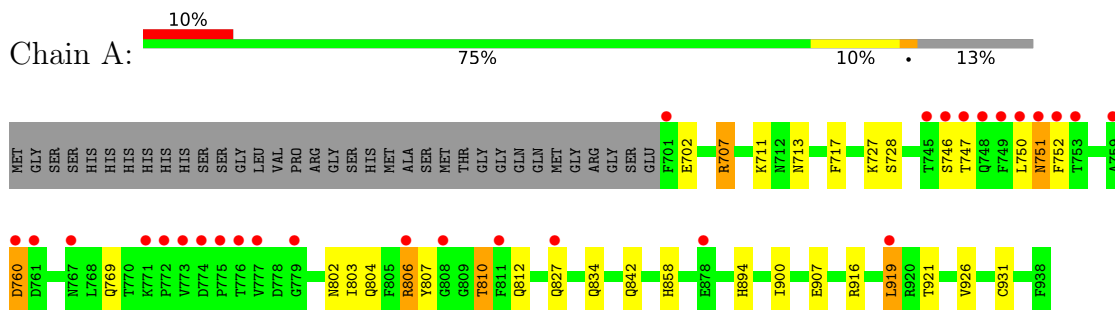
• Molecule 2: peptide from Intersectin-1, residues 840-851

Chain P:
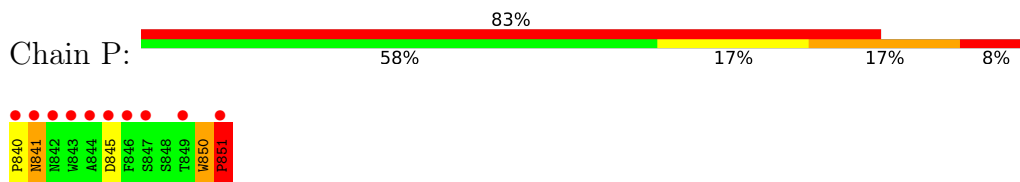
4 Data and refinement statistics ⓘ

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
$< I/\sigma(I) >$ [1]	6.12 (at 1.91Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.189　,　0.235 0.193　,　0.233	Depositor DCC
R_{free} test set	1000 reflections (5.22%)	wwPDB-VP
Wilson B-factor (Å^2)	23.0	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.0	EDS
L-test for twinning[2]	$< |L| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	2171	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage'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.*

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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 ⓘ

5.1 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 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(^{o})	Ideal(^{o})
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 Too-close contacts ⓘ

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	1910	0	1904	30	0
2	P	101	0	81	2	0
3	A	158	0	0	4	0
3	P	2	0	0	0	0
All	All	2171	0	1985	32	0

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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 8.

The worst 5 of 32 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: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%)	34	24
2	P	10/12 (83%)	7 (70%)	2 (20%)	1 (10%)	0	0
All	All	247/285 (87%)	239 (97%)	6 (2%)	2 (1%)	19	9

All (2) Ramachandran outliers are listed below:

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

5.3.2 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 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%)	38	29
2	P	11/11 (100%)	9 (82%)	2 (18%)	1	0
All	All	226/252 (90%)	217 (96%)	9 (4%)	31	22

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

Mol	Chain	Res	Type
2	P	845	ASP
2	P	851	PRO
1	A	810	THR
1	A	842	GLN
1	A	919	LEU

Sometimes 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	802	ASN
1	A	858	HIS
1	A	812	GLN
1	A	763	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides 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 ⓘ

6.1 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, 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(Å²)	Q<0.9
1	A	238/273 (87%)	0.54	28 (11%)	4	5	20, 26, 36, 48	1 (0%)
2	P	12/12 (100%)	4.78	10 (83%)	0	0	22, 25, 32, 32	0
All	All	250/285 (87%)	0.74	38 (15%)	2	2	20, 26, 35, 48	1 (0%)

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	851	PRO	9.2
2	P	842	ASN	7.5
2	P	840	PRO	7.2
2	P	841	ASN	6.9
1	A	767	ASN	5.8

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.

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