



wwPDB EM Validation Summary Report ⓘ

Mar 27, 2026 – 03:51 AM UTC

PDB ID : 8P12 / pdb_00008p12
EMDB ID : EMD-17343
Title : Cryo-EM structure of Rhodopsin-Gi bound to antibody fragment Fab13
Authors : Pamula, F.; Tejero, O.; Muehle, J.; Thoma, R.; Schertler, G.F.X.; Marino, J.;
Tsai, C.-J.
Deposited on : 2023-05-11
Resolution : 3.21 Å (reported)
Based on initial models : 5EN0, 6CRK, 6CMO, ., 1GOT

This is a wwPDB EM Validation Summary Report for a publicly released PDB 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

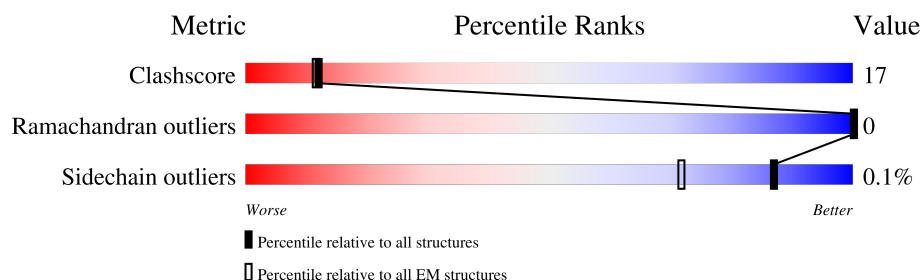
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.21 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	348	51% 38% 9%
2	A	376	38% 18% 44%
3	B	340	56% 37% 7%
4	G	74	24% 24% 51%
5	L	238	61% 31% 8%
6	H	258	63% 22% 16%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10266 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 Rhodopsin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	317	Total	C	N	O	S	0	0
			2530	1690	388	427	25		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	2	CYS	ASN	engineered mutation	UNP P02699
R	257	TYR	MET	engineered mutation	UNP P02699
R	282	CYS	ASP	engineered mutation	UNP P02699

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	210	Total	C	N	O	S	1	0
			1699	1085	282	319	13		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP P63096
A	-20	LYS	-	expression tag	UNP P63096
A	-19	LYS	-	expression tag	UNP P63096
A	-18	HIS	-	expression tag	UNP P63096
A	-17	HIS	-	expression tag	UNP P63096
A	-16	HIS	-	expression tag	UNP P63096
A	-15	HIS	-	expression tag	UNP P63096
A	-14	HIS	-	expression tag	UNP P63096
A	-13	HIS	-	expression tag	UNP P63096
A	-12	HIS	-	expression tag	UNP P63096
A	-11	HIS	-	expression tag	UNP P63096
A	-10	HIS	-	expression tag	UNP P63096
A	-9	HIS	-	expression tag	UNP P63096
A	-8	GLU	-	expression tag	UNP P63096

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ASN	-	expression tag	UNP P63096
A	-6	LEU	-	expression tag	UNP P63096
A	-5	TYR	-	expression tag	UNP P63096
A	-4	PHE	-	expression tag	UNP P63096
A	-3	GLN	-	expression tag	UNP P63096
A	-2	GLY	-	expression tag	UNP P63096
A	-1	GLY	-	expression tag	UNP P63096
A	0	SER	-	expression tag	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
3	B	316	Total	C	N	O	S	0	0
			2416	1494	429	472	21		

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(T) subunit gamma-T1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	36	Total	C	N	O	S	0	0
			293	183	47	60	3		

- Molecule 5 is a protein called Immunoglobulin G light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	219	Total	C	N	O	S	0	0
			1699	1063	287	342	7		

