



Full wwPDB X-ray Structure Validation Report

Mar 31, 2014 – 03:27 PM BST

PDB ID : 4JR8
Title : Crystal structure of cruxrhodopsin-3 from Haloarcula vallismortis at 2.3 angstrom resolution
Authors : Kouyama, T.; Chan, S.K.
Deposited on : 2013-03-21
Resolution : 2.30 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>

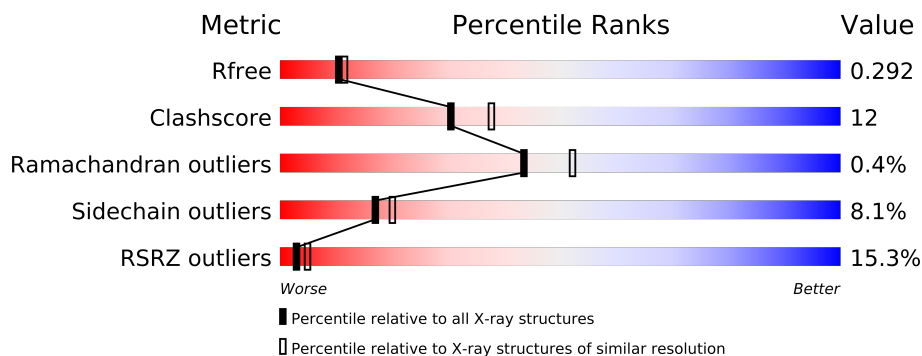
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable23004
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) : stable23004

1 Overall quality at a glance

The reported resolution of this entry is 2.30 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	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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	250	

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	RET	A	301	-	X
3	22B	A	302	-	X

2 Entry composition i

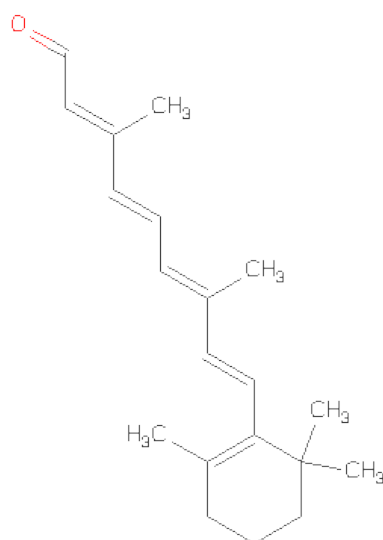
There are 4 unique types of molecules in this entry. The entry contains 1872 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Cruxrhodopsin-3.

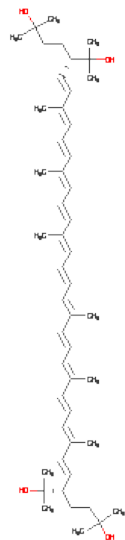
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	234	1801	1196	287	313	5	0	0	0

- Molecule 2 is RETINAL (three-letter code: RET) (formula: C₂₀H₂₈O).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	C	0	0
			20	20		

- Molecule 3 is BACTERIORUBERIN (three-letter code: 22B) (formula: C₅₀H₇₆O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			37	35	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	14	Total	O	0	0
			14	14		

4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	106.21 Å 106.21 Å 60.21 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.30 45.99 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (15.00-2.30) 88.9 (45.99-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 2.29 Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.245 , 0.295 0.249 , 0.292	Depositor DCC
R_{free} test set	763 reflections (4.89%)	DCC
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.631	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 62.8	EDS
Estimated twinning fraction	0.044 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 15669 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	1872	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% 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: 22B, RET

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	0.35	0/1846	0.55	0/2519

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	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	81	TYR	Sidechain

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	1801	0	1844	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	20	0	27	5	0
3	A	37	0	45	0	0
4	A	14	0	0	0	0
All	All	1872	0	1916	45	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 12.

