wwPDB X-ray Structure Validation Summary Report (i)

Apr 25, 2022 – 01:02 am BST

PDB ID	:	7OAD
Title	:	conserved hypothetical protein residues 311-335 from Candidatus Magnetomorum sp. HK-1 fused to GCN4 adaptors, mutant beta1/A, crystal form II
Authors	:	Adlakha, J.; Albrecht, R.; Hartmann, M.D.
Deposited on	:	2021-04-19
Resolution	:	2.00 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

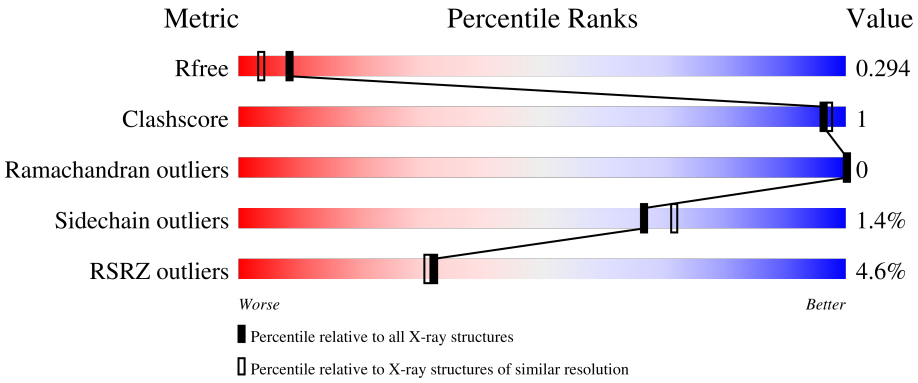
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.28
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

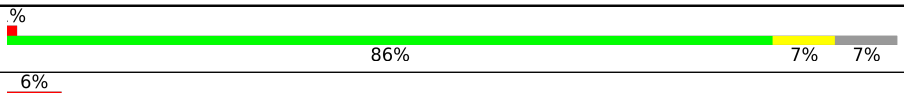
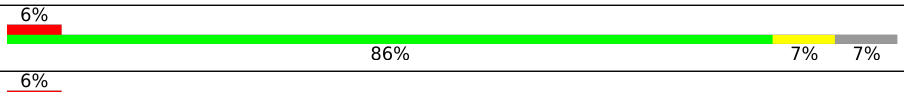
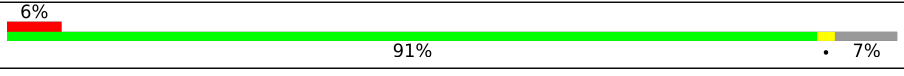
The reported resolution of this entry is 2.00 Å.

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	86	
1	B	86	
1	C	86	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4141 atoms, of which 2127 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 General control transcription factor GCN4,conserved hypothetical protein residues 311-335 from Candidatus Magnetomorum sp. HK-1 fused to GCN4 adaptors, mutant beta1/A,General control transcription factor GCN4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	80	Total	C	H	N	O	S	10	0	0
			1378	428	709	113	125	3			
1	B	80	Total	C	H	N	O	S	10	0	0
			1378	428	709	113	125	3			
1	C	80	Total	C	H	N	O	S	10	0	0
			1378	428	709	113	125	3			

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	278	GLY	-	expression tag	UNP P03069
A	279	GLY	-	expression tag	UNP P03069
A	280	GLY	-	expression tag	UNP P03069
A	281	SER	-	expression tag	UNP P03069
A	282	GLY	-	expression tag	UNP P03069
A	286	ILE	LEU	engineered mutation	UNP P03069
A	288	MET	ASP	engineered mutation	UNP P03069
A	290	ILE	VAL	engineered mutation	UNP P03069
A	293	ILE	LEU	engineered mutation	UNP P03069
A	297	ILE	ASN	engineered mutation	UNP P03069
A	300	ILE	LEU	engineered mutation	UNP P03069
A	304	ILE	VAL	engineered mutation	UNP P03069
A	307	ILE	LEU	engineered mutation	UNP P03069
A	320	ALA	VAL	engineered mutation	UNP A0A0N0D484
A	326	ALA	LEU	engineered mutation	UNP A0A0N0D484
A	339	ILE	LEU	engineered mutation	UNP P03069
A	341	TRP	ASP	engineered mutation	UNP P03069
A	343	ILE	VAL	engineered mutation	UNP P03069
A	346	ILE	LEU	engineered mutation	UNP P03069
A	350	ILE	ASN	engineered mutation	UNP P03069
A	353	ILE	LEU	engineered mutation	UNP P03069