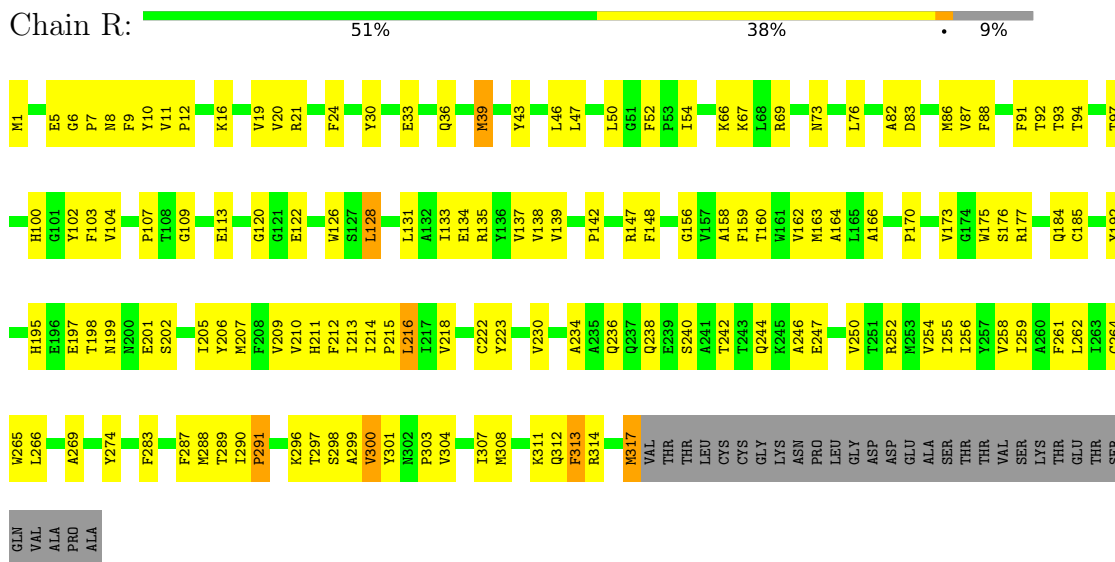
- Molecule 6 is a protein called Immunoglobulin G heavy chain FAB fragment.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	218	Total	C	N	O	S	0	0
			1629	1034	267	320	8		

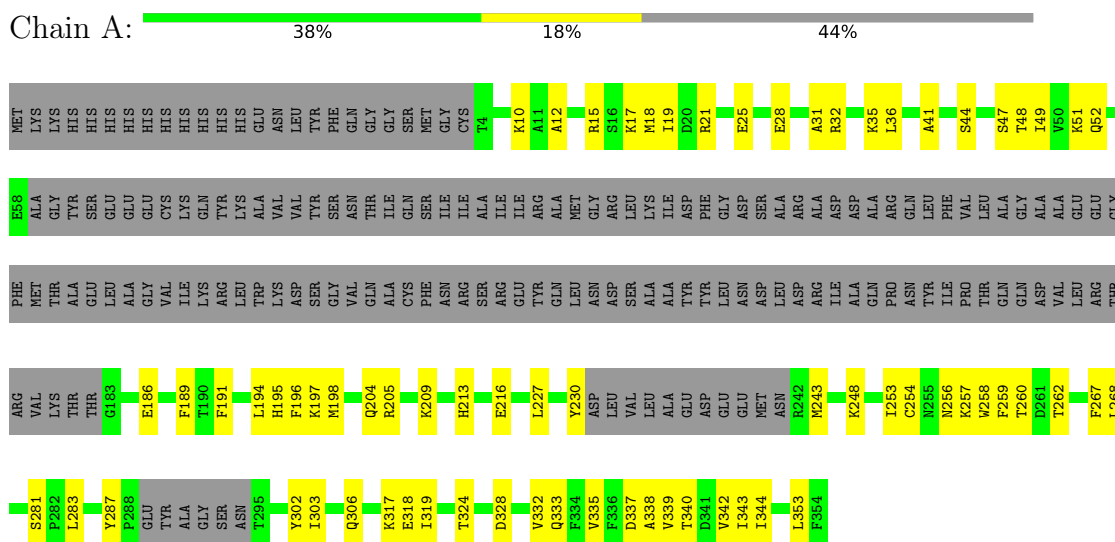
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Rhodopsin