All (45) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:181:LEU:O	1:A:185:VAL:HG12	1.88	0.73
1:A:34:ASP:O	1:A:38:GLN:HG2	1.90	0.72
1:A:98:LEU:HD12	1:A:175:PHE:HB2	1.75	0.69
1:A:168:PRO:HG2	1:A:171:THR:HG22	1.75	0.68
1:A:88:THR:OG1	1:A:89:PRO:HD3	1.94	0.67
1:A:179:ARG:HG2	1:A:179:ARG:HH11	1.62	0.65
1:A:47:ILE:HD13	1:A:91:LEU:HD13	1.78	0.64
1:A:190:PRO:HB3	2:A:301:RET:H183	1.81	0.62
1:A:167:LEU:HB3	1:A:171:THR:HG23	1.81	0.61
1:A:185:VAL:HG13	1:A:186:TRP:HD1	1.65	0.61
1:A:176:LYS:HG2	1:A:179:ARG:HH21	1.65	0.60
1:A:69:ILE:HD12	1:A:74:ARG:HE	1.71	0.55
1:A:145:SER:HB3	2:A:301:RET:H41	1.89	0.55
1:A:161:SER:O	1:A:164:VAL:HG12	2.07	0.53
1:A:230:SER:O	1:A:233:VAL:HG22	2.09	0.53
1:A:36:ARG:NH2	1:A:237:ALA:HB3	2.24	0.53
1:A:230:SER:HB2	1:A:233:VAL:HG13	1.91	0.52
1:A:28:ARG:HG2	1:A:41:TYR:HE1	1.74	0.52
1:A:160:LEU:HD13	1:A:163:ARG:HB3	1.91	0.51
1:A:74:ARG:HD2	1:A:76:ILE:HD11	1.93	0.49
1:A:164:VAL:HA	1:A:167:LEU:HD12	1.94	0.49
1:A:137:GLU:O	1:A:140:VAL:HG12	2.12	0.48
1:A:111:SER:O	1:A:115:LEU:HD13	2.14	0.48
1:A:176:LYS:HG2	1:A:179:ARG:NH2	2.29	0.47
1:A:152:LEU:HD23	1:A:152:LEU:C	2.36	0.47
1:A:40:PHE:CE2	1:A:234:LEU:HB2	2.50	0.46
1:A:214:VAL:O	1:A:218:VAL:HG23	2.16	0.46
1:A:231:HIS:O	1:A:234:LEU:HD23	2.16	0.45
1:A:141:TRP:HA	1:A:144:ILE:HG22	1.99	0.45
1:A:103:ARG:HD3	1:A:103:ARG:H	1.82	0.45
1:A:141:TRP:HA	1:A:144:ILE:CG2	2.47	0.44
1:A:179:ARG:CG	1:A:179:ARG:HH11	2.30	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:140:VAL:O	1:A:144:ILE:HG22	2.19	0.43
1:A:231:HIS:HA	1:A:234:LEU:CD2	2.50	0.42
1:A:145:SER:CB	2:A:301:RET:H41	2.49	0.42
2:A:301:RET:H181	2:A:301:RET:H7	1.89	0.42
1:A:227:LEU:HG	1:A:228:LEU:HD13	2.02	0.42
1:A:190:PRO:HB3	2:A:301:RET:C18	2.50	0.42
1:A:51:ALA:HB2	1:A:220:LYS:HE2	2.02	0.42
1:A:98:LEU:CD1	1:A:175:PHE:HB2	2.46	0.41
1:A:36:ARG:HH21	1:A:237:ALA:HB3	1.84	0.41
1:A:66:ILE:CG2	1:A:73:GLN:HB3	2.51	0.41
1:A:7:GLU:N	1:A:7:GLU:OE1	2.50	0.41
1:A:100:GLY:O	1:A:163:ARG:HD3	2.21	0.40
1:A:68:GLU:CD	1:A:68:GLU:H	2.25	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	232/250 (93%)	222 (96%)	9 (4%)	1 (0%)	43	52

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	SER

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	185/193 (96%)	170 (92%)	15 (8%)	17	20

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	20	LEU
1	A	23	LEU
1	A	28	ARG
1	A	91	LEU
1	A	92	LEU
1	A	95	LEU
1	A	103	ARG
1	A	156	LEU
1	A	160	LEU
1	A	166	ASP
1	A	205	ILE
1	A	228	LEU
1	A	229	ARG
1	A	234	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	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

