



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Apr 6, 2019 – 01:45 PM EDT

PDB ID : 6CMO
EMDB ID: : EMD-7517
Title : Rhodopsin-Gi complex
Authors : Kang, Y.; Kuybeda, O.; de Waal, P.W.; Mukherjee, S.; Van Eps, N.; Dutka, P.; Zhou, X.E.; Bartesaghi, A.; Erramilli, S.; Morizumi, T.; Gu, X.; Yin, Y.; Liu, P.; Jiang, Y.; Meng, X.; Zhao, G.; Melcher, K.; Earnst, O.P.; Kossiakoff, A.A.; Subramaniam, S.; Xu, H.E.
Deposited on : 2018-03-05
Resolution : 4.50 Å(reported)

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20031633

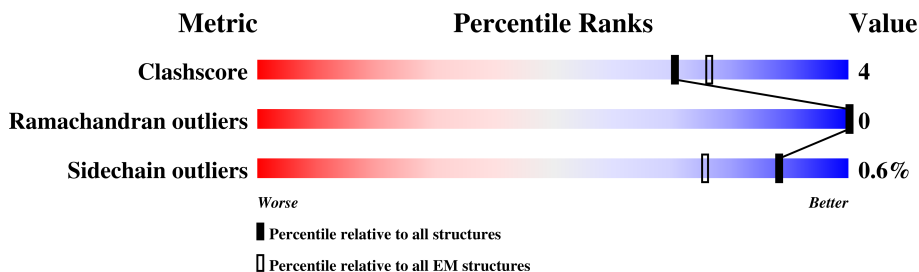
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	R	463	61% (green), 8% (yellow), 30% (grey)
2	A	354	86% (green), 14% (yellow)
3	B	345	86% (green), 12% (yellow), . (grey)
4	G	68	75% (green), 10% (yellow), 15% (grey)
5	L	215	85% (green), 13% (yellow), . (grey)
6	H	239	91% (green), 5% (yellow), . (grey)

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 11834 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 chimera protein of Soluble cytochrome b562 and Rhodopsin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	R	323	2567	1714	393	434	26	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-139	PHE	-	expression tag	UNP P0ABE7
R	-138	ALA	-	expression tag	UNP P0ABE7
R	-137	ASP	-	expression tag	UNP P0ABE7
R	-136	TYR	-	expression tag	UNP P0ABE7
R	-135	LYS	-	expression tag	UNP P0ABE7
R	-134	ASP	-	expression tag	UNP P0ABE7
R	-133	ASP	-	expression tag	UNP P0ABE7
R	-132	ASP	-	expression tag	UNP P0ABE7
R	-131	ASP	-	expression tag	UNP P0ABE7
R	-130	ALA	-	expression tag	UNP P0ABE7
R	-129	LYS	-	expression tag	UNP P0ABE7
R	-128	LEU	-	expression tag	UNP P0ABE7
R	-127	GLN	-	expression tag	UNP P0ABE7
R	-126	THR	-	expression tag	UNP P0ABE7
R	-125	MET	-	expression tag	UNP P0ABE7
R	-124	HIS	-	expression tag	UNP P0ABE7
R	-123	HIS	-	expression tag	UNP P0ABE7
R	-122	HIS	-	expression tag	UNP P0ABE7
R	-121	HIS	-	expression tag	UNP P0ABE7
R	-120	HIS	-	expression tag	UNP P0ABE7
R	-119	HIS	-	expression tag	UNP P0ABE7
R	-118	HIS	-	expression tag	UNP P0ABE7
R	-117	HIS	-	expression tag	UNP P0ABE7
R	-116	HIS	-	expression tag	UNP P0ABE7
R	-115	HIS	-	expression tag	UNP P0ABE7
R	-114	GLU	-	expression tag	UNP P0ABE7
R	-113	ASN	-	expression tag	UNP P0ABE7
R	-112	LEU	-	expression tag	UNP P0ABE7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
R	-111	TYR	-	expression tag	UNP P0ABE7
R	-110	PHE	-	expression tag	UNP P0ABE7
R	-109	GLN	-	expression tag	UNP P0ABE7
R	-108	GLY	-	expression tag	UNP P0ABE7
R	-107	GLY	-	expression tag	UNP P0ABE7
R	-106	THR	-	expression tag	UNP P0ABE7
R	-99	TRP	MET	conflict	UNP P0ABE7
R	-4	ILE	HIS	conflict	UNP P0ABE7
R	0	LEU	-	linker	UNP P0ABE7
R	1	MET	-	linker	UNP P0ABE7
R	2	CYS	-	linker	UNP P0ABE7
R	113	GLN	GLU	conflict	UNP P08100
R	257	TYR	MET	conflict	UNP P08100
R	282	CYS	ASN	conflict	UNP P08100