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Chain	Residue	Modelled	Actual	Comment	Reference
A	357	ILE	VAL	engineered mutation	UNP P03069
A	360	ILE	LEU	engineered mutation	UNP P03069
B	278	GLY	-	expression tag	UNP P03069
B	279	GLY	-	expression tag	UNP P03069
B	280	GLY	-	expression tag	UNP P03069
B	281	SER	-	expression tag	UNP P03069
B	282	GLY	-	expression tag	UNP P03069
B	286	ILE	LEU	engineered mutation	UNP P03069
B	288	MET	ASP	engineered mutation	UNP P03069
B	290	ILE	VAL	engineered mutation	UNP P03069
B	293	ILE	LEU	engineered mutation	UNP P03069
B	297	ILE	ASN	engineered mutation	UNP P03069
B	300	ILE	LEU	engineered mutation	UNP P03069
B	304	ILE	VAL	engineered mutation	UNP P03069
B	307	ILE	LEU	engineered mutation	UNP P03069
B	320	ALA	VAL	engineered mutation	UNP A0A0N0D484
B	326	ALA	LEU	engineered mutation	UNP A0A0N0D484
B	339	ILE	LEU	engineered mutation	UNP P03069
B	341	TRP	ASP	engineered mutation	UNP P03069
B	343	ILE	VAL	engineered mutation	UNP P03069
B	346	ILE	LEU	engineered mutation	UNP P03069
B	350	ILE	ASN	engineered mutation	UNP P03069
B	353	ILE	LEU	engineered mutation	UNP P03069
B	357	ILE	VAL	engineered mutation	UNP P03069
B	360	ILE	LEU	engineered mutation	UNP P03069
C	278	GLY	-	expression tag	UNP P03069
C	279	GLY	-	expression tag	UNP P03069
C	280	GLY	-	expression tag	UNP P03069
C	281	SER	-	expression tag	UNP P03069
C	282	GLY	-	expression tag	UNP P03069
C	286	ILE	LEU	engineered mutation	UNP P03069
C	288	MET	ASP	engineered mutation	UNP P03069
C	290	ILE	VAL	engineered mutation	UNP P03069
C	293	ILE	LEU	engineered mutation	UNP P03069
C	297	ILE	ASN	engineered mutation	UNP P03069
C	300	ILE	LEU	engineered mutation	UNP P03069
C	304	ILE	VAL	engineered mutation	UNP P03069
C	307	ILE	LEU	engineered mutation	UNP P03069
C	320	ALA	VAL	engineered mutation	UNP A0A0N0D484
C	326	ALA	LEU	engineered mutation	UNP A0A0N0D484
C	339	ILE	LEU	engineered mutation	UNP P03069
C	341	TRP	ASP	engineered mutation	UNP P03069

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Chain	Residue	Modelled	Actual	Comment	Reference
C	343	ILE	VAL	engineered mutation	UNP P03069
C	346	ILE	LEU	engineered mutation	UNP P03069
C	350	ILE	ASN	engineered mutation	UNP P03069
C	353	ILE	LEU	engineered mutation	UNP P03069
C	357	ILE	VAL	engineered mutation	UNP P03069
C	360	ILE	LEU	engineered mutation	UNP P03069

- Molecule 2 is water.

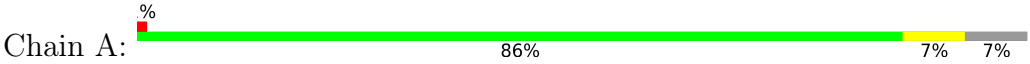
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total O 3 3	0	0
2	B	3	Total O 3 3	0	0
2	C	1	Total O 1 1	0	0

3 Residue-property plots (i)

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.

