



## wwPDB EM Validation Summary Report ⓘ

Nov 5, 2024 – 10:53 AM JST

PDB ID : 8ZPT  
EMDB ID : EMD-60354  
Title : Cryo-EM structure of prolactin-releasing peptide recognition with Gq  
Authors : Zhao, L.; Li, Y.; Yuan, Q.; Xu, H.E.  
Deposited on : 2024-05-31  
Resolution : 2.96 Å(reported)

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

The types of validation reports are described at

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

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

EMDB validation analysis : **FAILED**  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

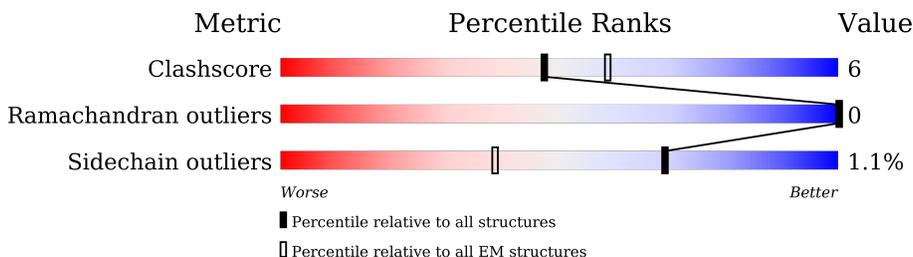
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.96 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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	A	361	
2	B	371	
3	E	247	
4	G	70	
5	L	21	
6	R	370	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9151 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 Guanine nucleotide-binding protein G(324) subunit alpha-1,.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	229	1875	1187	332	348	8	0	0

- Molecule 2 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		
2	B	336	2577	1590	462	504	21	0	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP P62873
B	2	GLY	-	expression tag	UNP P62873
B	3	SER	-	expression tag	UNP P62873
B	4	LEU	-	expression tag	UNP P62873
B	5	LEU	-	expression tag	UNP P62873
B	6	GLN	-	expression tag	UNP P62873
B	346	GLY	-	expression tag	UNP P62873
B	347	SER	-	expression tag	UNP P62873
B	348	SER	-	expression tag	UNP P62873
B	349	GLY	-	expression tag	UNP P62873
B	350	GLY	-	expression tag	UNP P62873
B	351	GLY	-	expression tag	UNP P62873
B	352	GLY	-	expression tag	UNP P62873
B	353	SER	-	expression tag	UNP P62873
B	354	GLY	-	expression tag	UNP P62873
B	355	GLY	-	expression tag	UNP P62873
B	356	GLY	-	expression tag	UNP P62873
B	357	GLY	-	expression tag	UNP P62873
B	358	SER	-	expression tag	UNP P62873
B	359	SER	-	expression tag	UNP P62873

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Chain	Residue	Modelled	Actual	Comment	Reference
B	360	GLY	-	expression tag	UNP P62873
B	361	VAL	-	expression tag	UNP P62873
B	362	SER	-	expression tag	UNP P62873
B	363	GLY	-	expression tag	UNP P62873
B	364	TRP	-	expression tag	UNP P62873
B	365	ARG	-	expression tag	UNP P62873
B	366	LEU	-	expression tag	UNP P62873
B	367	PHE	-	expression tag	UNP P62873
B	368	LYS	-	expression tag	UNP P62873
B	369	LYS	-	expression tag	UNP P62873
B	370	ILE	-	expression tag	UNP P62873
B	371	SER	-	expression tag	UNP P62873

- Molecule 3 is a protein called scfv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	232	1782	1131	295	346	10	0	0

- 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	53	403	254	72	74	3	0	0

- Molecule 5 is a protein called Prolactin-releasing peptide PrRP20.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	L	21	162	104	32	26	0	1

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	21	NH2	-	amidation	UNP P81277

