



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 04:00 PM GMT

PDB ID : 3N7N
Title : Structure of Csm1/Lrs4 complex
Authors : Corbett, K.D.; Harrison, S.C.
Deposited on : 2010-05-27
Resolution : 3.90 Å(reported)

This is a wwPDB validation summary 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>

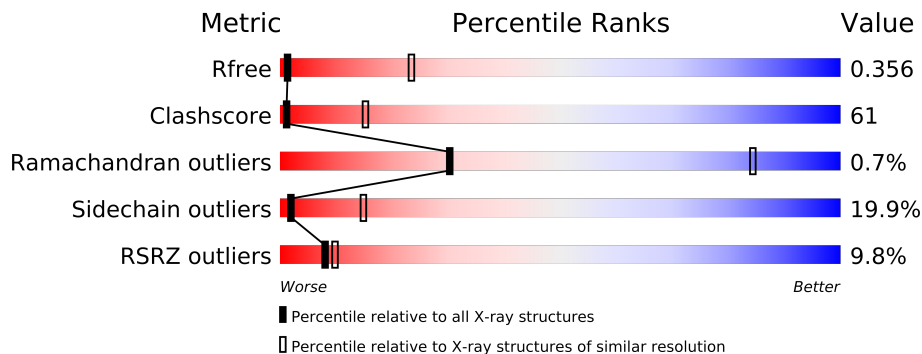
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.90 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	1022 (4.38-3.42)
Clashscore	79885	1173 (4.30-3.50)
Ramachandran outliers	78287	1118 (4.30-3.50)
Sidechain outliers	78261	1107 (4.30-3.50)
RSRZ outliers	66119	1000 (4.36-3.44)

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	190	
1	B	190	
1	C	190	
1	D	190	
2	E	95	
2	F	95	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5496 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 Monopolin complex subunit CSM1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	163	Total	C	N	O	S	0	0	0
			1313	840	208	263	2			
1	B	164	Total	C	N	O	S	0	0	0
			1326	847	212	265	2			
1	C	158	Total	C	N	O	S	0	0	0
			1271	810	203	256	2			
1	D	158	Total	C	N	O	S	0	0	0
			1281	821	202	256	2			

- Molecule 2 is a protein called Monopolin complex subunit LRS4.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	31	Total	C	N	O	0	0	0
			155	93	31	31			
2	F	30	Total	C	N	O	0	0	0
			150	90	30	30			

There are 14 discrepancies between the modelled and reference sequences:

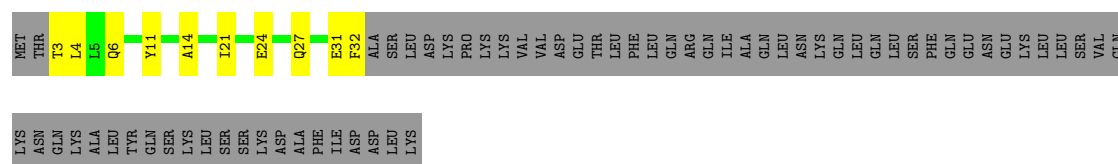
Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	LEU	DELETION	UNP Q04087
E	?	-	ASN	DELETION	UNP Q04087
E	?	-	ASN	DELETION	UNP Q04087
E	?	-	ASN	DELETION	UNP Q04087
E	?	-	LYS	DELETION	UNP Q04087
E	?	-	GLY	DELETION	UNP Q04087
E	?	-	ASP	DELETION	UNP Q04087
F	?	-	LEU	DELETION	UNP Q04087
F	?	-	ASN	DELETION	UNP Q04087
F	?	-	ASN	DELETION	UNP Q04087
F	?	-	ASN	DELETION	UNP Q04087
F	?	-	LYS	DELETION	UNP Q04087

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Chain	Residue	Modelled	Actual	Comment	Reference
F	?	-	GLY	DELETION	UNP Q04087
F	?	-	ASP	DELETION	UNP Q04087