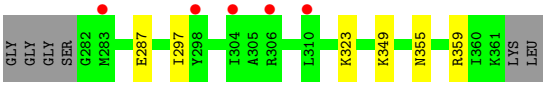
• Molecule 1: General control transcription factor GCN4,conserved hypothetical protein residues 311-335 from Candidatus Magnetomorum sp. HK-1 fused to GCN4 adaptors, mutant beta1/A,General control transcription factor GCN4

Chain A:



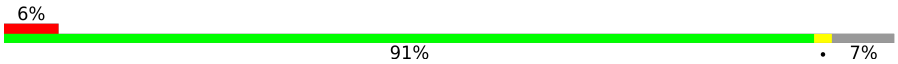
• Molecule 1: General control transcription factor GCN4,conserved hypothetical protein residues 311-335 from Candidatus Magnetomorum sp. HK-1 fused to GCN4 adaptors, mutant beta1/A,General control transcription factor GCN4

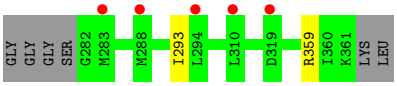
Chain B:



• Molecule 1: General control transcription factor GCN4,conserved hypothetical protein residues 311-335 from Candidatus Magnetomorum sp. HK-1 fused to GCN4 adaptors, mutant beta1/A,General control transcription factor GCN4

Chain C:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	36.35Å 38.56Å 99.25Å 90.00° 98.88° 90.00°	Depositor
Resolution (Å)	49.03 – 2.00 49.03 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.03-2.00) 99.7 (49.03-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0049 2013/06/30	Depositor
R, R_{free}	0.254 , 0.294 0.258 , 0.294	Depositor DCC
R_{free} test set	933 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	49.5	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4141	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[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	0.60	0/676	0.73	1/901 (0.1%)
1	B	0.61	0/676	0.69	1/901 (0.1%)
1	C	0.54	0/676	0.72	1/901 (0.1%)
All	All	0.58	0/2028	0.71	3/2703 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	359	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	B	359	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	A	306	ARG	NE-CZ-NH1	5.40	123.00	120.30

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	669	709	706	4	0
1	B	669	709	706	3	0
1	C	669	709	706	1	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	1	0	0	0	0
All	All	2014	2127	2118	4	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 1.

All (4) 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:286:ILE:HD11	1:B:287:GLU:HG3	1.82	0.62
1:A:293:ILE:HG23	1:B:297:ILE:HD11	1.94	0.48
1:A:297:ILE:HD11	1:C:293:ILE:HG23	1.99	0.44
1:A:321:TYR:CE2	1:B:323:LYS:HA	2.53	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 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	78/86 (91%)	78 (100%)	0	0	100	100
1	B	78/86 (91%)	78 (100%)	0	0	100	100
1	C	78/86 (91%)	78 (100%)	0	0	100	100
All	All	234/258 (91%)	234 (100%)	0	0	100	100

There are no Ramachandran outliers to report.

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	73/76 (96%)	72 (99%)	1 (1%)	67 72
1	B	73/76 (96%)	71 (97%)	2 (3%)	44 46
1	C	73/76 (96%)	73 (100%)	0	100 100
All	All	219/228 (96%)	216 (99%)	3 (1%)	67 72

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	302	ASN
1	B	349	LYS
1	B	355	ASN

Sometimes 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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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

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	80/86 (93%)	0.40	1 (1%)	77	76	41, 69, 100, 113	0
1	B	80/86 (93%)	0.69	5 (6%)	20	19	43, 79, 103, 116	0
1	C	80/86 (93%)	0.65	5 (6%)	20	19	50, 73, 105, 118	0
All	All	240/258 (93%)	0.58	11 (4%)	32	31	41, 74, 104, 118	0

The worst 5 of 11 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	283	MET	4.3
1	A	310	LEU	3.1
1	B	310	LEU	3.0
1	C	319	ASP	2.6
1	B	283	MET	2.5

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 (i)

There are no such residues in this entry.