



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2014 – 05:51 PM GMT

PDB ID : 4CEM
Title : Crystal structure of the first MIF4G domain of human nonsense mediated decay factor UPF2
Authors : Clerici, M.; Deniaud, A.; Boehm, V.; Gehring, N.H.; Schaffitzel, C.; Cusack, S.
Deposited on : 2013-11-11
Resolution : 2.60 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>

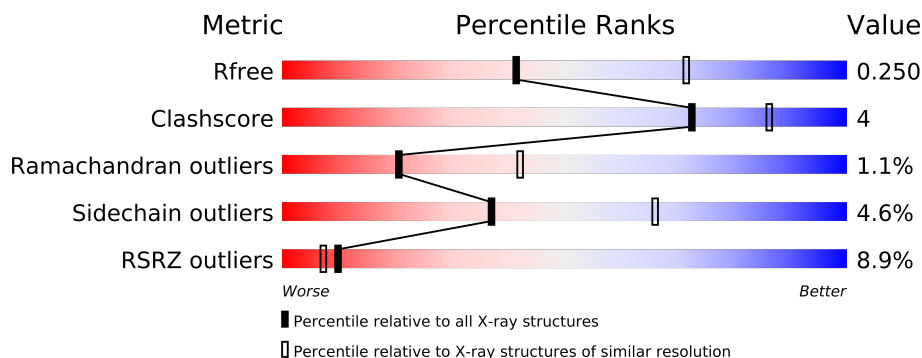
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : trunk22714
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk22714

1 Overall quality at a glance

The reported resolution of this entry is 2.60 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	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)

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	370	
1	B	370	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5115 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 REGULATOR OF NONSENSE TRANSCRIPTS 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	Se	0	0	0
			2526	1588	456	475	4	3			
1	B	309	Total	C	N	O	S	Se	0	0	0
			2535	1593	458	477	4	3			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	117	GLY	-	EXPRESSION TAG	UNP Q9HAU5
A	118	ALA	-	EXPRESSION TAG	UNP Q9HAU5
A	119	MSE	-	EXPRESSION TAG	UNP Q9HAU5
A	120	GLY	-	EXPRESSION TAG	UNP Q9HAU5
A	168	ILE	LEU	CONFLICT	UNP Q9HAU5
B	117	GLY	-	EXPRESSION TAG	UNP Q9HAU5
B	118	ALA	-	EXPRESSION TAG	UNP Q9HAU5
B	119	MSE	-	EXPRESSION TAG	UNP Q9HAU5
B	120	GLY	-	EXPRESSION TAG	UNP Q9HAU5
B	168	ILE	LEU	CONFLICT	UNP Q9HAU5

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	20	Total	O	0	0
			20	20		
2	B	34	Total	O	0	0
			34	34		

4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	101.08Å 101.08Å 158.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	87.54 – 2.60 48.16 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (87.54-2.60) 99.9 (48.16-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.6.0116	Depositor
R, R_{free}	0.205 , 0.251 0.209 , 0.250	Depositor DCC
R_{free} test set	1428 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	46.1	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 28.4	EDS
Estimated twinning fraction	0.058 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 28218 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5115	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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	0.48	0/2573	0.55	0/3457
1	B	0.49	0/2582	0.59	0/3469
All	All	0.48	0/5155	0.57	0/6926

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2526	0	2528	23	0
1	B	2535	0	2536	20	0
2	A	20	0	0	1	0
2	B	34	0	0	3	0
All	All	5115	0	5064	43	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 (43) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:414:GLN:HA	1:A:424:MSE:HE1	1.53	0.89