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	RET	A	301	1	19,20,21	2.96	5 (26%)	26,27,28	1.73	7 (26%)
3	22B	A	302	-	33,36,53	2.84	12 (36%)	38,45,72	1.99	10 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	RET	A	301	1	-	0/13/30/31	0/1/1/1
3	22B	A	302	-	-	0/37/41/65	0/0/0/0

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	22B	C1-C2	9.74	1.69	1.55
2	A	301	RET	C1-C6	8.36	1.65	1.53
2	A	301	RET	C5-C6	7.27	1.46	1.34
3	A	302	22B	C2-C3	4.95	1.55	1.49
3	A	302	22B	C20-C13	4.64	1.59	1.51
3	A	302	22B	C16-C1	4.25	1.60	1.52
3	A	302	22B	C17-C1	4.19	1.59	1.52
3	A	302	22B	C19-C9	4.00	1.58	1.51
3	A	302	22B	O27-C23	3.47	1.54	1.44
2	A	301	RET	C7-C6	3.44	1.58	1.46
3	A	302	22B	C18-C5	3.21	1.56	1.51
3	A	302	22B	C22-C23	3.19	1.60	1.52
2	A	301	RET	C10-C9	2.71	1.39	1.35
3	A	302	22B	C22-C21	2.58	1.58	1.53
2	A	301	RET	C2-C3	-2.53	1.45	1.52
3	A	302	22B	C42-C43	2.13	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	22B	C21-C2	2.01	1.56	1.54

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	22B	C21-C2-C3	-6.48	102.45	111.34
3	A	302	22B	C8-C9-C10	-3.76	113.19	118.97
3	A	302	22B	C4-C5-C6	-3.53	113.55	118.97
3	A	302	22B	C12-C13-C14	-3.41	113.73	118.97
2	A	301	RET	C3-C4-C5	3.30	118.74	113.74
3	A	302	22B	C20-C13-C12	3.09	123.09	118.09
2	A	301	RET	C4-C5-C6	-3.07	118.75	122.84
3	A	302	22B	C25-C23-C22	3.02	118.17	111.65
3	A	302	22B	C19-C9-C8	2.96	122.87	118.09
2	A	301	RET	C8-C9-C10	-2.95	114.43	118.97
3	A	302	22B	C18-C5-C4	2.71	122.47	118.09
3	A	302	22B	C17-C1-C16	-2.64	106.69	110.54
2	A	301	RET	C2-C1-C6	2.55	114.67	110.44
2	A	301	RET	C1-C6-C7	2.50	122.63	115.69
2	A	301	RET	C19-C9-C8	2.45	122.05	118.09
3	A	302	22B	C22-C21-C2	-2.24	108.48	113.64
2	A	301	RET	C18-C5-C4	2.19	117.37	113.34

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	A	234/250 (93%)	0.93	36 (15%) 3 5	21, 29, 55, 72	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	70	ALA	13.5
1	A	71	GLY	12.9
1	A	128	GLY	7.0
1	A	129	SER	6.8
1	A	233	VAL	6.7
1	A	130	GLY	6.2
1	A	236	GLY	6.0
1	A	164	VAL	5.5
1	A	127	ALA	5.1
1	A	72	GLU	5.0
1	A	69	ILE	4.5
1	A	171	THR	4.5
1	A	234	LEU	4.2
1	A	231	HIS	4.0
1	A	235	ASP	4.0
1	A	73	GLN	3.8
1	A	170	ASP	3.8
1	A	68	GLU	3.7
1	A	131	VAL	3.7
1	A	60	LEU	3.5
1	A	169	SER	3.2
1	A	232	GLY	3.1
1	A	5	GLU	3.0
1	A	30	TRP	2.9
1	A	136	ALA	2.8
1	A	155	PHE	2.7
1	A	132	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	61	GLY	2.7
1	A	168	PRO	2.7
1	A	66	ILE	2.6
1	A	229	ARG	2.6
1	A	230	SER	2.4
1	A	237	ALA	2.3
1	A	167	LEU	2.2
1	A	67	VAL	2.2
1	A	144	ILE	2.1

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	RET	A	301	20/21	0.22	2.57	18,23,27,28	0
3	22B	A	302	37/54	0.29	2.40	29,35,47,49	0

6.5 Other polymers ⓘ

There are no such residues in this entry.