Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	2WA0
Title	:	Crystal structure of the human MAGEA4
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Deposited on	:	2009-01-31
Resolution	:	2.30 Å(reported)

This is a full wwPDB validation 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

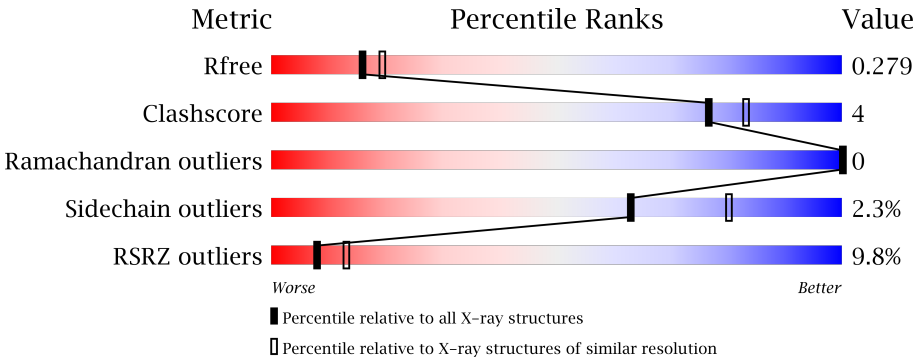
The following versions of software and data (see references) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.17 November 2013
Xtriage (Phenix)	:	dev-1439
EDS	:	stable24195
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.1.3
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable24195

1 Overall quality at a glance

The reported resolution of this entry is 2.30 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	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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	240	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1749 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 MELANOMA-ASSOCIATED ANTIGEN 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	214	1707	1103	280	317	7	0	3	0

- Molecule 2 is water.

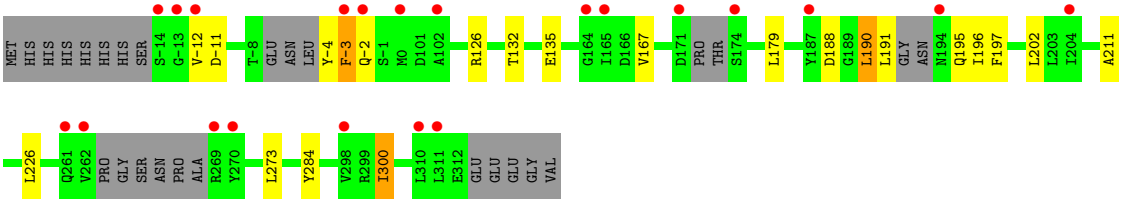
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	42	42	42	0	0

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: MELANOMA-ASSOCIATED ANTIGEN 4

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	81.63Å 81.63Å 210.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.81 – 2.30 40.82 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.81-2.30) 99.6 (40.82-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0070	Depositor
R, R_{free}	0.243 , 0.274 0.240 , 0.279	Depositor DCC
R_{free} test set	978 reflections (5.36%)	DCC
Wilson B-factor (Å^2)	55.0	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 34.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 19238 reflections (0.005%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	1749	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.86% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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	0.70	0/1746	0.72	0/2356

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	A	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	-2	GLN	Peptide
1	A	-3	PHE	Peptide

5.2 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 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	1707	0	1701	13	0
2	A	42	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	1749	0	1701	13	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 4.

All (13) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:167:VAL:HG22	1:A:179:LEU:HD22	1.71	0.73
1:A:196:ILE:HG23	1:A:197:PHE:H	1.67	0.58
1:A:132[A]:THR:HG23	1:A:135:GLU:H	1.70	0.57
1:A:126:ARG:HD3	1:A:195:GLN:O	2.05	0.57
1:A:188:ASP:CG	1:A:190:LEU:HD22	2.26	0.56
1:A:167:VAL:HG22	1:A:179:LEU:CD2	2.41	0.49
1:A:202:LEU:HD11	1:A:226:LEU:HD22	1.93	0.49
1:A:126:ARG:NH2	1:A:196:ILE:HG13	2.28	0.48
1:A:-4:TYR:HA	1:A:-3:PHE:HA	1.68	0.47
1:A:132[A]:THR:HG23	1:A:135:GLU:HB2	1.97	0.47
1:A:211:ALA:HA	1:A:284:TYR:CE1	2.52	0.45
1:A:300:ILE:H	1:A:300:ILE:HD12	1.86	0.41
1:A:-12:VAL:HG23	1:A:-11:ASP:N	2.36	0.40

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	207/240 (86%)	192 (93%)	15 (7%)	0	100 100

There are no Ramachandran outliers to report.

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	179/208 (86%)	175 (98%)	4 (2%)	64 81

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	190	LEU
1	A	191	LEU
1	A	273	LEU
1	A	300	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

There are no RNA chains 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 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

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, 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	A	214/240 (89%)	0.67	21 (9%) 8 13	27, 44, 73, 81	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	0	MET	6.0
1	A	171	ASP	4.7
1	A	262	VAL	4.3
1	A	269	ARG	4.1
1	A	-12	VAL	3.5
1	A	298	VAL	3.4
1	A	261	GLN	3.3
1	A	-13	GLY	3.3
1	A	194	ASN	2.8
1	A	-14	SER	2.7
1	A	174	SER	2.7
1	A	187	TYR	2.6
1	A	310	LEU	2.5
1	A	204	ILE	2.4
1	A	164	GLY	2.3
1	A	-3	PHE	2.3
1	A	270	TYR	2.2
1	A	165	ILE	2.2
1	A	102	ALA	2.2
1	A	-2	GLN	2.1
1	A	311	LEU	2.1

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 carbohydrates 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.