



wwPDB X-ray Structure Validation Summary Report i

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PDB ID : 2I36
Title : Crystal structure of trigonal crystal form of ground-state rhodopsin
Authors : Stenkamp, R.E.; Le Trong, I.; Lodowski, D.T.; Salom, D.; Palczewski, K.
Deposited on : 2006-08-17
Resolution : 4.10 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

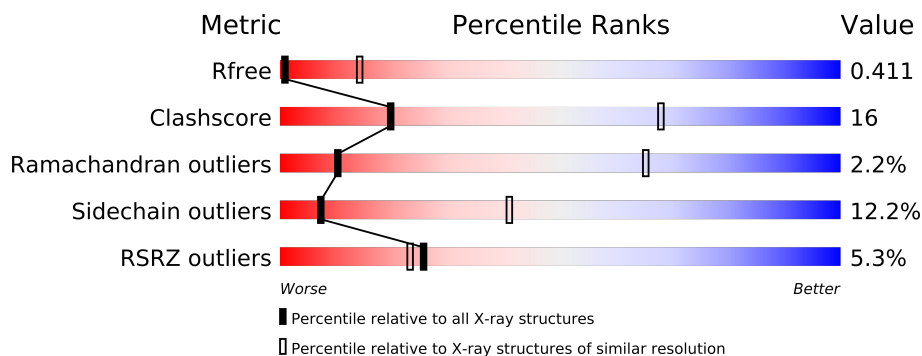
The following versions of software and data (see [references](#)) were used in the production of this report:

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 4.10 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	1002 (4.70-3.48)
Clashscore	79885	1248 (4.70-3.50)
Ramachandran outliers	78287	1183 (4.70-3.50)
Sidechain outliers	78261	1168 (4.70-3.50)
RSRZ outliers	66119	1002 (4.70-3.48)

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	349	
1	B	349	
1	C	349	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7883 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 Rhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	327	Total	C	N	O	S	0	0	0
			2595	1727	400	442	26			
1	B	315	Total	C	N	O	S	0	0	0
			2502	1667	384	427	24			
1	C	323	Total	C	N	O	S	0	0	0
			2568	1712	394	437	25			

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	3	Total	C	N	O	0	0
			39	22	2	15		
2	B	3	Total	C	N	O	0	0
			39	22	2	15		
2	C	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

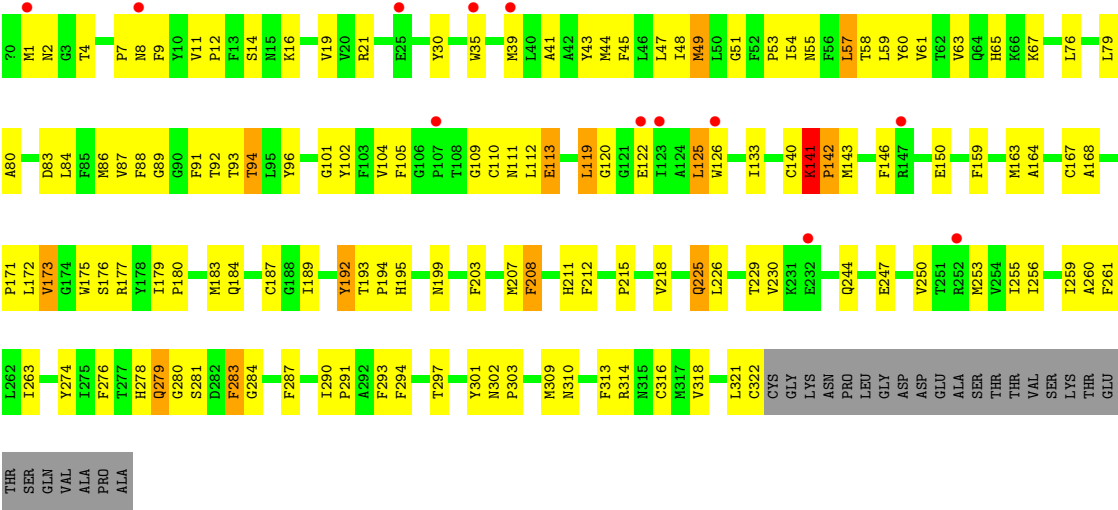
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		
3	C	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			17	16	1		

