



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 04:16 AM GMT

PDB ID : 2II0
Title : Crystal Structure of catalytic domain of Son of sevenless (Rem-Cdc25) in the absence of Ras
Authors : Freedman, T.S.; Sondermann, H.; Friedland, G.D.; Kortemme, T.; Bar-Sagi, D.; Marqusee, S.; Kuriyan, J.
Deposited on : 2006-09-27
Resolution : 2.02 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>

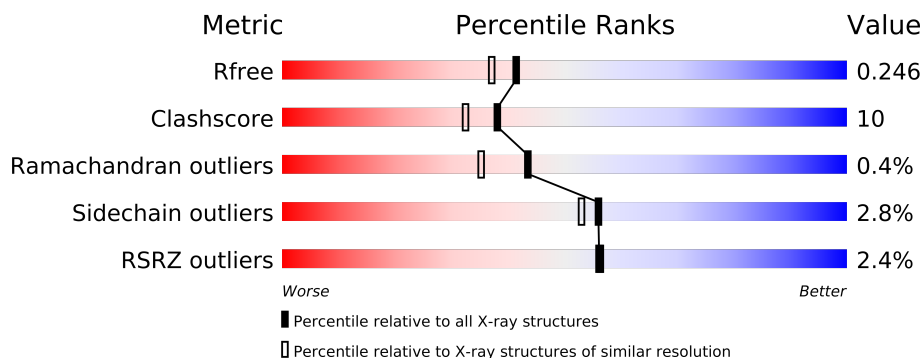
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.02 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	6003 (2.04-2.00)
Clashscore	79885	7467 (2.04-2.00)
Ramachandran outliers	78287	7370 (2.04-2.00)
Sidechain outliers	78261	7368 (2.04-2.00)
RSRZ outliers	66119	6006 (2.04-2.00)

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 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	490	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4089 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 Son of sevenless homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	463	3842	2468	661	700	13	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	560	GLY	-	CLONING ARTIFACT	UNP Q07889
A	561	ALA	-	CLONING ARTIFACT	UNP Q07889
A	562	MET	-	CLONING ARTIFACT	UNP Q07889
A	563	ALA	-	CLONING ARTIFACT	UNP Q07889

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	247	Total	O	0	0
			247	247		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	82.77Å 66.80Å 119.65Å 90.00° 108.91° 90.00°	Depositor
Resolution (Å)	34.39 – 2.02 42.52 – 2.02	Depositor EDS
% Data completeness (in resolution range)	90.9 (34.39-2.02) 91.0 (42.52-2.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.248 0.217 , 0.246	Depositor DCC
R_{free} test set	2436 reflections (6.58%)	DCC
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.3	EDS
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 39596 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4089	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.43% 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	0.34	0/3935	0.55	0/5324

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	3842	0	3865	76	0
2	A	247	0	0	10	0
All	All	4089	0	3865	76	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 10.

