



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Jan 4, 2020 – 09:32 AM EST

PDB ID : 6E3Y  
EMDB ID: : EMD-8978  
Title : Cryo-EM structure of the active, Gs-protein complexed, human CGRP receptor  
Authors : Liang, Y.L.; Khoshouei, M.; Deganutti, G.; Glukhova, A.; Koole, C.; Peat, T.S.; Radjainia, M.; Plitzko, J.M.; Baumeister, W.; Miller, L.J.; Hay, D.L.; Christopoulos, A.; Reynolds, C.A.; Wootten, D.; Sexton, P.M.  
Deposited on : 2018-07-16  
Resolution : 3.30 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](mailto: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.

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MolProbity : 4.02b-467  
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) : 2.4

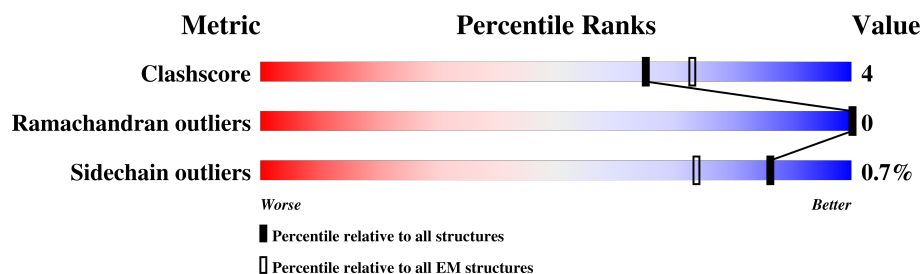
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 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  $\geq 3$ , 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	P	38	74% 18% 8%
2	N	138	81% 10% 9%
3	A	394	44% 52%
4	B	350	80% 16% .
5	G	71	65% 31%
6	R	490	61% 9% 29%
7	E	149	68% 9% 23%

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9434 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 Calcitonin gene-related peptide 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	P	35	Total	C	N	O	S	0	1
			240	149	45	44	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	38	NH2	-	amidation	UNP P06881

- Molecule 2 is a protein called Nanobody 35.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	N	126	Total	C	N	O	S	0	0
			961	599	168	188	6		

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	188	Total	C	N	O	S	0	0
			1578	1009	290	274	5		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	ASN	SER	engineered mutation	UNP P63092
A	226	ALA	GLY	engineered mutation	UNP P63092
A	268	ALA	GLU	engineered mutation	UNP P63092
A	271	LYS	ASN	engineered mutation	UNP P63092
A	274	ASP	LYS	engineered mutation	UNP P63092
A	280	LYS	ARG	engineered mutation	UNP P63092
A	284	ASP	THR	engineered mutation	UNP P63092
A	285	THR	ILE	engineered mutation	UNP P63092

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	336	Total	C	N	O	S	0	0
			2545	1573	455	496	21		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	MET	-	initiating methionine	UNP P62873
B	-8	HIS	-	expression tag	UNP P62873
B	-7	HIS	-	expression tag	UNP P62873
B	-6	HIS	-	expression tag	UNP P62873
B	-5	HIS	-	expression tag	UNP P62873
B	-4	HIS	-	expression tag	UNP P62873
B	-3	HIS	-	expression tag	UNP P62873
B	-2	GLY	-	expression tag	UNP P62873
B	-1	SER	-	expression tag	UNP P62873
B	0	SER	-	expression tag	UNP P62873
B	1	GLY	-	expression tag	UNP P62873

- Molecule 5 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	49	Total	C	N	O	S	0	0
			372	234	63	72	3		

- Molecule 6 is a protein called Calcitonin gene-related peptide type 1 receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	346	Total	C	N	O	S	0	0
			2813	1859	459	471	24		

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-9	MET	-	initiating methionine	UNP Q16602
R	-8	LYS	-	expression tag	UNP Q16602
R	-7	THR	-	expression tag	UNP Q16602
R	-6	ILE	-	expression tag	UNP Q16602
R	-5	ILE	-	expression tag	UNP Q16602
R	-4	ALA	-	expression tag	UNP Q16602

