



Full wwPDB X-ray Structure Validation Report i

Feb 28, 2014 – 12:49 PM GMT

PDB ID : 3UR3
Title : Structure of the Cmr2 subunit of the CRISPR RNA silencing complex
Authors : Cocozaki, A.I.; Ramia, N.F.; Shao, Y.; Hale, C.R.; Terns, R.M.; Terns, M.P.;
Li, H.
Deposited on : 2011-11-21
Resolution : 2.40 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>

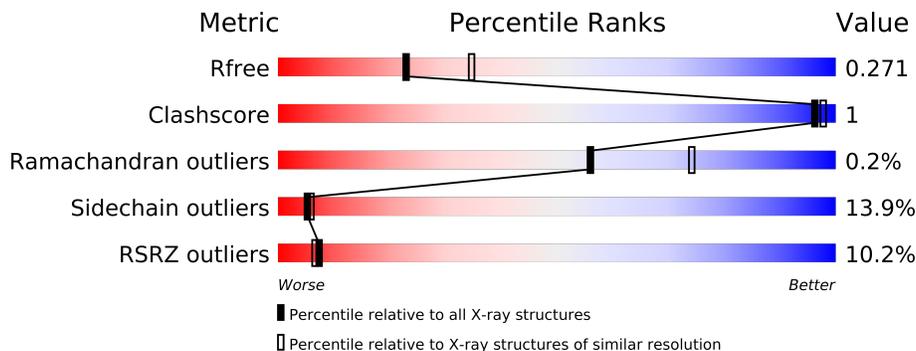
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
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) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.40 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	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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	C	693	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	CA	C	902	-	X

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 4502 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 Cmr2dHD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	548	4470	2907	740	810	13	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	179	MET	-	EXPRESSION TAG	UNP Q8U1S6
C	180	ARG	-	EXPRESSION TAG	UNP Q8U1S6
C	181	GLY	-	EXPRESSION TAG	UNP Q8U1S6
C	182	SER	-	EXPRESSION TAG	UNP Q8U1S6
C	183	HIS	-	EXPRESSION TAG	UNP Q8U1S6
C	184	HIS	-	EXPRESSION TAG	UNP Q8U1S6
C	185	HIS	-	EXPRESSION TAG	UNP Q8U1S6
C	186	HIS	-	EXPRESSION TAG	UNP Q8U1S6
C	187	HIS	-	EXPRESSION TAG	UNP Q8U1S6
C	188	HIS	-	EXPRESSION TAG	UNP Q8U1S6
C	189	GLY	-	EXPRESSION TAG	UNP Q8U1S6
C	190	MET	-	EXPRESSION TAG	UNP Q8U1S6
C	191	ALA	-	EXPRESSION TAG	UNP Q8U1S6
C	192	SER	-	EXPRESSION TAG	UNP Q8U1S6
C	193	MET	-	EXPRESSION TAG	UNP Q8U1S6
C	194	THR	-	EXPRESSION TAG	UNP Q8U1S6
C	195	GLY	-	EXPRESSION TAG	UNP Q8U1S6
C	196	GLY	-	EXPRESSION TAG	UNP Q8U1S6
C	197	GLN	-	EXPRESSION TAG	UNP Q8U1S6
C	198	GLN	-	EXPRESSION TAG	UNP Q8U1S6
C	199	MET	-	EXPRESSION TAG	UNP Q8U1S6
C	200	GLY	-	EXPRESSION TAG	UNP Q8U1S6
C	201	ARG	-	EXPRESSION TAG	UNP Q8U1S6
C	202	ASP	-	EXPRESSION TAG	UNP Q8U1S6
C	203	LEU	-	EXPRESSION TAG	UNP Q8U1S6
C	204	TYR	-	EXPRESSION TAG	UNP Q8U1S6
C	205	ASP	-	EXPRESSION TAG	UNP Q8U1S6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	206	ASP	-	EXPRESSION TAG	UNP Q8U1S6
C	207	ASP	-	EXPRESSION TAG	UNP Q8U1S6
C	208	ASP	-	EXPRESSION TAG	UNP Q8U1S6
C	209	LYS	-	EXPRESSION TAG	UNP Q8U1S6
C	210	ASP	-	EXPRESSION TAG	UNP Q8U1S6
C	211	HIS	-	EXPRESSION TAG	UNP Q8U1S6
C	212	PRO	-	EXPRESSION TAG	UNP Q8U1S6
C	213	PHE	-	EXPRESSION TAG	UNP Q8U1S6
C	214	THR	-	EXPRESSION TAG	UNP Q8U1S6

