wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 09:38 PM GMT

PDB ID	:	1PZ8
Title	:	Modulation of agrin function by alternative splicing and Ca2+ binding
Authors	:	Stetefeld, J.; Alexandrescu, A.T.; Maciejewski, M.W.; Jenny, M.; Rathgeb-Szabo, K.; Schulthess, T.; Landwehr, R.; Frank, S.; Ruegg, M.A.; Kammerer, R.A.
Deposited on	:	2003-07-10
Resolution	:	2.35 Å(reported)

This is a wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

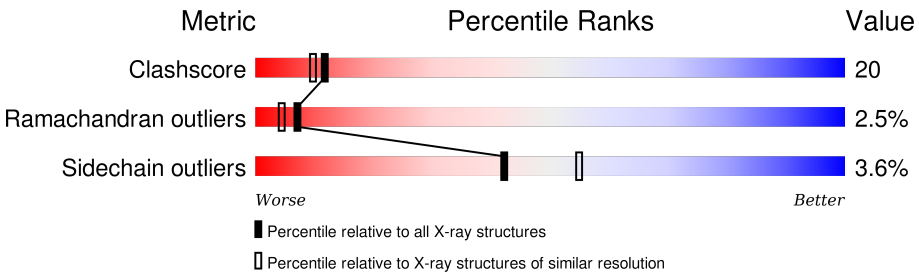
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.35 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))
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)

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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	201	57% 27% • 12%
1	B	201	65% 18% • • 11%
1	C	201	67% 17% • 12%
1	D	201	63% 19% 5% 12%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6058 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 Agrin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	176	1365	863	238	258	6	0	0	0
			Total	C	N	O	S			
1	B	179	1385	874	241	264	6	0	0	0
			Total	C	N	O	S			
1	C	176	1365	863	238	258	6	0	0	0
			Total	C	N	O	S			
1	D	177	1370	866	239	259	6	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	HIS	PRO	SEE REMARK 999	UNP P31696
A	34	LEU	ASP	SEE REMARK 999	UNP P31696
A	35	SER	ALA	SEE REMARK 999	UNP P31696
A	36	ASN	LEU	SEE REMARK 999	UNP P31696
A	37	GLU	ASP	SEE REMARK 999	UNP P31696
A	38	ILE	TYR	SEE REMARK 999	UNP P31696
A	42	-	PRO	SEE REMARK 999	UNP P31696
A	43	-	SER	SEE REMARK 999	UNP P31696
A	44	-	GLU	SEE REMARK 999	UNP P31696
B	33	HIS	PRO	SEE REMARK 999	UNP P31696
B	34	LEU	ASP	SEE REMARK 999	UNP P31696
B	35	SER	ALA	SEE REMARK 999	UNP P31696
B	36	ASN	LEU	SEE REMARK 999	UNP P31696
B	37	GLU	ASP	SEE REMARK 999	UNP P31696
B	38	ILE	TYR	SEE REMARK 999	UNP P31696
B	42	-	PRO	SEE REMARK 999	UNP P31696
B	43	-	SER	SEE REMARK 999	UNP P31696
B	44	-	GLU	SEE REMARK 999	UNP P31696
C	33	HIS	PRO	SEE REMARK 999	UNP P31696
C	34	LEU	ASP	SEE REMARK 999	UNP P31696
C	35	SER	ALA	SEE REMARK 999	UNP P31696

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Chain	Residue	Modelled	Actual	Comment	Reference
C	36	ASN	LEU	SEE REMARK 999	UNP P31696
C	37	GLU	ASP	SEE REMARK 999	UNP P31696
C	38	ILE	TYR	SEE REMARK 999	UNP P31696
C	42	-	PRO	SEE REMARK 999	UNP P31696
C	43	-	SER	SEE REMARK 999	UNP P31696
C	44	-	GLU	SEE REMARK 999	UNP P31696
D	33	HIS	PRO	SEE REMARK 999	UNP P31696
D	34	LEU	ASP	SEE REMARK 999	UNP P31696
D	35	SER	ALA	SEE REMARK 999	UNP P31696
D	36	ASN	LEU	SEE REMARK 999	UNP P31696
D	37	GLU	ASP	SEE REMARK 999	UNP P31696
D	38	ILE	TYR	SEE REMARK 999	UNP P31696
D	42	-	PRO	SEE REMARK 999	UNP P31696
D	43	-	SER	SEE REMARK 999	UNP P31696
D	44	-	GLU	SEE REMARK 999	UNP P31696

