



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:19 PM GMT

PDB ID : 1JV6
Title : BACTERIORHODOPSIN D85S/F219L DOUBLE MUTANT AT 2.00
ANGSTROM RESOLUTION
Authors : Rouhani, S.; Cartailier, J.-P.; Facciotti, M.T.; Walian, P.; Needleman, R.;
Lanyi, J.K.; Glaeser, R.M.; Luecke, H.
Deposited on : 2001-08-28
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure 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/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

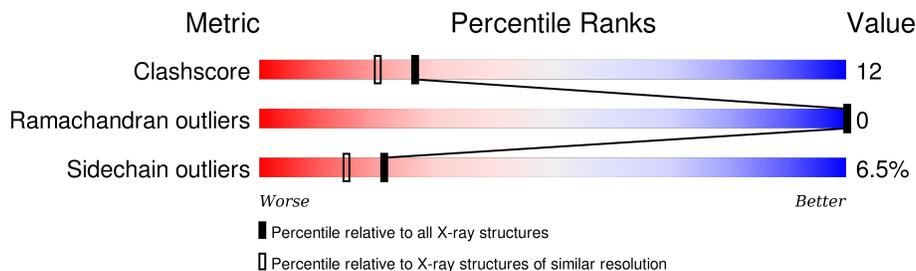
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	249	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	LI1	A	701	X	-	-	-

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 1788 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

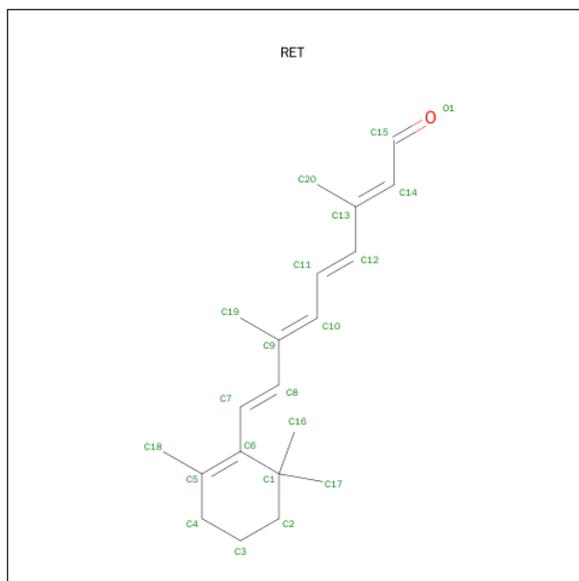
- Molecule 1 is a protein called Bacteriorhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	208	1613	1089	244	272	8	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

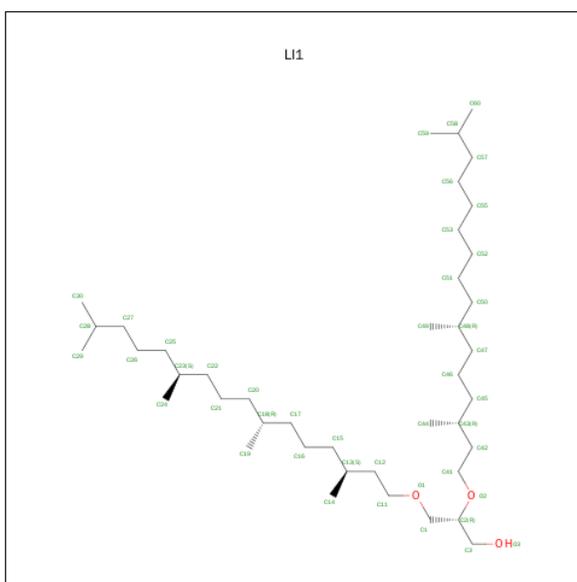
Chain	Residue	Modelled	Actual	Comment	Reference
A	85	SER	ASP	ENGINEERED	UNP P02945
A	219	LEU	PHE	ENGINEERED	UNP P02945

- 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 1-[2,6,10,14-TETRAMETHYL-HEXADECAN-16-YL]-2-[2,10,14-TRIMETHYLHEXADECAN-16-YL]GLYCEROL (three-letter code: LI1) (formula: C₄₂H₈₆O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C 19 19	0	0
3	A	1	Total C O 20 19 1	0	0
3	A	1	Total C O 12 11 1	0	0
3	A	1	Total C O 21 20 1	0	0
3	A	1	Total C 11 11	0	0
3	A	1	Total C O 17 16 1	0	0
3	A	1	Total C O 12 11 1	0	0
3	A	1	Total C 9 9	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	34	Total O 34 34	0	0

4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	51.80Å 121.30Å 85.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (12.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.222 , 0.240	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	1788	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: LI1, 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	0/1654	0.54	0/2258

