wwPDB EM Map/Model Validation Report (i)

May 16, 2016 – 05:51 PM EDT

PDB ID	:	3JD6
EMDB ID:	:	EMD-6425
Title	:	Double octamer structure of retinoschisin, a cell-cell adhesion protein of the retina
Authors	:	Tolun, G.; Vijayasarathy, C.; Huang, R.; Zeng, Y.; Li, Y.; Steven, A.C.; Sieving, P.A.; Heymann, J.B.
Deposited on	:	2016-04-12
Resolution	:	4.10 Å(reported)
Based on PDB ID	:	1SDD

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

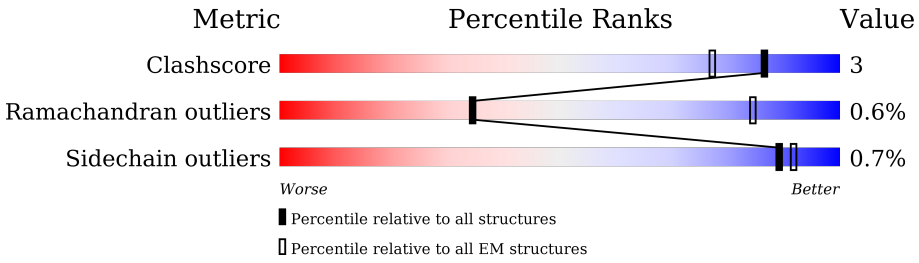
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027457

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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%

Mol	Chain	Length	Quality of chain
1	O	207	70% 11% 19%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2693 atoms, of which 1326 are hydrogens and 0 are deuteriums.

In the tables below, 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 Retinoschisin.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	O	167	2693	869	1326	237	252	9	0	0

There are 6 discrepancies between the modelled and reference sequences:

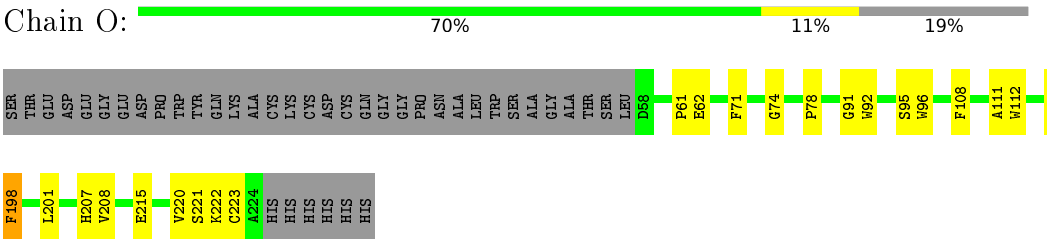
Chain	Residue	Modelled	Actual	Comment	Reference
O	225	HIS	-	EXPRESSION TAG	UNP O15537
O	226	HIS	-	EXPRESSION TAG	UNP O15537
O	227	HIS	-	EXPRESSION TAG	UNP O15537
O	228	HIS	-	EXPRESSION TAG	UNP O15537
O	229	HIS	-	EXPRESSION TAG	UNP O15537
O	230	HIS	-	EXPRESSION TAG	UNP O15537

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. 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: Retinoschisin

Chain O:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D	Depositor
Number of images	9096	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Included in iterative refinement	Depositor
Microscope	FEI POLARA F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	30	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	39000	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor

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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	O	1.34	6/1403 (0.4%)	1.37	7/1905 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	O	0	3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	112	TRP	CD2-CE3	-6.38	1.30	1.40
1	O	201	LEU	N-CA	-5.68	1.34	1.46
1	O	112	TRP	CD2-CE2	5.55	1.48	1.41
1	O	178	GLY	CA-C	-5.49	1.43	1.51
1	O	198	PHE	CB-CG	5.36	1.60	1.51

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	111	ALA	N-CA-CB	6.62	119.37	110.10
1	O	156	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	O	156	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	O	220	VAL	N-CA-C	-6.35	93.86	111.00
1	O	112	TRP	CA-CB-CG	5.67	124.47	113.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	O	221	SER	Peptide
1	O	62	GLU	Peptide
1	O	95	SER	Peptide

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	O	1367	1326	1327	7	0
All	All	1367	1326	1327	7	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 3.

The worst 5 of 7 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:O:222:LYS:O	1:O:223:CYS:HB2	2.12	0.49
1:O:207:HIS:O	1:O:208:VAL:HB	2.16	0.46
1:O:91:GLY:O	1:O:92:TRP:HB2	2.17	0.44
1:O:108:PHE:O	1:O:108:PHE:CG	2.71	0.44
1:O:222:LYS:O	1:O:223:CYS:CB	2.68	0.42

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 PDB entries followed by that with respect to all EM entries.

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	O	165/207 (80%)	142 (86%)	22 (13%)	1 (1%)	30 73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	61	PRO

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 PDB entries followed by that with respect to all EM entries.

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	O	152/184 (83%)	151 (99%)	1 (1%)	88 94

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	198	PHE

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)

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.