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	2	Total Ca 2 2	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total Zn 1 1	0	0

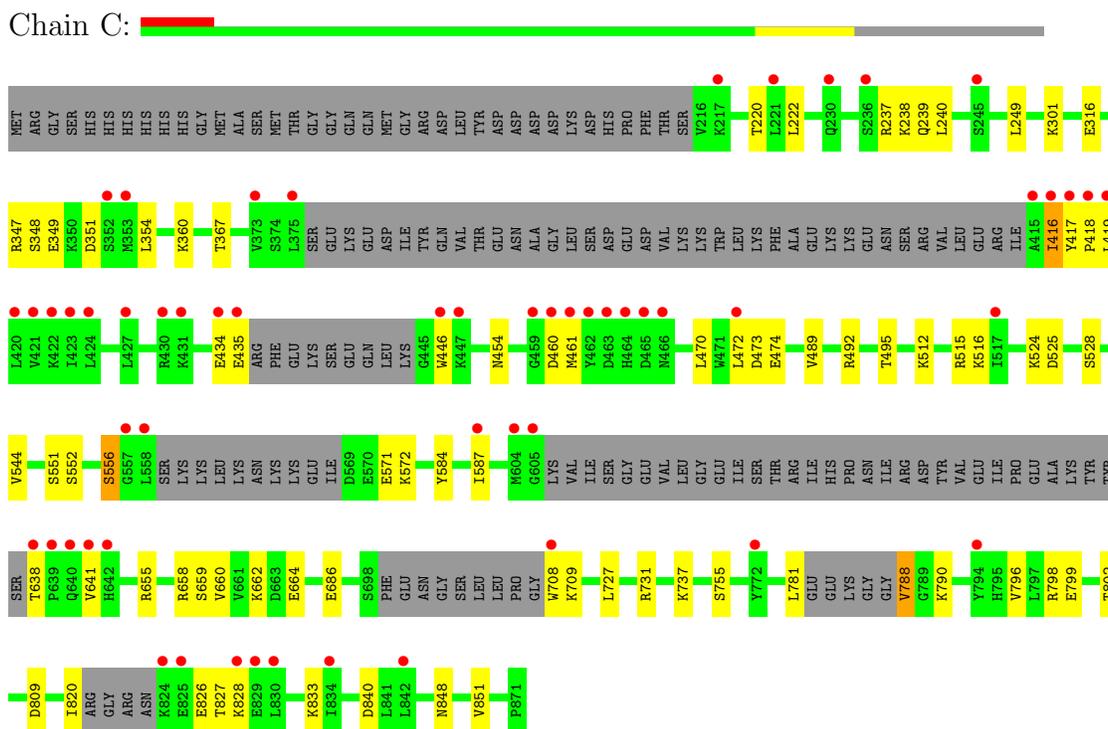
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	29	Total O 29 29	0	0

3 Residue-property plots

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: Cmr2dHD



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.64Å 80.21Å 143.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.68 – 2.40 49.74 – 2.40	Depositor EDS
% Data completeness (in resolution range)	83.9 (42.68-2.40) 82.8 (49.74-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.76 (at 2.39Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.218 , 0.273 0.213 , 0.271	Depositor DCC
R_{free} test set	1851 reflections (6.87%)	DCC
Wilson B-factor (Å ²)	51.7	Xtrriage
Anisotropy	0.722	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 70.8	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Outliers	0 of 29245 reflections	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4502	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	C	0.40	0/4559	0.53	0/6147

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	C	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	C	556	SER	Peptide
1	C	788	VAL	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	C	4470	0	0	5	0
2	C	2	0	0	0	0
3	C	1	0	0	0	0
4	C	29	0	0	0	0
All	All	4502	0	0	5	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 1.