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	354	2834	1790	481	544	19	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	203	ALA	GLY	conflict	UNP P63096
A	326	SER	ALA	conflict	UNP P63096

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	B	340	2616	1612	470	513	21	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	MET	-	initiating methionine	UNP P54311
B	-3	GLY	-	expression tag	UNP P54311
B	-2	SER	-	expression tag	UNP P54311
B	-1	LEU	-	expression tag	UNP P54311
B	0	LEU	-	expression tag	UNP P54311

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	GLN	-	expression tag	UNP P54311

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	G	58	444	277	79	85	3	0	0

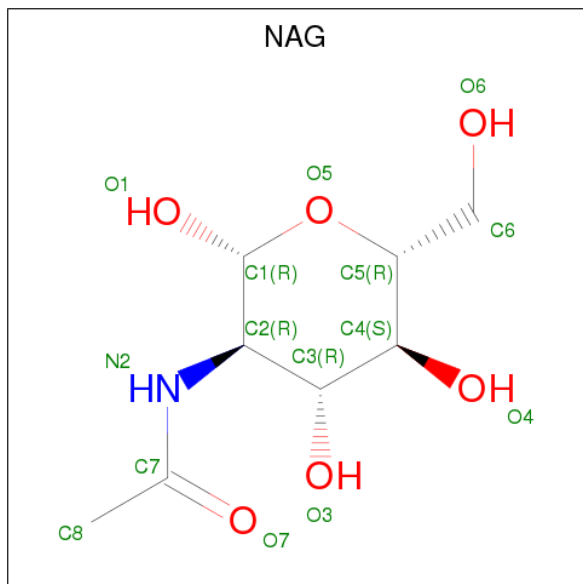
- Molecule 5 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	L	211	1602	997	270	329	6	0	0

- Molecule 6 is a protein called Fab Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	H	230	1743	1113	284	338	8	0	0

- Molecule 7 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	R	1	28	16	2	10	0

Continued on next page...

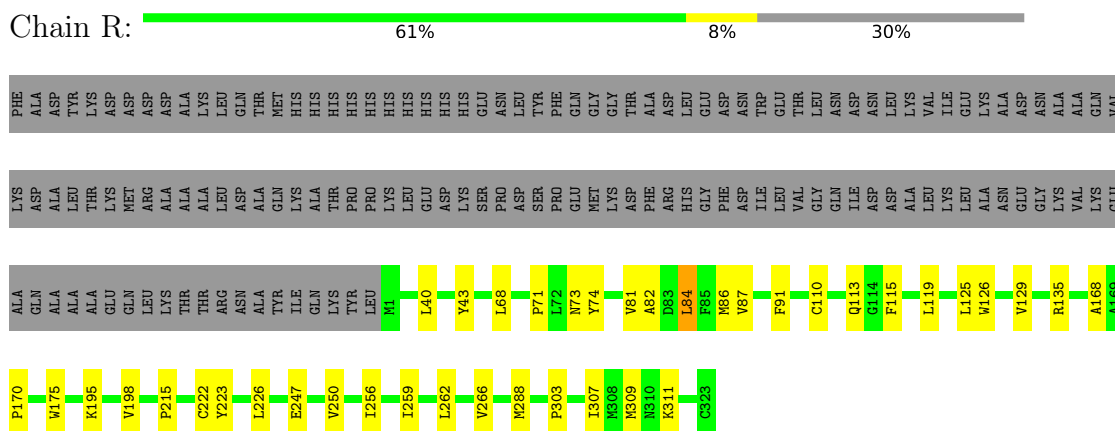
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	R	1	28	16	2	10	0

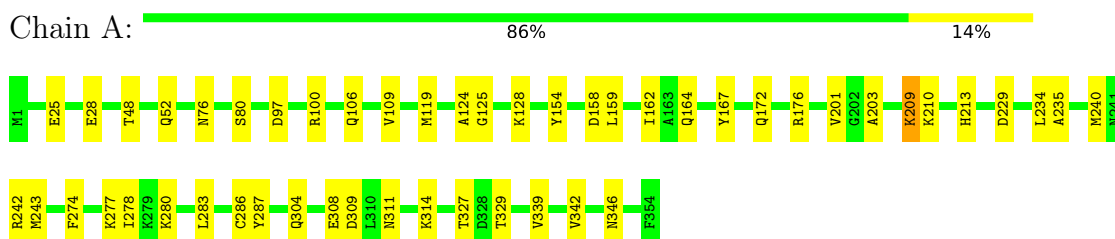
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