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-3	LEU	-	expression tag	UNP Q16602
R	-2	SER	-	expression tag	UNP Q16602
R	-1	TYR	-	expression tag	UNP Q16602
R	0	ILE	-	expression tag	UNP Q16602
R	1	PHE	-	expression tag	UNP Q16602
R	2	CYS	-	expression tag	UNP Q16602
R	3	LEU	-	expression tag	UNP Q16602
R	4	VAL	-	expression tag	UNP Q16602
R	5	PHE	-	expression tag	UNP Q16602
R	6	ALA	-	expression tag	UNP Q16602
R	7	ASP	-	expression tag	UNP Q16602
R	8	TYR	-	expression tag	UNP Q16602
R	9	LYS	-	expression tag	UNP Q16602
R	10	ASP	-	expression tag	UNP Q16602
R	11	ASP	-	expression tag	UNP Q16602
R	12	ASP	-	expression tag	UNP Q16602
R	13	ASP	-	expression tag	UNP Q16602
R	14	LEU	-	expression tag	UNP Q16602
R	15	GLU	-	expression tag	UNP Q16602
R	16	VAL	-	expression tag	UNP Q16602
R	17	LEU	-	expression tag	UNP Q16602
R	18	PHE	-	expression tag	UNP Q16602
R	19	GLN	-	expression tag	UNP Q16602
R	20	GLY	-	expression tag	UNP Q16602
R	21	PRO	-	expression tag	UNP Q16602
R	462	PRO	-	expression tag	UNP Q16602
R	463	ALA	-	expression tag	UNP Q16602
R	464	GLY	-	expression tag	UNP Q16602
R	465	LEU	-	expression tag	UNP Q16602
R	466	GLU	-	expression tag	UNP Q16602
R	467	VAL	-	expression tag	UNP Q16602
R	468	LEU	-	expression tag	UNP Q16602
R	469	PHE	-	expression tag	UNP Q16602
R	470	GLN	-	expression tag	UNP Q16602
R	471	GLY	-	expression tag	UNP Q16602
R	472	PRO	-	expression tag	UNP Q16602
R	473	HIS	-	expression tag	UNP Q16602
R	474	HIS	-	expression tag	UNP Q16602
R	475	HIS	-	expression tag	UNP Q16602
R	476	HIS	-	expression tag	UNP Q16602
R	477	HIS	-	expression tag	UNP Q16602
R	478	HIS	-	expression tag	UNP Q16602

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Chain	Residue	Modelled	Actual	Comment	Reference
R	479	HIS	-	expression tag	UNP Q16602
R	480	HIS	-	expression tag	UNP Q16602

- Molecule 7 is a protein called Receptor activity-modifying protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	115	Total	C	N	O	S	0	0
			925	600	158	160	7		

There are 27 discrepancies between the modelled and reference sequences:

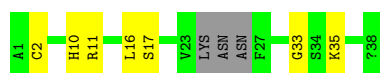
Chain	Residue	Modelled	Actual	Comment	Reference
E	0	MET	-	initiating methionine	UNP O60894
E	1	LYS	-	expression tag	UNP O60894
E	2	THR	-	expression tag	UNP O60894
E	3	ILE	-	expression tag	UNP O60894
E	4	ILE	-	expression tag	UNP O60894
E	5	ALA	-	expression tag	UNP O60894
E	6	LEU	-	expression tag	UNP O60894
E	7	SER	-	expression tag	UNP O60894
E	8	TYR	-	expression tag	UNP O60894
E	9	ILE	-	expression tag	UNP O60894
E	10	PHE	-	expression tag	UNP O60894
E	11	CYS	-	expression tag	UNP O60894
E	12	LEU	-	expression tag	UNP O60894
E	13	VAL	-	expression tag	UNP O60894
E	14	PHE	-	expression tag	UNP O60894
E	15	ALA	-	expression tag	UNP O60894
E	16	ASP	-	expression tag	UNP O60894
E	17	TYR	-	expression tag	UNP O60894
E	18	LYS	-	expression tag	UNP O60894
E	19	ASP	-	expression tag	UNP O60894
E	20	ASP	-	expression tag	UNP O60894
E	21	ASP	-	expression tag	UNP O60894
E	22	ASP	-	expression tag	UNP O60894
E	23	LYS	-	expression tag	UNP O60894
E	24	HIS	-	expression tag	UNP O60894
E	25	GLY	-	expression tag	UNP O60894
E	26	SER	-	expression tag	UNP O60894

### 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: Calcitonin gene-related peptide 1

Chain P: 



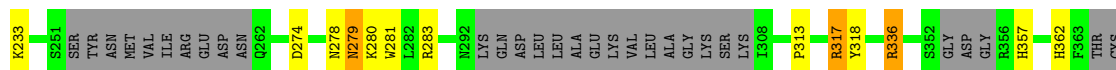
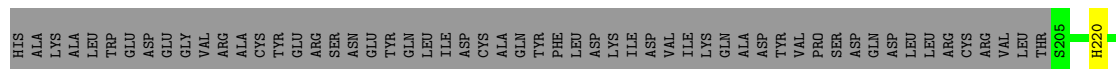
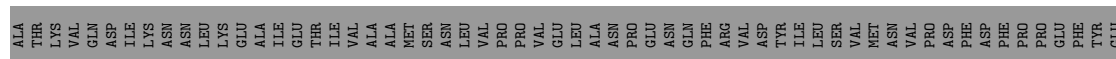
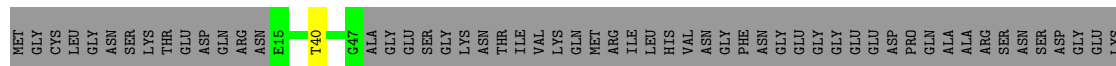
- Molecule 2: Nanobody 35

