



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 05:43 am GMT

PDB ID : 2F95
Title : M intermediate structure of sensory rhodopsin II/transducer complex in combination with the ground state structure
Authors : Moukhametzianov, R.I.; Klare, J.P.; Efremov, R.G.; Baecken, C.; Goepfner, A.; Labahn, J.; Engelhard, M.; Bueldt, G.; Gordeliy, V.I.
Deposited on : 2005-12-05
Resolution : 2.20 Å(reported)

This is a wwPDB X-ray Structure 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/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

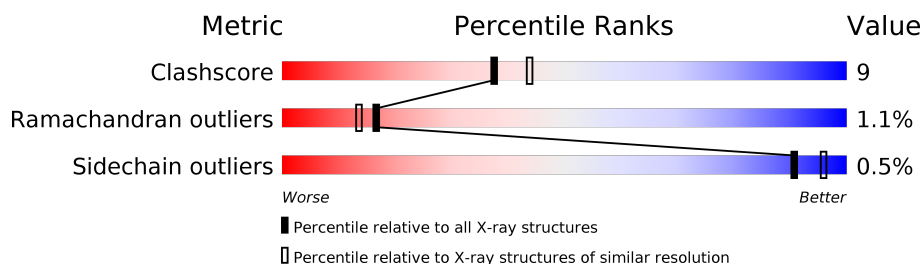
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)

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	1-A	248	
1	2-A	248	
2	1-B	163	
2	2-B	163	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4183 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 Sensory rhodopsin II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	220	Total	C	N	O	S	0	220	0
			1664	1113	264	281	6			
1	2-A	220	Total	C	N	O	S	0	220	0
			1664	1113	264	281	6			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	240	GLU	-	CLONING ARTIFACT	UNP P42196
A	241	ASN	-	CLONING ARTIFACT	UNP P42196
A	242	SER	-	CLONING ARTIFACT	UNP P42196
A	243	HIS	-	EXPRESSION TAG	UNP P42196
A	244	HIS	-	EXPRESSION TAG	UNP P42196
A	245	HIS	-	EXPRESSION TAG	UNP P42196
A	246	HIS	-	EXPRESSION TAG	UNP P42196
A	247	HIS	-	EXPRESSION TAG	UNP P42196
A	248	HIS	-	EXPRESSION TAG	UNP P42196
A	249	HIS	-	EXPRESSION TAG	UNP P42196

- Molecule 2 is a protein called Sensory rhodopsin II transducer.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	1-B	53	Total	C	N	O	0	53	0
			356	235	55	66			
2	2-B	53	Total	C	N	O	0	53	0
			356	235	55	66			

There are 10 discrepancies between the modelled and reference sequences:

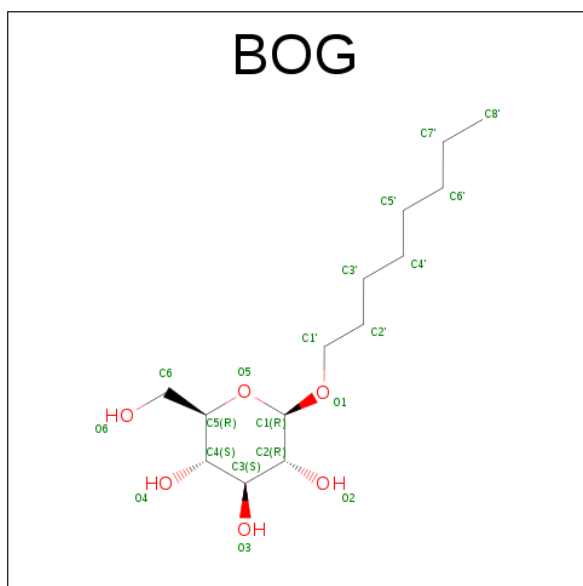
Chain	Residue	Modelled	Actual	Comment	Reference
B	4	ALA	-	CLONING ARTIFACT	UNP P42259
B	158	ASN	-	CLONING ARTIFACT	UNP P42259

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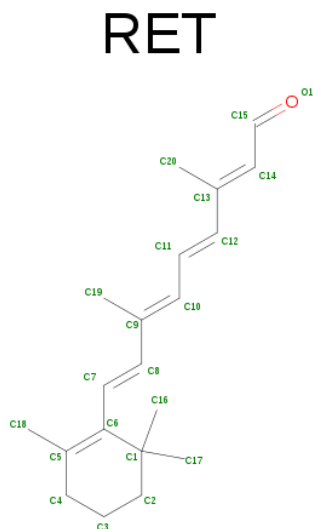
Chain	Residue	Modelled	Actual	Comment	Reference
B	159	SER	-	CLONING ARTIFACT	UNP P42259
B	160	HIS	-	EXPRESSION TAG	UNP P42259
B	161	HIS	-	EXPRESSION TAG	UNP P42259
B	162	HIS	-	EXPRESSION TAG	UNP P42259
B	163	HIS	-	EXPRESSION TAG	UNP P42259
B	164	HIS	-	EXPRESSION TAG	UNP P42259
B	165	HIS	-	EXPRESSION TAG	UNP P42259
B	166	HIS	-	EXPRESSION TAG	UNP P42259

- Molecule 3 is M intermediate of sensory rhodopsin II (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	1-A	1	Total	C	O	0	1
			20	14	6		
3	2-A	1	Total	C	O	0	1
			20	14	6		

- Molecule 4 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$).



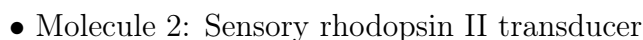
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	1-A	1	Total C 20 20	0	1
4	2-A	1	Total C 20 20	0	1

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	1-A	32	Total O 32 32	0	32
5	2-A	28	Total O 28 28	0	28
5	1-B	1	Total O 1 1	0	1
5	2-B	2	Total O 2 2	0	2

Note EDS was not executed.