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Ca 1 1	0	0
2	A	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	155	Total O 155 155	0	0
3	B	150	Total O 150 150	0	0
3	C	143	Total O 143 143	0	0
3	D	121	Total O 121 121	0	0

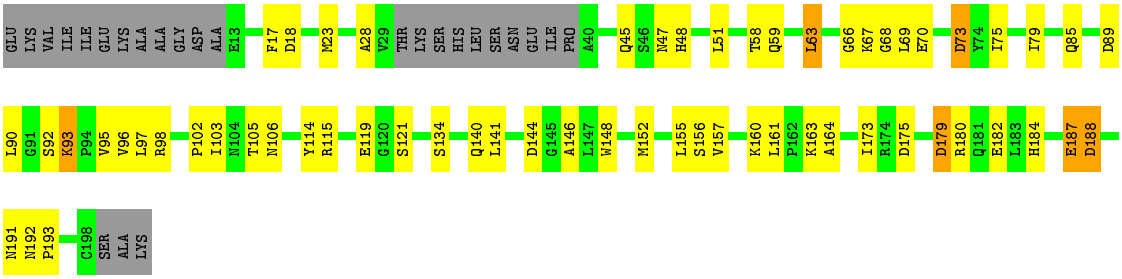
3 Residue-property plots (i)

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.

Note EDS was not executed.

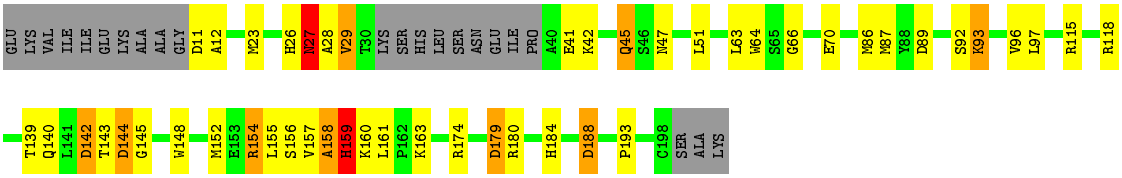
- Molecule 1: Agrin

Chain A:



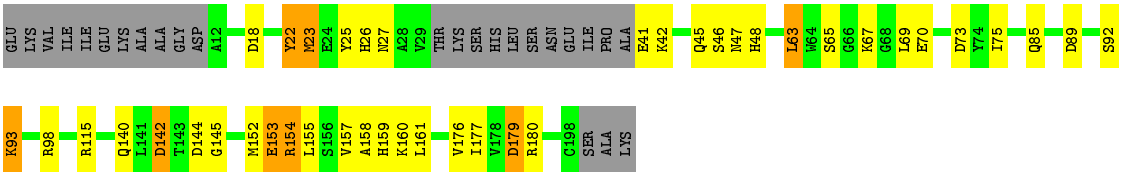
- Molecule 1: Agrin

Chain B:



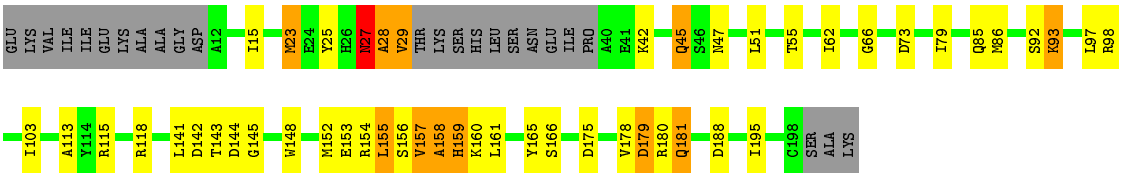
- Molecule 1: Agrin

Chain C:



- Molecule 1: Agrin

Chain D:


GLU
LYS
VAL
ILE
ILE
GLU
LYS
ALA
ALA
GLY
ASP
A12
I15
M23
E24
Y25
H26
M27
A28
V29
THR
LYS
SER
HIS
LEU
SER
ASN
GLU
ILE
PRO
A40
E41
K42
Q45
S46
N47
L51
T55
I62
G66
D73
I79
Q85
M86
S92
K93
L97
R98
I103
A113
Y114
R115
R118
L141
D142
T143
D144
G145
W148
M152
E153
R154
L155
S156
V157
A158
H159
K160
L161
Y165
S166
D175
V178
D179
R180
Q181
D188
I195
C198
SER
ALA
LYS

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.85Å 56.56Å 84.59Å 90.00° 99.75° 90.00°	Depositor
Resolution (Å)	20.00 – 2.35	Depositor
% Data completeness (in resolution range)	100.0 (20.00-2.35)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.218 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6058	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

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: CA

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	0.65	0/1392	0.83	6/1888 (0.3%)
1	B	0.71	0/1412	0.89	6/1916 (0.3%)
1	C	0.74	0/1392	0.89	6/1888 (0.3%)
1	D	0.78	0/1397	0.97	9/1895 (0.5%)
All	All	0.72	0/5593	0.90	27/7587 (0.4%)

There are no bond length outliers.

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	175	ASP	CB-CG-OD2	8.44	125.90	118.30
1	C	144	ASP	CB-CG-OD2	8.01	125.51	118.30
1	B	188	ASP	CB-CG-OD2	7.88	125.40	118.30
1	C	89	ASP	CB-CG-OD2	7.86	125.37	118.30
1	B	89	ASP	CB-CG-OD2	7.52	125.06	118.30

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	1365	0	1349	62	0
1	B	1385	0	1365	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1365	0	1349	57	0
1	D	1370	0	1354	57	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	155	0	0	14	0
3	B	150	0	0	9	0
3	C	143	0	0	13	0
3	D	121	0	0	4	0
All	All	6058	0	5417	220	0

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 20.

The worst 5 of 220 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:D:29:VAL:CG1	1:D:181:GLN:HB3	1.62	1.28
1:D:29:VAL:HG22	1:D:181:GLN:CG	1.64	1.26
1:D:29:VAL:HG13	1:D:181:GLN:CB	1.79	1.12
1:D:27:ASN:OD1	1:D:145:GLY:HA3	1.58	1.01
1:D:29:VAL:HG22	1:D:181:GLN:HG2	1.00	1.00

There are no symmetry-related clashes.

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	172/201 (86%)	157 (91%)	12 (7%)	3 (2%)	11 9
1	B	175/201 (87%)	158 (90%)	11 (6%)	6 (3%)	5 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	172/201 (86%)	160 (93%)	10 (6%)	2 (1%)	16	15
1	D	173/201 (86%)	159 (92%)	8 (5%)	6 (4%)	4	2
All	All	692/804 (86%)	634 (92%)	41 (6%)	17 (2%)	7	4

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	28	ALA
1	B	29	VAL
1	B	159	HIS
1	D	27	ASN
1	D	28	ALA

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	146/166 (88%)	143 (98%)	3 (2%)	61	76
1	B	148/166 (89%)	142 (96%)	6 (4%)	37	48
1	C	146/166 (88%)	142 (97%)	4 (3%)	52	67
1	D	146/166 (88%)	138 (94%)	8 (6%)	27	32
All	All	586/664 (88%)	565 (96%)	21 (4%)	42	55

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	22	TYR
1	C	63	LEU
1	D	143	THR
1	B	159	HIS
1	D	155	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	181	GLN
1	C	85	GLN
1	D	123	GLN
1	C	47	ASN
1	A	123	GLN

5.3.3 RNA (i)

There are no RNA molecules 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 (i)

Of 4 ligands modelled in this entry, 4 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.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.