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	152.62Å 152.62Å 118.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.90 49.96 – 3.91	Depositor EDS
% Data completeness (in resolution range)	44.5 (50.00-3.90) 44.7 (49.96-3.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.82 (at 3.88Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.333 , 0.355 0.332 , 0.356	Depositor DCC
R_{free} test set	321 reflections (4.83%)	DCC
Wilson B-factor (Å ²)	65.7	Xtriage
Anisotropy	1.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 290.8	EDS
Estimated twinning fraction	0.056 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 6642 reflections	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	5496	wwPDB-VP
Average B, all atoms (Å ²)	358.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% 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	0.67	0/1332	0.83	2/1800 (0.1%)
1	B	0.57	1/1345 (0.1%)	0.74	1/1817 (0.1%)
1	C	0.68	0/1288	0.85	2/1738 (0.1%)
1	D	0.60	1/1300 (0.1%)	0.74	1/1756 (0.1%)
2	E	0.25	0/154	0.41	0/214
2	F	0.21	0/149	0.34	0/207
All	All	0.61	2/5568 (0.0%)	0.77	6/7532 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	159	GLU	CG-CD	5.49	1.60	1.51
1	D	159	GLU	CG-CD	5.46	1.60	1.51

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	96	LEU	CB-CG-CD1	-5.75	101.22	111.00
1	D	149	LEU	CA-CB-CG	-5.73	102.13	115.30
1	A	81	LEU	CA-CB-CG	-5.72	102.15	115.30
1	B	149	LEU	CA-CB-CG	-5.69	102.22	115.30
1	A	96	LEU	CB-CG-CD1	-5.68	101.34	111.00

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	1313	0	1310	149	0
1	B	1326	0	1328	175	0
1	C	1271	0	1265	214	1
1	D	1281	0	1281	217	1
2	E	155	0	67	14	0
2	F	150	0	62	19	0
All	All	5496	0	5313	659	1

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 61.

The worst 5 of 659 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:26:VAL:HG12	1:C:30:PHE:CE2	1.24	1.69
1:A:7:TYR:CD1	1:B:7:TYR:CE1	2.02	1.47
1:D:14:GLN:HB3	2:F:14:ALA:CB	1.46	1.43
1:C:36:LEU:CD1	1:D:36:LEU:HD12	1.54	1.36
1:D:14:GLN:CB	2:F:14:ALA:HB1	1.53	1.35

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:39:LYS:CE	1:D:30:PHE:CD2[2.545]	1.98	0.22

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	157/190 (83%)	143 (91%)	14 (9%)	0	100	100
1	B	160/190 (84%)	148 (92%)	11 (7%)	1 (1%)	33	86
1	C	152/190 (80%)	139 (91%)	12 (8%)	1 (1%)	30	84

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	152/190 (80%)	132 (87%)	17 (11%)	3 (2%)	11	68
2	E	29/95 (30%)	29 (100%)	0	0	100	100
2	F	28/95 (30%)	27 (96%)	1 (4%)	0	100	100
All	All	678/950 (71%)	618 (91%)	55 (8%)	5 (1%)	30	84

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	33	SER
1	D	80	TYR
1	B	136	PRO
1	C	136	PRO
1	D	158	PHE

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	151/176 (86%)	125 (83%)	26 (17%)	3	22
1	B	152/176 (86%)	123 (81%)	29 (19%)	2	16
1	C	146/176 (83%)	121 (83%)	25 (17%)	3	23
1	D	148/176 (84%)	109 (74%)	39 (26%)	1	7
All	All	597/704 (85%)	478 (80%)	119 (20%)	2	15

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	162	SER
1	C	83	ASN
1	D	134	TYR
1	C	10	SER
1	C	45	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	169	ASN
1	C	13	GLN
1	D	13	GLN
1	B	67	GLN
1	B	83	ASN

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	163/190 (85%)	0.09	3 (1%) 65 50	195, 331, 461, 500	0
1	B	164/190 (86%)	0.19	7 (4%) 34 27	149, 319, 447, 500	0
1	C	158/190 (83%)	0.78	24 (15%) 3 4	182, 398, 500, 500	0
1	D	158/190 (83%)	1.33	35 (22%) 1 3	142, 400, 500, 500	0
2	E	31/95 (32%)	-0.25	0 100 100	107, 270, 426, 483	0
2	F	30/95 (31%)	-0.54	0 100 100	201, 272, 384, 500	0
All	All	704/950 (74%)	0.51	69 (9%) 8 10	107, 349, 500, 500	0

The worst 5 of 69 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	116	MET	17.2
1	D	115	ILE	14.4
1	D	85	ARG	13.2
1	D	87	HIS	10.4
1	D	86	VAL	10.4

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.