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:384:ILE:HG22	1:B:384:ILE:O	1.94	0.67
1:A:148:ASN:HD22	1:A:275:VAL:HG13	1.59	0.67
1:A:148:ASN:ND2	1:A:275:VAL:HG13	2.11	0.65
1:A:141:ARG:HD3	1:A:274:ILE:HG21	1.78	0.65
1:A:404:MSE:HE2	1:A:408:LYS:HE3	1.80	0.64
1:B:148:ASN:HD22	1:B:275:VAL:HG13	1.63	0.63
1:A:414:GLN:HG2	1:A:424:MSE:HE3	1.82	0.61
1:A:364:THR:HG23	1:A:425:PRO:HG3	1.83	0.61
1:B:148:ASN:ND2	1:B:275:VAL:HG13	2.18	0.58
1:A:182:THR:HG23	1:A:184:GLN:OE1	2.05	0.56
1:B:182:THR:HG21	2:B:2006:HOH:O	2.05	0.56
1:B:182:THR:HG23	1:B:184:GLN:OE1	2.06	0.55
1:B:237:ALA:HB3	1:B:238:PRO:HD3	1.87	0.55
1:B:214:LEU:HB2	1:B:264:THR:HG21	1.90	0.52
1:B:168:ILE:HD12	1:B:168:ILE:H	1.74	0.51
1:A:159:ASN:OD1	1:A:160:PHE:N	2.44	0.51
1:A:414:GLN:HA	1:A:424:MSE:CE	2.34	0.50
1:A:237:ALA:HB3	1:A:238:PRO:HD3	1.92	0.50
1:A:239:SER:O	1:A:243:VAL:HG23	2.11	0.50
1:A:128:ILE:HG23	2:A:2002:HOH:O	2.12	0.49
1:B:219:VAL:HG21	1:B:267:ARG:HD3	1.93	0.49
1:B:275:VAL:O	1:B:275:VAL:HG13	2.13	0.48
1:A:295:ILE:HD11	1:A:355:LEU:O	2.13	0.48
1:B:270:ALA:HA	1:B:287:ILE:HD11	1.95	0.47
1:A:315:CYS:HB3	1:A:319:ILE:HD12	1.97	0.46
1:B:271:GLU:O	1:B:275:VAL:HB	2.16	0.46
1:B:141:ARG:HD3	1:B:274:ILE:HG21	1.98	0.45
1:B:384:ILE:HG21	1:B:391:LEU:HD23	1.99	0.44
1:B:242:GLN:HG3	2:B:2019:HOH:O	2.17	0.44
1:B:251:ARG:HD2	2:B:2021:HOH:O	2.18	0.44
1:A:424:MSE:HB2	1:A:424:MSE:HE2	1.74	0.44
1:B:302:HIS:O	1:B:305:VAL:HG22	2.18	0.43
1:A:384:ILE:HD12	1:A:395:ARG:HH12	1.84	0.43
1:B:399:TYR:O	1:B:403:ALA:N	2.50	0.42
1:B:144:LEU:HB3	1:B:275:VAL:HG22	2.01	0.42
1:A:259:ILE:HG23	1:A:307:VAL:CG2	2.49	0.42
1:A:384:ILE:HG22	1:A:384:ILE:O	2.19	0.42
1:A:350:GLN:HB3	1:A:351:PRO:HD3	2.02	0.42
1:A:266:LEU:HD23	1:A:311:PHE:HB2	2.02	0.42
1:B:182:THR:CG2	1:B:184:GLN:HG2	2.50	0.41
1:A:302:HIS:O	1:A:305:VAL:HG23	2.21	0.41
1:A:270:ALA:HA	1:A:287:ILE:HD11	2.02	0.41

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	306/370 (83%)	290 (95%)	12 (4%)	4 (1%)	18	35
1	B	307/370 (83%)	294 (96%)	10 (3%)	3 (1%)	22	45
All	All	613/740 (83%)	584 (95%)	22 (4%)	7 (1%)	21	42

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	393	GLU
1	A	389	GLY
1	A	391	LEU
1	A	393	GLU
1	B	389	GLY
1	B	391	LEU
1	A	256	THR

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	283/329 (86%)	273 (96%)	10 (4%)	48	77
1	B	284/329 (86%)	268 (94%)	16 (6%)	30	55
All	All	567/658 (86%)	541 (95%)	26 (5%)	37	66

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	157	GLU
1	A	165	ASP
1	A	182	THR
1	A	184	GLN
1	A	242	GLN
1	A	268	PHE
1	A	275	VAL
1	A	291	LEU
1	A	364	THR
1	A	386	HIS
1	B	121	MSE
1	B	157	GLU
1	B	165	ASP
1	B	176	LYS
1	B	177	LYS
1	B	182	THR
1	B	184	GLN
1	B	215	LYS
1	B	255	LYS
1	B	268	PHE
1	B	275	VAL
1	B	291	LEU
1	B	300	GLU
1	B	305	VAL
1	B	364	THR
1	B	402	PHE

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, 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(Å ²)	Q<0.9
1	A	308/370 (83%)	0.44	30 (9%) 8 6	31, 49, 116, 148	0
1	B	309/370 (83%)	0.30	25 (8%) 12 9	27, 40, 109, 141	0
All	All	617/740 (83%)	0.37	55 (8%) 10 7	27, 44, 113, 148	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	390	GLU	10.7
1	B	391	LEU	8.4
1	A	391	LEU	8.1
1	A	386	HIS	7.3
1	A	388	LYS	7.0
1	B	392	SER	6.8
1	A	389	GLY	6.8
1	B	385	LEU	6.5
1	B	383	ARG	5.8
1	A	382	ARG	5.8
1	B	382	ARG	5.7
1	A	387	SER	5.7
1	B	381	ASN	5.7
1	B	389	GLY	5.5
1	A	384	ILE	5.5
1	B	386	HIS	5.5
1	B	395	ARG	5.4
1	A	379	ARG	5.2
1	B	380	GLN	5.1
1	B	388	LYS	5.1
1	A	399	TYR	5.0
1	B	396	HIS	5.0
1	A	392	SER	5.0
1	B	384	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	396	HIS	4.6
1	A	383	ARG	4.2
1	A	385	LEU	4.2
1	A	377	THR	4.1
1	B	390	GLU	4.0
1	B	393	GLU	3.8
1	A	394	ASP	3.6
1	B	379	ARG	3.6
1	A	375	GLN	3.6
1	A	402	PHE	3.5
1	A	395	ARG	3.4
1	A	374	LEU	3.3
1	B	377	THR	3.1
1	B	399	TYR	3.1
1	B	394	ASP	3.1
1	B	400	GLU	3.0
1	B	387	SER	3.0
1	A	404	MSE	2.8
1	B	402	PHE	2.7
1	B	378	GLU	2.7
1	A	397	LYS	2.7
1	B	398	GLN	2.7
1	B	397	LYS	2.6
1	A	381	ASN	2.5
1	A	378	GLU	2.4
1	A	400	GLU	2.3
1	A	398	GLN	2.3
1	A	380	GLN	2.3
1	A	168	ILE	2.3
1	A	405	SER	2.2
1	A	371	HIS	2.2

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.