



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:09 AM GMT

PDB ID : 4KMH
Title : Crystal structure of Suppressor of Fused d20
Authors : Zhang, Y.; Qi, X.; Zhang, Z.; Wu, G.
Deposited on : 2013-05-08
Resolution : 3.04 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>

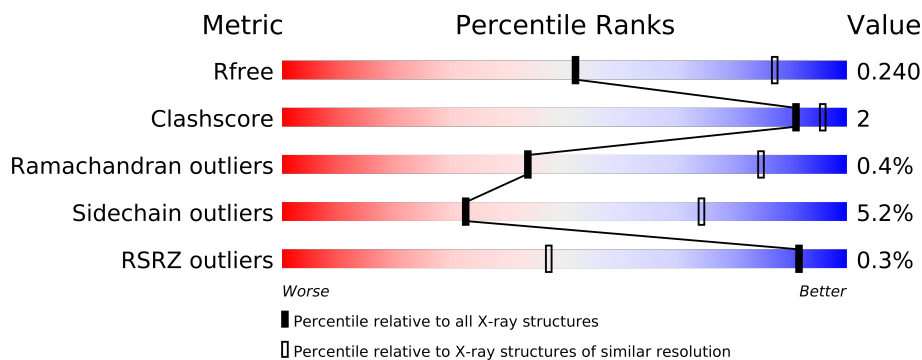
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.04 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	1460 (3.08-3.00)
Clashscore	79885	1881 (3.08-3.00)
Ramachandran outliers	78287	1814 (3.08-3.00)
Sidechain outliers	78261	1817 (3.08-3.00)
RSRZ outliers	66119	1462 (3.08-3.00)

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	484	
1	B	484	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6075 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 Suppressor of fused homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	S	0	0	0
			3012	1922	509	568	13			
1	B	389	Total	C	N	O	S	0	0	0
			3051	1948	515	575	13			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q9UMX1
A	-18	GLY	-	EXPRESSION TAG	UNP Q9UMX1
A	-17	SER	-	EXPRESSION TAG	UNP Q9UMX1
A	-16	SER	-	EXPRESSION TAG	UNP Q9UMX1
A	-15	HIS	-	EXPRESSION TAG	UNP Q9UMX1
A	-14	HIS	-	EXPRESSION TAG	UNP Q9UMX1
A	-13	HIS	-	EXPRESSION TAG	UNP Q9UMX1
A	-12	HIS	-	EXPRESSION TAG	UNP Q9UMX1
A	-11	HIS	-	EXPRESSION TAG	UNP Q9UMX1
A	-10	HIS	-	EXPRESSION TAG	UNP Q9UMX1
A	-9	SER	-	EXPRESSION TAG	UNP Q9UMX1
A	-8	SER	-	EXPRESSION TAG	UNP Q9UMX1
A	-7	GLY	-	EXPRESSION TAG	UNP Q9UMX1
A	-6	LEU	-	EXPRESSION TAG	UNP Q9UMX1
A	-5	VAL	-	EXPRESSION TAG	UNP Q9UMX1
A	-4	PRO	-	EXPRESSION TAG	UNP Q9UMX1
A	-3	ARG	-	EXPRESSION TAG	UNP Q9UMX1
A	-2	GLY	-	EXPRESSION TAG	UNP Q9UMX1
A	-1	SER	-	EXPRESSION TAG	UNP Q9UMX1
A	0	HIS	-	EXPRESSION TAG	UNP Q9UMX1
B	-19	MET	-	EXPRESSION TAG	UNP Q9UMX1
B	-18	GLY	-	EXPRESSION TAG	UNP Q9UMX1
B	-17	SER	-	EXPRESSION TAG	UNP Q9UMX1
B	-16	SER	-	EXPRESSION TAG	UNP Q9UMX1
B	-15	HIS	-	EXPRESSION TAG	UNP Q9UMX1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	EXPRESSION TAG	UNP Q9UMX1
B	-13	HIS	-	EXPRESSION TAG	UNP Q9UMX1
B	-12	HIS	-	EXPRESSION TAG	UNP Q9UMX1
B	-11	HIS	-	EXPRESSION TAG	UNP Q9UMX1
B	-10	HIS	-	EXPRESSION TAG	UNP Q9UMX1
B	-9	SER	-	EXPRESSION TAG	UNP Q9UMX1
B	-8	SER	-	EXPRESSION TAG	UNP Q9UMX1
B	-7	GLY	-	EXPRESSION TAG	UNP Q9UMX1
B	-6	LEU	-	EXPRESSION TAG	UNP Q9UMX1
B	-5	VAL	-	EXPRESSION TAG	UNP Q9UMX1
B	-4	PRO	-	EXPRESSION TAG	UNP Q9UMX1
B	-3	ARG	-	EXPRESSION TAG	UNP Q9UMX1
B	-2	GLY	-	EXPRESSION TAG	UNP Q9UMX1
B	-1	SER	-	EXPRESSION TAG	UNP Q9UMX1
B	0	HIS	-	EXPRESSION TAG	UNP Q9UMX1