- Chain 1-A:



ASN	SER	HIS	HIS	HIS	HIS	HIS	HIS	SER	ARG	ALA	127	F36	A40	V44	Q57	V61	S62	A63	M74	L75	V78	A79	ALA	THR	LEU	GLY	GLY	ASP	THR	ALA	ALA	ALA	GLN	LYS	ARG	ALA	GLU	GLU	THR	ASN	THR										
SER	ARG	MET	GLY	ASP	GLY	ASP	VAL	ASP	VAL	LEU	TYR	ALA	ALA	GLU	MET	ARG	GLN	SER	VAL	ARG	THR	SER	LEU	GLU	ASP	ALA	LYS	ASN	ALA	ARG	GLU	ASP	ALA	GLU	GLN	ALA	GLN	LYS	ARG	ALA	GLU	ILE	ASN	THR							
ALA	VAL	SER	ARG	LEU	LEU	PRO	SER	ARG	VAL	HIS	SER	TYR	THR	GLY	LYS	GLY	MET	GLY	ALA	VAL	PHE	127	F36	A40	V44	Q57	V61	S62	A63	M74	L75	V78	A79	ALA	THR	LEU	GLY	GLY	ASP	THR	ALA	ALA	GLN	LYS	ARG	ALA	GLU	GLU	THR	ASN	THR

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	124.62Å 46.90Å 53.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.01 – 2.20	Depositor
% Data completeness (in resolution range)	94.0 (22.01-2.20)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.217 , 0.241	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4183	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: RET, BOG

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	1-A	0.35	0/1706	0.54	0/2335
2	1-B	0.26	0/358	0.45	0/490
All	All	0.34	0/2064	0.52	0/2825

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

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	1-A	1664	0	1730	16	0
1	2-A	1664	0	1731	48	0
2	1-B	356	0	381	3	0
2	2-B	356	0	381	7	0
3	1-A	20	0	28	5	0
3	2-A	20	0	28	3	0
4	1-A	20	0	27	1	0
4	2-A	20	0	27	1	0
5	1-A	32	0	0	0	0
5	1-B	1	0	0	0	0
5	2-A	28	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	2-B	2	0	0	1	0
All	All	4183	0	4333	74	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 9.

The worst 5 of 74 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:66[B]:ARG:HD3	1:A:182[B]:PRO:O	1.69	0.93
1:A:31[B]:SER:O	1:A:33[B]:GLU:N	2.13	0.80
1:A:185[B]:VAL:HG23	1:A:187[B]:LEU:HG	1.66	0.77
1:A:213[A]:LEU:HD12	3:A:300[A]:BOG:H8'1	1.70	0.74
1:A:142[B]:VAL:O	1:A:146[B]:THR:HB	1.91	0.70

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	1-A	218/248 (88%)	215 (99%)	2 (1%)	1 (0%)	32	34
1	2-A	218/248 (88%)	205 (94%)	8 (4%)	5 (2%)	7	4
2	1-B	51/163 (31%)	50 (98%)	1 (2%)	0	100	100
2	2-B	51/163 (31%)	48 (94%)	3 (6%)	0	100	100
All	All	538/822 (66%)	518 (96%)	14 (3%)	6 (1%)	17	13

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2-A	31[B]	SER

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Mol	Chain	Res	Type
1	2-A	32[B]	GLY
1	2-A	120[B]	GLY
1	2-A	143[B]	GLY
1	1-A	64[A]	ALA

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	1-A	167/189 (88%)	166 (99%)	1 (1%)	89	94
2	1-B	32/120 (27%)	32 (100%)	0	100	100
All	All	199/309 (64%)	198 (100%)	1 (0%)	91	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	66[A]	ARG

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

Mol	Chain	Res	Type
2	1-B	74[A]	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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$
3	BOG	1-A	300[A]	-	20,20,20	1.03	2 (10%)	25,25,25	0.67	0
4	RET	1-A	301[A]	1	19,20,21	1.56	4 (21%)	27,27,28	2.25	11 (40%)
3	BOG	2-A	300[B]	-	20,20,20	1.03	2 (10%)	25,25,25	0.67	0
4	RET	2-A	301[B]	-	19,20,21	1.81	6 (31%)	27,27,28	2.36	10 (37%)

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
3	BOG	1-A	300[A]	-	-	0/11/31/31	0/1/1/1
4	RET	1-A	301[A]	1	-	0/13/30/31	0/1/1/1
3	BOG	2-A	300[B]	-	-	0/11/31/31	0/1/1/1
4	RET	2-A	301[B]	-	-	0/13/30/31	0/1/1/1

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2-A	301[B]	RET	C11-C10	2.01	1.49	1.43
4	1-A	301[A]	RET	C16-C1	2.10	1.58	1.53
4	2-A	301[B]	RET	C11-C12	2.34	1.40	1.34
4	2-A	301[B]	RET	C10-C9	2.44	1.39	1.35
3	1-A	300[A]	BOG	O5-C1	2.52	1.48	1.41

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	2-A	301[B]	RET	C11-C10-C9	-5.61	119.30	127.31
4	1-A	301[A]	RET	C11-C10-C9	-4.60	120.75	127.31
4	1-A	301[A]	RET	C8-C9-C10	-3.90	112.96	118.94
4	2-A	301[B]	RET	C20-C13-C14	-3.50	113.15	123.66
4	1-A	301[A]	RET	C7-C6-C5	-3.11	114.12	121.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	1-A	300[A]	BOG	5	0
4	1-A	301[A]	RET	1	0
3	2-A	300[B]	BOG	3	0
4	2-A	301[B]	RET	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.