Chain N: 




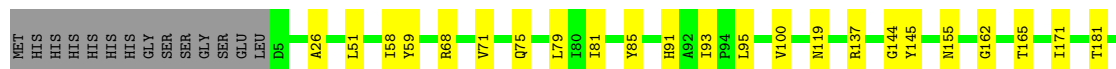
- Molecule 3: Guanine nucleotide-binding protein G(s) subunit alpha isoforms short

Chain A: 



- Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B: 





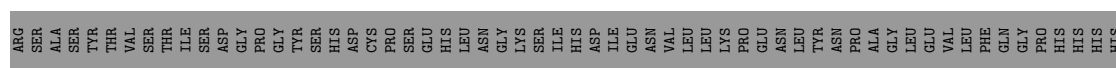
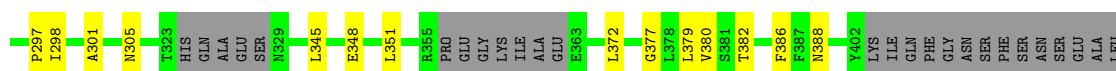
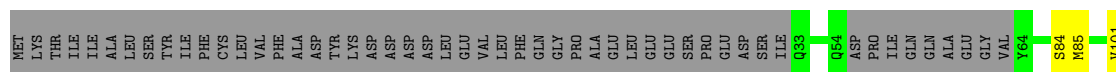
- Molecule 5: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain G: 65% 31%



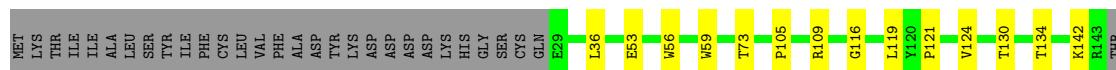
- Molecule 6: Calcitonin gene-related peptide type 1 receptor

Chain R: 61% 9% 29%



- Molecule 7: Receptor activity-modifying protein 1

Chain E: 68% 9% 23%





## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	407000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; phase plate CTF correction	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50.0	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	47170	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: NH2

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	P	0.32	0/241	0.53	0/325
2	N	0.43	0/981	0.58	0/1329
3	A	0.38	0/1610	0.54	0/2162
4	B	0.43	0/2592	0.60	0/3519
5	G	0.31	0/378	0.51	0/513
6	R	0.38	0/2893	0.60	1/3942 (0.0%)
7	E	0.33	0/952	0.53	0/1299
All	All	0.39	0/9647	0.58	1/13089 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	252	LEU	CA-CB-CG	5.33	127.55	115.30

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	P	240	0	243	6	0
2	N	961	0	928	9	0
3	A	1578	0	1552	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2545	0	2427	32	0
5	G	372	0	367	2	0
6	R	2813	0	2778	27	0
7	E	925	0	903	9	0
All	All	9434	0	9198	83	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 83 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)
6:R:297:PRO:HB3	7:E:130:THR:HG21	1.74	0.68
4:B:71:VAL:HG22	4:B:81:ILE:HG12	1.77	0.65
3:A:313:PRO:O	3:A:317:ARG:NH1	2.32	0.63
6:R:172:GLN:HE21	6:R:252:LEU:HB2	1.65	0.61
4:B:95:LEU:HD13	4:B:100:VAL:HG21	1.83	0.61

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	P	31/38 (82%)	29 (94%)	2 (6%)	0	100	100
2	N	124/138 (90%)	120 (97%)	4 (3%)	0	100	100
3	A	176/394 (45%)	176 (100%)	0	0	100	100
4	B	334/350 (95%)	317 (95%)	17 (5%)	0	100	100
5	G	47/71 (66%)	47 (100%)	0	0	100	100
6	R	336/490 (69%)	329 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	E	113/149 (76%)	113 (100%)	0	0	100	100
All	All	1161/1630 (71%)	1131 (97%)	30 (3%)	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	P	26/29 (90%)	26 (100%)	0	100	100
2	N	104/115 (90%)	104 (100%)	0	100	100
3	A	166/349 (48%)	163 (98%)	3 (2%)	62	81
4	B	270/291 (93%)	269 (100%)	1 (0%)	92	95
5	G	39/58 (67%)	39 (100%)	0	100	100
6	R	306/437 (70%)	303 (99%)	3 (1%)	78	87
7	E	98/129 (76%)	98 (100%)	0	100	100
All	All	1009/1408 (72%)	1002 (99%)	7 (1%)	86	91

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	155	ASN
6	R	388	ASN
6	R	208	ASN
3	A	317	ARG
6	R	226	ASN

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

Mol	Chain	Res	Type
4	B	155	ASN
4	B	259	GLN

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Mol	Chain	Res	Type
6	R	54	GLN
4	B	88	ASN
6	R	50	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](#)

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.