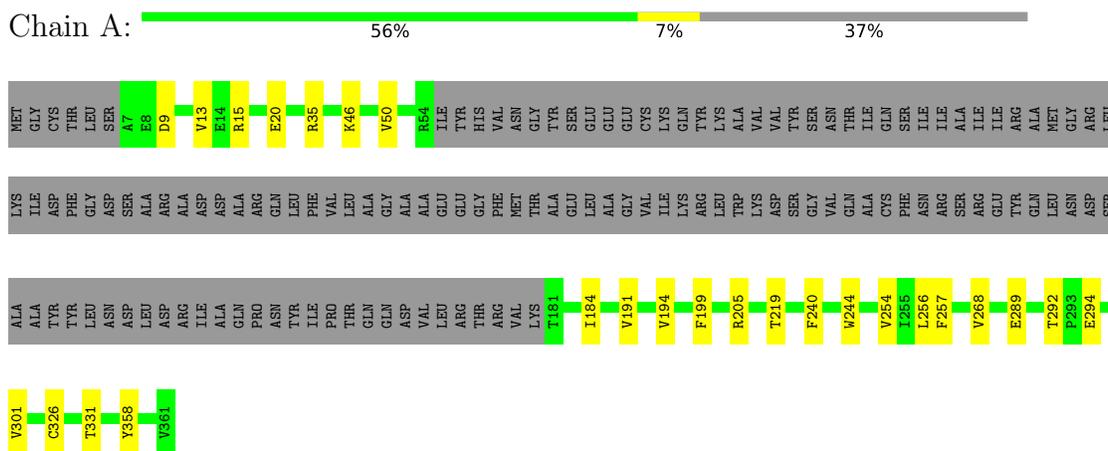
- Molecule 6 is a protein called Prolactin-releasing peptide receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	R	292	2352	1561	408	372	11	0	0

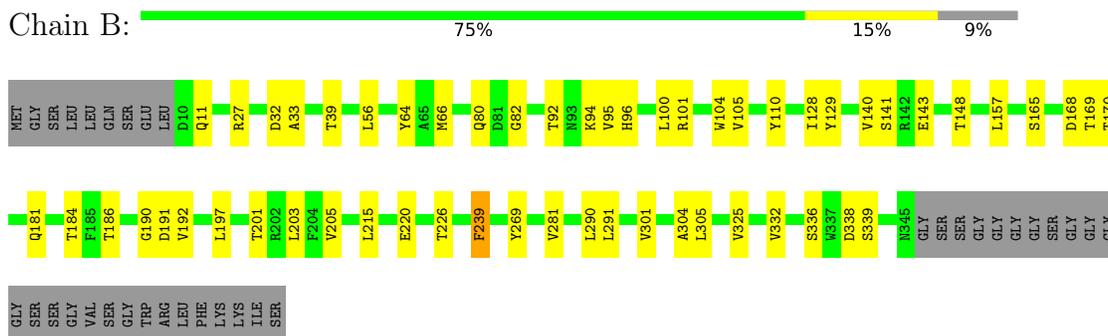
### 3 Residue-property plots [i](#)

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.

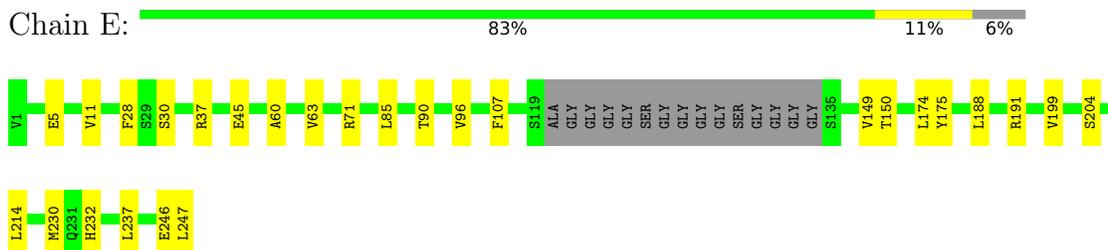
- Molecule 1: Guanine nucleotide-binding protein G(324) subunit alpha-1,



- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1



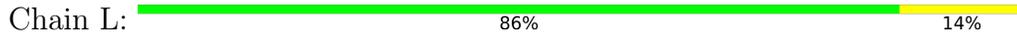
- Molecule 3: scfv16



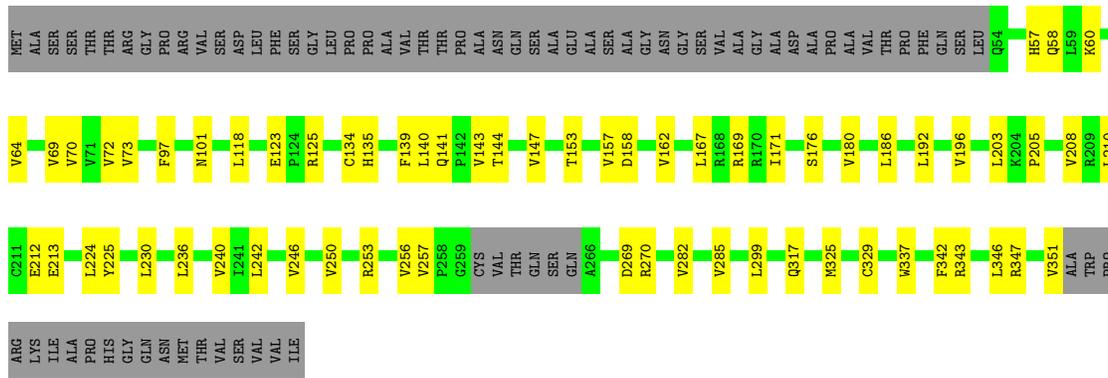
- Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



- Molecule 5: Prolactin-releasing peptide PrRP20



- Molecule 6: Prolactin-releasing peptide receptor



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	634723	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 ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	8000	Depositor
Maximum defocus (nm)	18000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

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  >5	RMSZ	# Z  >5
1	A	0.24	0/1909	0.48	0/2571
2	B	0.24	0/2624	0.50	0/3559
3	E	0.25	0/1826	0.48	0/2476
4	G	0.25	0/409	0.42	0/552
5	L	0.26	0/167	0.56	0/228
6	R	0.24	0/2414	0.48	0/3304
All	All	0.24	0/9349	0.49	0/12690

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	A	1875	0	1863	17	0
2	B	2577	0	2477	36	0
3	E	1782	0	1724	17	0
4	G	403	0	412	2	0
5	L	162	0	159	3	0
6	R	2352	0	2459	37	0
All	All	9151	0	9094	106	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 6.

The worst 5 of 106 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:35:ARG:O	1:A:219:THR:OG1	1.97	0.80
1:A:256:LEU:HD13	1:A:326:CYS:SG	2.21	0.80
2:B:56:LEU:HD13	2:B:92:THR:HG23	1.70	0.74
2:B:181:GLN:NE2	2:B:184:THR:OG1	2.21	0.73
2:B:281:VAL:HG13	2:B:290:LEU:HD21	1.69	0.73

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	A	225/361 (62%)	223 (99%)	2 (1%)	0	100	100
2	B	334/371 (90%)	330 (99%)	4 (1%)	0	100	100
3	E	228/247 (92%)	228 (100%)	0	0	100	100
4	G	51/70 (73%)	51 (100%)	0	0	100	100
5	L	19/21 (90%)	18 (95%)	1 (5%)	0	100	100
6	R	288/370 (78%)	269 (93%)	19 (7%)	0	100	100
All	All	1145/1440 (80%)	1119 (98%)	26 (2%)	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	A	204/315 (65%)	204 (100%)	0	100	100
2	B	278/302 (92%)	274 (99%)	4 (1%)	62	79
3	E	196/198 (99%)	195 (100%)	1 (0%)	86	93
4	G	41/57 (72%)	40 (98%)	1 (2%)	44	68
5	L	16/16 (100%)	16 (100%)	0	100	100
6	R	256/317 (81%)	251 (98%)	5 (2%)	50	72
All	All	991/1205 (82%)	980 (99%)	11 (1%)	69	83

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	R	253	ARG
6	R	325	MET
6	R	343	ARG
6	R	337	TRP
3	E	191	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	181	GLN
2	B	235	ASN

### 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.