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, α , β , γ	159.87Å 159.87Å 142.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 4.10 29.83 – 4.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-4.10) 99.8 (29.83-4.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 4.11Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.382 , 0.412 0.388 , 0.411	Depositor DCC
R_{free} test set	832 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	200.1	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.13 , -10.0	EDS
Estimated twinning fraction	0.069 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 16375 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	7883	wwPDB-VP
Average B, all atoms (Å ²)	185.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% 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: PLM, NAG, ACE, MAN

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	0.50	0/2675	0.59	0/3645
1	B	0.54	2/2579 (0.1%)	0.60	3/3514 (0.1%)
1	C	0.60	1/2648 (0.0%)	0.58	0/3610
All	All	0.55	3/7902 (0.0%)	0.59	3/10769 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	141	LYS	CE-NZ	17.19	1.92	1.49
1	B	148	PHE	CG-CD2	7.43	1.50	1.38
1	B	148	PHE	CE1-CZ	5.81	1.48	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	148	PHE	CB-CG-CD1	-5.52	116.94	120.80
1	B	322	CYS	CA-C-N	-5.35	105.43	117.20
1	B	57	LEU	CA-CB-CG	5.14	127.13	115.30

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	2595	0	2569	87	0
1	B	2502	0	2469	85	0
1	C	2568	0	2543	85	0
2	A	39	0	34	1	0
2	B	39	0	34	5	0
2	C	39	0	34	2	0
3	A	28	0	25	1	0
3	B	28	0	25	0	0
3	C	28	0	25	1	0
4	A	17	0	31	0	0
All	All	7883	0	7789	252	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 16.

The worst 5 of 252 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:141:LYS:NZ	1:C:141:LYS:CE	1.92	1.29
1:A:179:ILE:HG13	1:A:180:PRO:HD2	1.54	0.88
2:B:505:NAG:H2	2:C:505:NAG:H83	1.60	0.84
1:C:179:ILE:HG13	1:C:180:PRO:HD2	1.63	0.81
1:B:179:ILE:HG13	1:B:180:PRO:HD2	1.65	0.78

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	325/349 (93%)	270 (83%)	47 (14%)	8 (2%)	9	62
1	B	311/349 (89%)	265 (85%)	40 (13%)	6 (2%)	12	68
1	C	321/349 (92%)	270 (84%)	44 (14%)	7 (2%)	10	65
All	All	957/1047 (91%)	805 (84%)	131 (14%)	21 (2%)	10	65

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	279	GLN
1	B	279	GLN
1	C	279	GLN
1	A	111	ASN
1	A	144	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	278/296 (94%)	242 (87%)	36 (13%)	6	38
1	B	266/296 (90%)	235 (88%)	31 (12%)	8	43
1	C	275/296 (93%)	242 (88%)	33 (12%)	7	41
All	All	819/888 (92%)	719 (88%)	100 (12%)	7	41

5 of 100 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	96	TYR
1	B	183	MET
1	C	207	MET
1	B	113	GLU
1	B	150	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	73	ASN
1	B	199	ASN
1	C	73	ASN
1	A	310	ASN
1	C	8	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 ⓘ

15 carbohydrates 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	MAN	A	503	2	10,11,12	0.59	0	11,15,17	1.42	1 (9%)
2	NAG	A	504	2	12,14,15	0.90	1 (8%)	15,19,21	1.31	2 (13%)
2	NAG	A	505	1,2	12,14,15	0.86	0	15,19,21	1.58	3 (20%)
3	NAG	A	704	3	12,14,15	0.64	0	15,19,21	1.52	1 (6%)
3	NAG	A	705	1,3	12,14,15	0.70	0	15,19,21	1.66	2 (13%)
2	MAN	B	503	2	10,11,12	0.60	0	11,15,17	1.55	3 (27%)
2	NAG	B	504	2	12,14,15	0.62	0	15,19,21	0.73	0
2	NAG	B	505	1,2	12,14,15	0.69	1 (8%)	15,19,21	1.55	1 (6%)
3	NAG	B	704	3	12,14,15	0.47	0	15,19,21	1.10	2 (13%)
3	NAG	B	705	1,3	12,14,15	0.61	0	15,19,21	1.33	3 (20%)
2	MAN	C	503	2	10,11,12	0.65	0	11,15,17	1.87	3 (27%)
2	NAG	C	504	2	12,14,15	0.52	0	15,19,21	1.10	1 (6%)
2	NAG	C	505	1,2	12,14,15	0.71	0	15,19,21	1.64	4 (26%)
3	NAG	C	704	3	12,14,15	0.49	0	15,19,21	1.29	1 (6%)
3	NAG	C	705	1,3	12,14,15	0.72	0	15,19,21	1.51	3 (20%)