All (76) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:804:LEU:HD23	1:A:937:ILE:HD12	1.64	0.77
1:A:614:THR:OG1	1:A:647:ARG:NH1	2.19	0.75
1:A:619:ALA:HB2	1:A:688:ARG:HH21	1.54	0.72
1:A:587:ILE:HD11	1:A:950:ARG:HG3	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:585:ASN:HD22	1:A:586:ILE:N	1.91	0.67
1:A:924:PRO:HB2	1:A:977:GLN:HB3	1.76	0.67
1:A:606:VAL:HG22	1:A:956:ILE:HD11	1.76	0.67
1:A:893:ILE:O	1:A:898:LYS:HE3	1.94	0.67
1:A:1003:LYS:O	1:A:1006:THR:HG22	1.96	0.66
1:A:1020:ASN:HB3	1:A:1021:PRO:HD3	1.78	0.64
1:A:869:ASN:O	1:A:873:GLU:HG3	1.97	0.64
1:A:694:ARG:HH11	1:A:694:ARG:HB3	1.63	0.64
1:A:610:ILE:HD13	1:A:643:LEU:HB3	1.82	0.62
1:A:610:ILE:HD12	1:A:643:LEU:HD13	1.82	0.62
1:A:846:GLU:CA	1:A:846:GLU:OE1	2.48	0.61
1:A:846:GLU:HA	1:A:846:GLU:OE1	2.00	0.61
1:A:804:LEU:CD2	1:A:937:ILE:HD12	2.31	0.61
1:A:606:VAL:HG23	2:A:13:HOH:O	2.00	0.60
1:A:1044:ASN:N	1:A:1045:PRO:HD2	2.16	0.60
1:A:843:GLU:OE1	1:A:1012:LYS:NZ	2.34	0.60
1:A:859:LEU:C	1:A:859:LEU:HD23	2.22	0.60
1:A:585:ASN:ND2	1:A:586:ILE:HG22	2.18	0.59
1:A:585:ASN:HD22	1:A:585:ASN:C	2.06	0.58
1:A:772:GLU:H	1:A:772:GLU:CD	2.05	0.58
1:A:972:GLN:HA	1:A:975:GLN:OE1	2.03	0.57
1:A:683:GLN:HG2	2:A:203:HOH:O	2.03	0.57
1:A:902:GLU:O	1:A:906:GLU:HG3	2.06	0.56
1:A:606:VAL:HG21	2:A:137:HOH:O	2.06	0.55
1:A:582:SER:H	1:A:585:ASN:HD21	1.53	0.55
1:A:728:LYS:HG3	2:A:78:HOH:O	2.07	0.54
1:A:898:LYS:O	1:A:902:GLU:HG3	2.07	0.54
1:A:890:PHE:O	1:A:898:LYS:HE2	2.08	0.53
1:A:727:LYS:O	1:A:731:GLU:HG2	2.09	0.53
1:A:681:TYR:O	1:A:684:PRO:HG2	2.07	0.53
1:A:764:HIS:CD2	1:A:765:ILE:HG13	2.44	0.53
1:A:619:ALA:CB	1:A:688:ARG:HH21	2.21	0.52
1:A:742:ILE:HG13	1:A:743:ALA:N	2.24	0.52
1:A:801:PRO:HB3	1:A:968:THR:HB	1.92	0.51
1:A:1020:ASN:CB	1:A:1021:PRO:HD3	2.40	0.50
1:A:918:LYS:O	1:A:922:ILE:HG12	2.12	0.50
1:A:754:PHE:HB3	1:A:756:SER:O	2.11	0.50
1:A:902:GLU:HG3	2:A:147:HOH:O	2.11	0.49
1:A:665:ASN:HB2	1:A:667:ASP:OD1	2.13	0.48
1:A:701:PHE:CD2	1:A:740:LYS:HB3	2.49	0.48
1:A:950:ARG:HH11	1:A:950:ARG:HG2	1.79	0.48
1:A:804:LEU:HB3	1:A:937:ILE:CD1	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:582:SER:H	1:A:585:ASN:ND2	2.12	0.48
1:A:846:GLU:N	1:A:846:GLU:OE1	2.47	0.47
1:A:791:LEU:C	1:A:791:LEU:HD23	2.34	0.47
1:A:610:ILE:CD1	1:A:643:LEU:HD13	2.44	0.47
1:A:610:ILE:HD13	1:A:643:LEU:CB	2.45	0.47
1:A:738:GLN:NE2	2:A:211:HOH:O	2.48	0.47
1:A:631:TYR:HA	1:A:634:PHE:CE2	2.51	0.46
1:A:908:SER:HA	1:A:912:TYR:CD1	2.52	0.45
1:A:905:HIS:HD2	1:A:909:GLU:OE2	2.00	0.44
1:A:734:THR:O	1:A:738:GLN:HG2	2.17	0.44
1:A:619:ALA:CA	1:A:688:ARG:HH21	2.31	0.43
1:A:763:TRP:CE2	1:A:768:PRO:HG3	2.53	0.43
1:A:988:LYS:O	1:A:992:GLU:HG3	2.19	0.43
1:A:619:ALA:N	1:A:688:ARG:NH2	2.66	0.43
1:A:988:LYS:NZ	1:A:992:GLU:OE2	2.48	0.42
1:A:606:VAL:HG22	1:A:956:ILE:CD1	2.47	0.42
1:A:688:ARG:HD2	2:A:121:HOH:O	2.19	0.42
1:A:944:ASN:HB2	1:A:960:LYS:HE3	2.01	0.42
1:A:637:PRO:HD2	2:A:83:HOH:O	2.20	0.42
1:A:647:ARG:HA	1:A:647:ARG:HD2	1.96	0.41
1:A:577:PHE:HE1	1:A:646:GLU:HG2	1.85	0.41
1:A:615:TYR:CE2	1:A:617:MET:HB2	2.55	0.41
1:A:814:LYS:HG3	1:A:815:GLU:N	2.35	0.41
1:A:816:ILE:HG12	2:A:142:HOH:O	2.20	0.41
1:A:634:PHE:CD1	1:A:956:ILE:HD13	2.55	0.41
1:A:847:GLU:HG2	1:A:1035:LEU:HD11	2.03	0.41
1:A:804:LEU:HB3	1:A:937:ILE:HD13	2.02	0.41
1:A:834:TRP:HB2	1:A:996:PRO:HG3	2.04	0.40
1:A:607:ILE:HG12	2:A:118:HOH:O	2.21	0.40
1:A:654:GLU:HA	1:A:655:PRO:HD3	1.88	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	457/490 (93%)	443 (97%)	12 (3%)	2 (0%)	43	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1020	ASN
1	A	598	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	A	432/452 (96%)	420 (97%)	12 (3%)	56	53

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	567	MET
1	A	585	ASN
1	A	609	LEU
1	A	688	ARG
1	A	694	ARG
1	A	722	ARG
1	A	772	GLU
1	A	846	GLU
1	A	930	PHE
1	A	932	ILE
1	A	950	ARG
1	A	1003	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	585	ASN
1	A	830	ASN
1	A	892	GLN
1	A	905	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	944	ASN
1	A	973	GLN
1	A	1020	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	463/490 (94%)	-0.09	11 (2%) 56 56	22, 36, 64, 89	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1045	PRO	8.0
1	A	1044	ASN	6.1
1	A	566	GLN	3.7
1	A	655	PRO	3.4
1	A	654	GLU	3.3
1	A	597	GLY	3.0
1	A	568	ARG	2.5
1	A	896	ARG	2.5
1	A	1043	SER	2.4
1	A	656	THR	2.2
1	A	999	ASN	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 ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.