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	6	Total O 6 6	0	0
2	B	6	Total O 6 6	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	73.63Å 122.33Å 118.75Å 90.00° 90.41° 90.00°	Depositor
Resolution (Å)	50.00 – 3.04 42.60 – 3.04	Depositor EDS
% Data completeness (in resolution range)	97.5 (50.00-3.04) 97.5 (42.60-3.04)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 3.06Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.224 , 0.277 0.215 , 0.240	Depositor DCC
R_{free} test set	1010 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	83.4	Xtriage
Anisotropy	0.024	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.6	EDS
Estimated twinning fraction	0.632 for H,K,L 0.368 for -H,-K,L 0.022 for -1/2*h+1/2*k,3/2*h+1/2*k,-l 0.021 for -1/2*h-1/2*k,-3/2*h+1/2*k,-l 0.019 for 1/2*h+1/2*k,3/2*h-1/2*k,-l 0.018 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.406 for -h,-k,l	Xtriage
Reported twinning fraction	0.632 for H,K,L 0.368 for -H,-K,L	Depositor
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 19784 reflections	Xtriage
F_o , F_c correlation	0.94	EDS
Total number of atoms	6075	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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	0.33	0/3098	0.52	1/4217 (0.0%)
1	B	0.33	0/3138	0.52	1/4274 (0.0%)
All	All	0.33	0/6236	0.52	2/8491 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	20	PRO	N-CA-CB	5.98	110.48	103.30
1	A	20	PRO	N-CA-CB	5.91	110.39	103.30

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	3012	0	0	2	0
1	B	3051	0	0	10	0
2	A	6	0	0	0	0
2	B	6	0	0	0	0
All	All	6075	0	0	12	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 2.

All (12) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:278:LEU:CB	1:A:368:SER:OG	2.41	0.69
1:B:278:LEU:CB	1:B:368:SER:OG	2.48	0.61
1:B:279:SER:O	1:B:280:ARG:CB	2.54	0.55
1:A:371:LEU:CD1	1:A:433:ILE:CD1	2.84	0.55
1:B:449:ASP:CA	1:B:450:LEU:C	2.78	0.52
1:B:22:ALA:O	1:B:42:ARG:NH2	2.45	0.50
1:B:168:ASP:CG	1:B:170:SER:OG	2.50	0.50
1:B:279:SER:OG	1:B:367:GLU:N	2.47	0.47
1:B:30:PHE:N	1:B:30:PHE:CD2	2.83	0.47
1:B:168:ASP:OD1	1:B:168:ASP:N	2.51	0.44
1:B:166:PRO:CB	1:B:170:SER:O	2.67	0.42
1:B:448:GLU:O	1:B:449:ASP:C	2.59	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	375/484 (78%)	364 (97%)	11 (3%)	0	100	100
1	B	381/484 (79%)	363 (95%)	15 (4%)	3 (1%)	27	74
All	All	756/968 (78%)	727 (96%)	26 (3%)	3 (0%)	43	85

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	172	SER
1	B	21	THR
1	B	174	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	325/418 (78%)	307 (94%)	18 (6%)	30	71
1	B	329/418 (79%)	313 (95%)	16 (5%)	35	77
All	All	654/836 (78%)	620 (95%)	34 (5%)	32	74

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	THR
1	A	76	ASN
1	A	125	LYS
1	A	128	THR
1	A	144	LEU
1	A	209	HIS
1	A	215	ASN
1	A	256	ASP
1	A	266	LEU
1	A	278	LEU
1	A	279	SER
1	A	362	ARG
1	A	364	ARG
1	A	368	SER
1	A	374	ASN
1	A	383	LEU
1	A	447	LEU
1	A	469	LEU
1	B	4	LEU
1	B	5	ARG
1	B	55	THR
1	B	76	ASN
1	B	125	LYS
1	B	215	ASN
1	B	266	LEU
1	B	278	LEU
1	B	363	THR
1	B	374	ASN
1	B	384	CYS

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Mol	Chain	Res	Type
1	B	386	ARG
1	B	433	ILE
1	B	434	LEU
1	B	469	LEU
1	B	476	ASP

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	383/484 (79%)	0.05	1 (0%)	91 47	63, 82, 108, 149	15 (3%)
1	B	389/484 (80%)	0.10	1 (0%)	91 47	63, 82, 113, 202	15 (3%)
All	All	772/968 (79%)	0.08	2 (0%)	91 47	63, 82, 111, 202	30 (3%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	450	LEU	3.2
1	A	450	LEU	2.3

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.