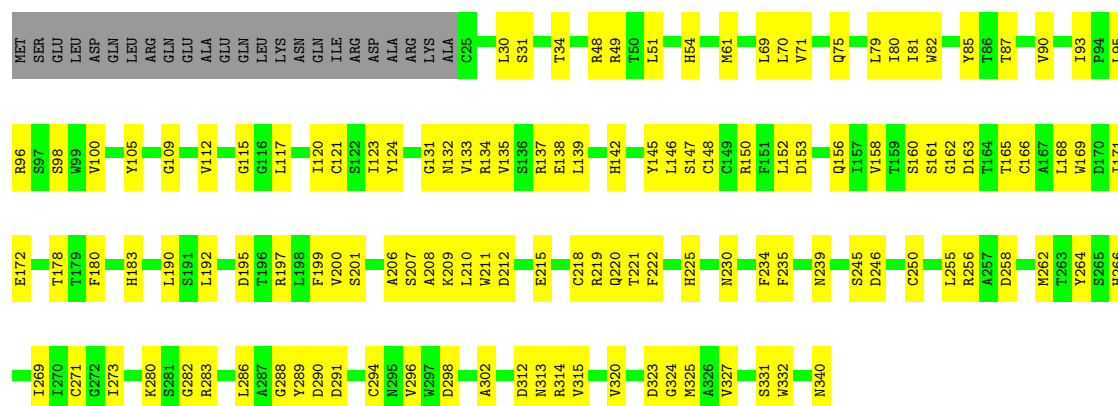


• Molecule 2: Guanine nucleotide-binding protein G(i) subunit alpha-1



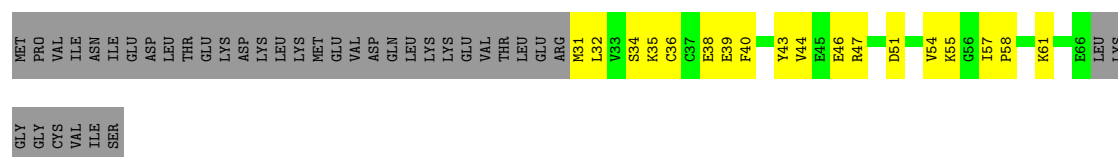
• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B: 



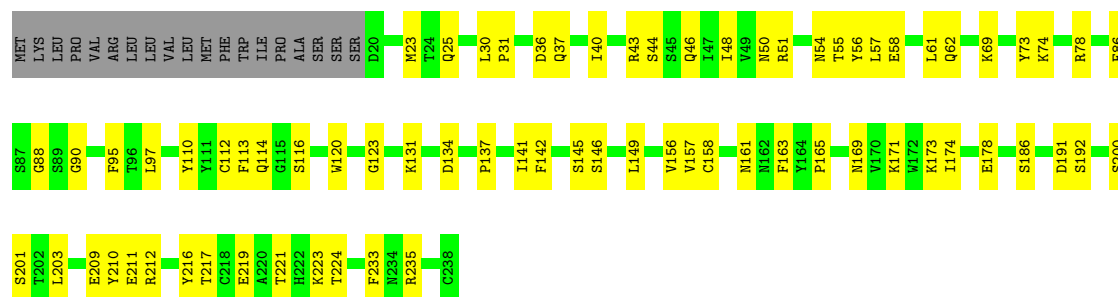
- Molecule 4: Guanine nucleotide-binding protein G(T) subunit gamma-T1

Chain G: 