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	MAN	A	503	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	504	2	-	0/6/23/26	0/1/1/1
2	NAG	A	505	1,2	-	0/6/23/26	0/1/1/1
3	NAG	A	704	3	-	0/6/23/26	0/1/1/1
3	NAG	A	705	1,3	-	0/6/23/26	0/1/1/1
2	MAN	B	503	2	-	0/2/19/22	0/1/1/1
2	NAG	B	504	2	-	1/6/23/26	0/1/1/1
2	NAG	B	505	1,2	-	1/6/23/26	0/1/1/1
3	NAG	B	704	3	-	0/6/23/26	0/1/1/1
3	NAG	B	705	1,3	-	0/6/23/26	0/1/1/1
2	MAN	C	503	2	-	0/2/19/22	0/1/1/1
2	NAG	C	504	2	-	0/6/23/26	0/1/1/1
2	NAG	C	505	1,2	-	0/6/23/26	0/1/1/1
3	NAG	C	704	3	-	0/6/23/26	0/1/1/1
3	NAG	C	705	1,3	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	504	NAG	O5-C5	-2.65	1.40	1.45
2	B	505	NAG	O5-C5	-2.07	1.41	1.45

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	704	NAG	O5-C5-C6	5.00	112.23	106.98
2	B	505	NAG	C3-C2-N2	-4.59	104.78	111.76
3	A	705	NAG	O5-C5-C6	4.55	111.75	106.98
3	C	704	NAG	O5-C5-C6	4.22	111.41	106.98
2	A	503	MAN	O5-C5-C6	4.20	111.39	106.98

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	504	NAG	O7-C7-N2-C2
2	B	505	NAG	O7-C7-N2-C2

There are no ring outliers.

5.6 Ligand geometry ⓘ

1 ligand is 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	$\# Z > 2$
4	PLM	A	401	1	16,16,17	4.06	1 (6%)	13,15,17	0.60	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
4	PLM	A	401	1	-	0/13/14/15	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	401	PLM	O2-C1	16.14	1.22	1.11

There are no bond angle outliers.

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	327/349 (93%)	0.24	17 (5%) 26 23	185, 185, 185, 185	0
1	B	315/349 (90%)	0.32	22 (6%) 16 17	185, 185, 185, 185	0
1	C	323/349 (92%)	0.16	12 (3%) 39 32	185, 185, 185, 185	0
All	All	965/1047 (92%)	0.24	51 (5%) 25 23	185, 185, 185, 185	0

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	185	CYS	6.3
1	A	67	LYS	6.1
1	B	243	THR	5.0
1	A	185	CYS	4.6
1	B	244	GLN	4.6

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 ⓘ

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	NAG	B	504	14/15	0.17	-	185,185,185,185	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	B	704	14/15	0.59	-	185,185,185,185	0
3	NAG	C	704	14/15	0.33	-	185,185,185,185	0
3	NAG	B	705	14/15	0.34	-	185,185,185,185	0
3	NAG	C	705	14/15	0.18	-	185,185,185,185	0
2	NAG	C	505	14/15	0.18	-	185,185,185,185	0
2	NAG	A	505	14/15	0.19	-	185,185,185,185	0
2	NAG	B	505	14/15	0.13	-	185,185,185,185	0
2	MAN	C	503	11/12	0.17	-	185,185,185,185	0
2	NAG	A	504	14/15	0.12	-	185,185,185,185	0
2	MAN	A	503	11/12	0.21	-	185,185,185,185	0
2	NAG	C	504	14/15	0.27	-	185,185,185,185	0
3	NAG	A	705	14/15	0.19	-	185,185,185,185	0
2	MAN	B	503	11/12	0.23	-	185,185,185,185	0
3	NAG	A	704	14/15	0.35	-	185,185,185,185	0

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(\AA^2)	Q<0.9
4	PLM	A	401	17/18	0.15	-	185,185,185,185	0

6.5 Other polymers ⓘ

There are no such residues in this entry.