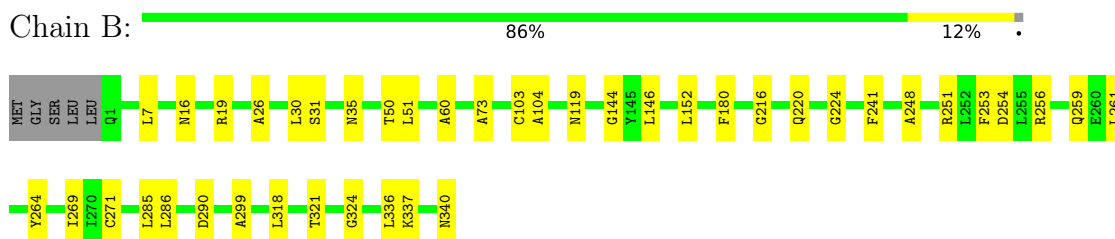
- Molecule 1: chimera protein of Soluble cytochrome b562 and Rhodopsin



- Molecule 2: Guanine nucleotide-binding protein G(i) subunit alpha-1



- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1



- Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2





- Molecule 5: Fab light chain

Chain L: 85% 13%



- Molecule 6: Fab Heavy chain

Chain H: 91% 5%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	227386	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.92	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

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: NAG

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 >2	RMSZ	# Z >2
1	R	0.33	0/2649	0.65	4/3611 (0.1%)
2	A	0.29	0/2881	0.61	1/3874 (0.0%)
3	B	0.28	0/2663	0.60	2/3609 (0.1%)
4	G	0.25	0/450	0.50	0/608
5	L	0.26	0/1634	0.54	0/2215
6	H	0.27	0/1794	0.56	0/2449
All	All	0.29	0/12071	0.60	7/16366 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	84	LEU	CA-CB-CG	6.81	130.96	115.30
1	R	40	LEU	CA-CB-CG	6.07	129.27	115.30
2	A	309	ASP	CB-CG-OD1	5.67	123.41	118.30
3	B	152	LEU	CA-CB-CG	5.46	127.85	115.30
1	R	43	TYR	CA-CB-CG	5.44	123.74	113.40

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	R	2567	0	2553	19	0
2	A	2834	0	2813	25	0
3	B	2616	0	2521	22	0
4	G	444	0	454	6	0
5	L	1602	0	1565	16	0
6	H	1743	0	1684	7	0
7	R	28	0	25	0	0
All	All	11834	0	11615	91	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 4.

The worst 5 of 91 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:R:115:PHE:O	1:R:119:LEU:HB2	1.91	0.70
1:R:87:VAL:O	1:R:91:PHE:HB2	1.93	0.68
5:L:90:GLN:HE22	5:L:92:SER:HB2	1.60	0.66
2:A:209:LYS:HG2	2:A:210:LYS:HG3	1.79	0.64
1:R:125:LEU:HD11	1:R:215:PRO:HG3	1.80	0.63

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 PDB entries followed by that with respect to all EM entries.

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	R	321/463 (69%)	319 (99%)	2 (1%)	0	100	100
2	A	352/354 (99%)	344 (98%)	8 (2%)	0	100	100
3	B	338/345 (98%)	335 (99%)	3 (1%)	0	100	100
4	G	56/68 (82%)	56 (100%)	0	0	100	100
5	L	209/215 (97%)	205 (98%)	4 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	H	228/239 (95%)	226 (99%)	2 (1%)	0	100	100
All	All	1504/1684 (89%)	1485 (99%)	19 (1%)	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 PDB entries followed by that with respect to all EM entries.

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	R	275/391 (70%)	273 (99%)	2 (1%)	85	92
2	A	306/306 (100%)	302 (99%)	4 (1%)	71	85
3	B	283/287 (99%)	282 (100%)	1 (0%)	92	95
4	G	47/56 (84%)	47 (100%)	0	100	100
5	L	186/190 (98%)	186 (100%)	0	100	100
6	H	193/202 (96%)	192 (100%)	1 (0%)	90	94
All	All	1290/1432 (90%)	1282 (99%)	8 (1%)	88	93

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	243	MET
6	H	31	ASN
2	A	346	ASN
2	A	209	LYS
2	A	283	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	220	GLN
3	B	259	GLN
5	L	91	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	119	ASN
5	L	90	GLN

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](#)

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
7	NAG	R	501	1,7	14,14,15	0.30	0	17,19,21	0.52	0
7	NAG	R	502	7	14,14,15	0.28	0	17,19,21	0.52	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
7	NAG	R	501	1,7	-	0/6/23/26	0/1/1/1
7	NAG	R	502	7	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.