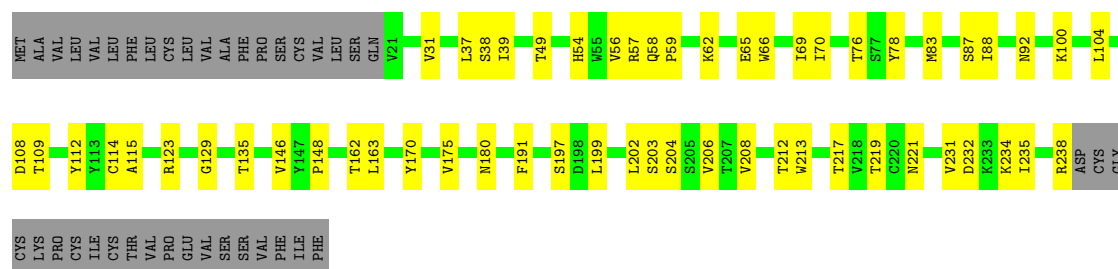
- Molecule 5: Immunoglobulin G light chain

Chain L: 



- Molecule 6: Immunoglobulin G heavy chain FAB fragment

Chain H: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	587113	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	66	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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	R	0.38	2/2613 (0.1%)	0.97	12/3561 (0.3%)
2	A	0.16	0/1727	0.47	0/2313
3	B	0.16	0/2463	0.46	0/3343
4	G	0.30	0/298	0.79	2/398 (0.5%)
5	L	0.14	0/1738	0.36	0/2360
6	H	0.15	0/1673	0.39	0/2290
All	All	0.24	2/10512 (0.0%)	0.62	14/14265 (0.1%)

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	R	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	291	PRO	CB-CG	-12.25	0.88	1.49
1	R	291	PRO	CG-CD	-8.50	1.21	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	291	PRO	N-CD-CG	-17.20	77.39	103.20
1	R	291	PRO	CA-CB-CG	-16.62	72.93	104.50
1	R	291	PRO	CB-CG-CD	16.32	158.31	106.10
4	G	58	PRO	N-CD-CG	-8.48	90.47	103.20
1	R	291	PRO	CA-N-CD	-7.84	101.02	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	R	312	GLN	Mainchain

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	R	2530	0	2503	115	0
2	A	1699	0	1689	56	0
3	B	2416	0	2317	95	0
4	G	293	0	280	11	0
5	L	1699	0	1632	53	0
6	H	1629	0	1597	40	0
All	All	10266	0	10018	351	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 17.

The worst 5 of 351 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:304:VAL:HA	1:R:308:MET:HG2	1.45	0.98
5:L:173:LYS:HB2	5:L:217:THR:HB	1.64	0.80
2:A:204:GLN:H	2:A:205:ARG:HH21	1.34	0.75
5:L:78:ARG:HH12	5:L:88:GLY:H	1.34	0.74
3:B:150:ARG:HB3	3:B:192:LEU:HD11	1.70	0.73

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 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	315/348 (90%)	295 (94%)	20 (6%)	0	100	100
2	A	203/376 (54%)	196 (97%)	7 (3%)	0	100	100
3	B	314/340 (92%)	301 (96%)	13 (4%)	0	100	100
4	G	34/74 (46%)	31 (91%)	3 (9%)	0	100	100
5	L	217/238 (91%)	214 (99%)	3 (1%)	0	100	100
6	H	216/258 (84%)	211 (98%)	5 (2%)	0	100	100
All	All	1299/1634 (80%)	1248 (96%)	51 (4%)	0	100	100

There are no Ramachandran outliers to report.

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 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	270/296 (91%)	269 (100%)	1 (0%)	84	85
2	A	187/325 (58%)	187 (100%)	0	100	100
3	B	262/283 (93%)	262 (100%)	0	100	100
4	G	34/70 (49%)	34 (100%)	0	100	100
5	L	195/213 (92%)	195 (100%)	0	100	100
6	H	186/223 (83%)	186 (100%)	0	100	100
All	All	1134/1410 (80%)	1133 (100%)	1 (0%)	87	89

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

Mol	Chain	Res	Type
1	R	128	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
2	A	256	ASN
2	A	306	GLN
5	L	66	GLN
3	B	155	ASN
2	A	244	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 Map visualisation

This section contains visualisations of the EMDB entry EMD-17343. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.