All (5) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:492:ARG:O	1:C:495:THR:O	2.24	0.56
1:C:238:LYS:CD	1:C:239:GLN:N	2.75	0.49
1:C:551:SER:OG	1:C:584:TYR:CE2	2.66	0.47
1:C:799:GLU:O	1:C:802:THR:O	2.33	0.46
1:C:417:TYR:N	1:C:418:PRO:CD	2.80	0.45

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	C	532/693 (77%)	500 (94%)	31 (6%)	1 (0%)	56 74

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	416	ILE

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	C	489/617 (79%)	421 (86%)	68 (14%)	5 6

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	220	THR
1	C	222	LEU
1	C	237	ARG
1	C	240	LEU
1	C	249	LEU
1	C	301	LYS
1	C	316	GLU
1	C	347	ARG
1	C	348	SER
1	C	349	GLU
1	C	351	ASP
1	C	354	LEU
1	C	360	LYS
1	C	367	THR
1	C	416	ILE
1	C	419	LEU
1	C	434	GLU
1	C	435	GLU
1	C	446	TRP
1	C	454	ASN
1	C	460	ASP
1	C	461	MET
1	C	470	LEU
1	C	472	LEU
1	C	473	ASP
1	C	474	GLU
1	C	489	VAL
1	C	512	LYS
1	C	515	ARG
1	C	516	LYS
1	C	524	LYS
1	C	525	ASP
1	C	528	SER
1	C	544	VAL
1	C	552	SER
1	C	556	SER

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Mol	Chain	Res	Type
1	C	571	GLU
1	C	572	LYS
1	C	587	ILE
1	C	638	THR
1	C	641	VAL
1	C	655	ARG
1	C	658	ARG
1	C	659	SER
1	C	660	VAL
1	C	662	LYS
1	C	664	GLU
1	C	686	GLU
1	C	708	TRP
1	C	709	LYS
1	C	727	LEU
1	C	731	ARG
1	C	737	LYS
1	C	755	SER
1	C	781	LEU
1	C	788	VAL
1	C	790	LYS
1	C	796	VAL
1	C	798	ARG
1	C	809	ASP
1	C	820	ILE
1	C	826	GLU
1	C	827	THR
1	C	828	LYS
1	C	833	LYS
1	C	840	ASP
1	C	848	ASN
1	C	851	VAL

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

Of 3 ligands modelled in this entry, 3 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.

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	C	548/693 (79%)	0.63	56 (10%) 7 6	46, 75, 132, 165	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	417	TYR	8.2
1	C	605	GLY	7.9
1	C	446	TRP	7.8
1	C	420	LEU	7.6
1	C	419	LEU	6.8
1	C	641	VAL	6.6
1	C	416	ILE	6.1
1	C	460	ASP	6.0
1	C	461	MET	6.0
1	C	427	LEU	5.6
1	C	418	PRO	5.1
1	C	604	MET	4.7
1	C	421	VAL	4.5
1	C	464	HIS	4.4
1	C	640	GLN	3.8
1	C	465	ASP	3.7
1	C	434	GLU	3.7
1	C	415	ALA	3.7
1	C	517	ILE	3.7
1	C	830	LEU	3.6
1	C	424	LEU	3.5
1	C	463	ASP	3.3
1	C	558	LEU	3.3
1	C	638	THR	3.3
1	C	639	PRO	3.3
1	C	708	TRP	3.1
1	C	422	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	353	MET	3.0
1	C	587	ILE	2.9
1	C	825	GLU	2.9
1	C	447	LYS	2.8
1	C	373	VAL	2.8
1	C	824	LYS	2.8
1	C	230	GLN	2.8
1	C	459	GLY	2.7
1	C	462	TYR	2.6
1	C	375	LEU	2.6
1	C	221	LEU	2.5
1	C	430	ARG	2.5
1	C	217	LYS	2.4
1	C	431	LYS	2.3
1	C	829	GLU	2.3
1	C	435	GLU	2.3
1	C	828	LYS	2.2
1	C	794	TYR	2.2
1	C	466	ASN	2.2
1	C	245	SER	2.2
1	C	352	SER	2.2
1	C	423	ILE	2.1
1	C	842	LEU	2.1
1	C	772	TYR	2.1
1	C	642	HIS	2.1
1	C	557	GLY	2.0
1	C	236	SER	2.0
1	C	834	ILE	2.0
1	C	472	LEU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	CA	C	902	1/1	0.21	3.64	85,85,85,85	0
3	ZN	C	903	1/1	0.17	1.05	96,96,96,96	0
2	CA	C	901	1/1	0.16	-0.35	81,81,81,81	0

6.5 Other polymers

There are no such residues in this entry.