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1613	0	1685	44	0
2	A	20	0	27	2	0
3	A	121	0	215	10	0
4	A	34	0	0	3	0
All	All	1788	0	1927	45	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (45) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:MET:HE3	1:A:81:ALA:O	1.69	0.92
1:A:190:LEU:HD22	3:A:712:LI1:H193	1.62	0.82
1:A:84:ALA:HB1	3:A:702:LI1:H202	1.70	0.74
1:A:129:LYS:HD3	1:A:129:LYS:N	2.05	0.71
1:A:129:LYS:HD3	1:A:129:LYS:H	1.57	0.69
1:A:52:ILE:HG12	3:A:702:LI1:H272	1.75	0.68
1:A:56:MET:CE	1:A:84:ALA:HB3	2.26	0.66
1:A:176:ASN:HD22	3:A:710:LI1:H142	1.60	0.65
1:A:129:LYS:CD	1:A:129:LYS:H	2.09	0.64
1:A:135:PHE:HA	3:A:712:LI1:H172	1.79	0.63
1:A:56:MET:HE2	1:A:84:ALA:HB3	1.81	0.63
1:A:56:MET:HG3	1:A:85:SER:HB3	1.83	0.61
1:A:157:THR:O	1:A:161:GLU:HG3	2.00	0.61
1:A:15:LEU:HD23	1:A:209:MET:HE1	1.84	0.58
1:A:153:PHE:CE1	1:A:175:ARG:HD3	2.41	0.56
1:A:93:LEU:HD13	4:A:501:HOH:O	2.07	0.55
1:A:25:LEU:C	1:A:25:LEU:HD23	2.28	0.54
1:A:90:THR:OG1	1:A:91:PRO:HD3	2.08	0.53
1:A:156:PHE:HB3	1:A:171:PHE:CZ	2.43	0.53
1:A:135:PHE:CD1	3:A:712:LI1:H18	2.44	0.53
1:A:190:LEU:CD2	3:A:712:LI1:H193	2.38	0.52
1:A:153:PHE:CD1	1:A:175:ARG:HD3	2.45	0.51
1:A:36:ASP:O	1:A:40:LYS:HG2	2.10	0.51
1:A:199:VAL:HG13	3:A:701:LI1:H492	1.93	0.49
1:A:15:LEU:HD23	1:A:209:MET:CE	2.42	0.49
1:A:95:LEU:O	1:A:99:LEU:HG	2.12	0.49
1:A:14:ALA:HA	1:A:61:LEU:HD11	1.95	0.49
1:A:202:ASN:ND2	1:A:202:ASN:C	2.64	0.49
1:A:31:GLY:O	1:A:40:LYS:NZ	2.46	0.48
1:A:166:GLU:HG3	4:A:516:HOH:O	2.14	0.47
1:A:129:LYS:N	1:A:129:LYS:CD	2.72	0.46
1:A:45:ILE:HD11	1:A:99:LEU:HD11	1.97	0.46
1:A:123:LEU:HD13	1:A:123:LEU:C	2.35	0.46
1:A:164:ARG:HG3	4:A:516:HOH:O	2.16	0.46
2:A:301:RET:H171	2:A:301:RET:H8	1.99	0.45
1:A:123:LEU:HD11	1:A:127:LEU:HD11	1.98	0.45
1:A:199:VAL:HG22	3:A:701:LI1:H493	1.99	0.44
1:A:80:TRP:HB2	3:A:702:LI1:H122	2.00	0.44
1:A:36:ASP:HA	1:A:37:PRO:HD3	1.93	0.42
1:A:206:LEU:HD23	1:A:206:LEU:O	2.20	0.42
1:A:202:ASN:HD22	1:A:202:ASN:C	2.22	0.41
1:A:86:TRP:CD1	2:A:301:RET:H14	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ARG:HD2	1:A:176:ASN:OD1	2.21	0.41
1:A:152:LEU:O	1:A:156:PHE:HB2	2.21	0.41
1:A:56:MET:HE3	1:A:81:ALA:C	2.39	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	204/249 (82%)	203 (100%)	1 (0%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	168/195 (86%)	157 (94%)	11 (6%)	21 15

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LEU
1	A	28	LEU
1	A	96	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	97	LEU
1	A	129	LYS
1	A	130	VAL
1	A	158	SER
1	A	201	LEU
1	A	202	ASN
1	A	206	LEU
1	A	211	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	202	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

9 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	1.58	3 (15%)	27,27,28	1.17	1 (3%)
3	LI1	A	701	-	18,18,44	1.04	0	20,20,51	1.05	2 (10%)
3	LI1	A	702	-	19,19,44	1.06	0	20,21,51	0.97	0
3	LI1	A	703	-	11,11,44	0.91	0	11,12,51	0.67	0
3	LI1	A	710	-	20,20,44	1.10	0	22,23,51	1.00	1 (4%)
3	LI1	A	711	-	10,10,44	0.77	0	11,11,51	0.73	0
3	LI1	A	712	-	16,16,44	1.10	0	17,18,51	1.06	2 (11%)
3	LI1	A	713	-	11,11,44	0.93	0	11,12,51	0.76	0
3	LI1	A	722	-	8,8,44	0.68	0	8,8,51	0.61	0

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	LI1	A	701	-	1/1/3/8	0/18/18/49	0/0/0/0
3	LI1	A	702	-	-	0/19/19/49	0/0/0/0
3	LI1	A	703	-	-	0/11/11/49	0/0/0/0
3	LI1	A	710	-	-	0/21/21/49	0/0/0/0
3	LI1	A	711	-	-	0/10/10/49	0/0/0/0
3	LI1	A	712	-	-	0/17/17/49	0/0/0/0
3	LI1	A	713	-	-	0/11/11/49	0/0/0/0
3	LI1	A	722	-	-	0/6/6/49	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	RET	C15-C14	-2.25	1.40	1.49
2	A	301	RET	C2-C3	-2.06	1.46	1.52
2	A	301	RET	C1-C6	4.69	1.60	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	RET	C18-C5-C4	-2.01	109.61	113.43
3	A	701	LI1	C46-C45-C43	2.04	122.24	115.49
3	A	712	LI1	C16-C15-C13	2.14	122.57	115.49
3	A	712	LI1	C16-C17-C18	2.40	123.46	115.49
3	A	710	LI1	C16-C17-C18	2.52	123.86	115.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	LI1	C46-C47-C48	2.67	124.33	115.49

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	701	LI1	C43

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	RET	2	0
3	A	701	LI1	2	0
3	A	702	LI1	3	0
3	A	710	LI1	1	0
3	A	712	LI1	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.