W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB EM Validation Summary Report ⓘ

Oct 16, 2024 – 12:34 AM JST

PDB ID	:	8JIS
EMDB ID	:	EMD-36326
Title	:	Cryo-EM structure of the GLP-1R/GCGR dual agonist peptide15-bound human GLP-1R-Gs complex
Authors	:	Yang, L.; Zhou, Q.T.; Dai, A.T.; Zhao, F.H.; Chang, R.L.; Ying, T.L.; Wu, B.L.; Yang, D.H.; Wang, M.W.; Cong, Z.T.
Deposited on	:	2023-05-27
Resolution	:	2.46 Å(reported)

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 ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.46 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	Percentile Ranks	Value
Clashscore		8
Ramachandran outliers		0.9%
Sidechain outliers		15.5%

Worse   *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures
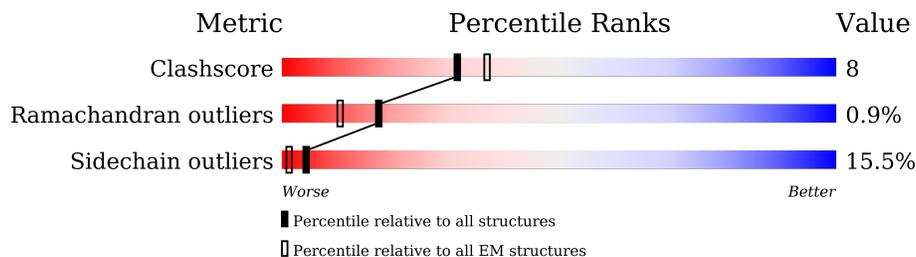
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	356	47% 17% • 33%
2	B	338	79% 18% •
3	P	29	76% 21% •
4	G	57	75% 19% 5%
5	N	126	70% 25% 5% •
6	R	394	75% 20% • •

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 9158 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(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	238	1856	1166	338	344	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	338	2572	1591	457	503	21	0	0

- Molecule 3 is a protein called Peptide 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	P	29	238	152	37	48	1	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	57	427	269	74	81	3	0	0

- Molecule 5 is a protein called Nanobody 35.

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

- Molecule 6 is a protein called Glucagon-like peptide 1 receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	386	Total 3104	C 2051	N 500	O 535	S 18	0	0

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

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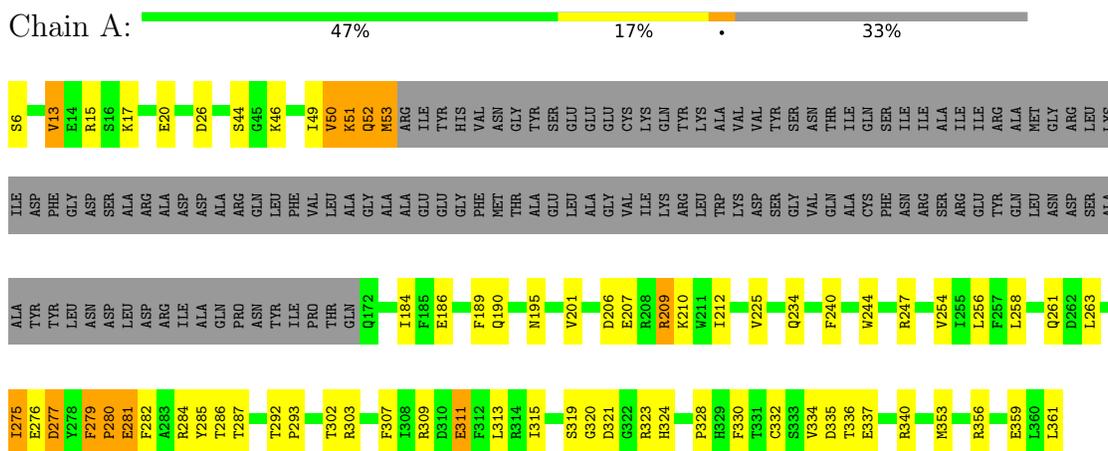
• Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B:
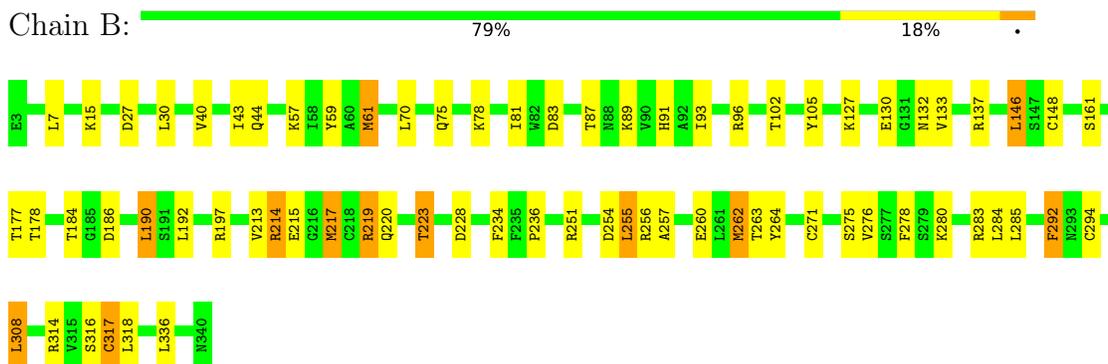
• Molecule 3: Peptide 15

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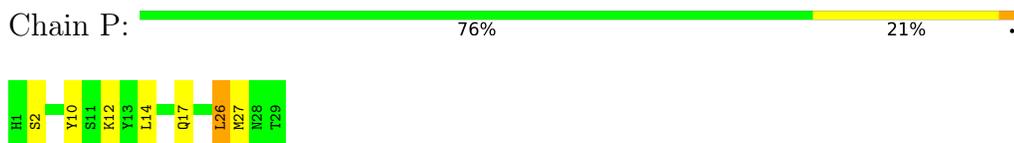
• Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain G:

T6 I9 L19 K20 I28 A34 M38 C41 A45 K46 E47 D48 P49 L50 L51 T52 R62

• Molecule 5: Nanobody 35

Chain N: 70% 25% 5% •

Q1 V2 Q3 L4 Q5 V12 Q13 P14 G15 L18 C22 S25 K33 Q39 K43 G44 L45 I51 S52 Q53 S54 G55 T61 R67 F68 T69 R72 T78 N84 S85 L86 K87 P88 E89 D90 T91 C99 R105 D109 V110 T111 S112 T113 T114

Y117 T122 V126

• Molecule 6: Glucagon-like peptide 1 receptor

Chain R: 75% 20% • •

V30 S31 L32 W33 E34 K38 Y42 Q47 L50 T51 A57 T58 D59 L60 F61 C62 N63 R64 W72 P73 D74 G78 V81 N82 V83 S84 C85 Y88 L89 P90 W91 A92 G98 H99 V100 T105 A106 E107 G108 L109 W110 L111 Q112 K113 L118 L123 S124

E125 E128 SER LYS ARG GLY GLU ARG SER SER. P137 S157 I179 H180 K197 L201 K202 W203 M204 T207 Q213 G216 L217 L218 S219 Y220 Q221 L224 Q234 Y235 L245 V246 E247 G248 S261 I265 I272 V276 V281 W284 K288

D293 N320 I323 R326 L335 K336 A337 N338 L339 M340 C341 K342 T343 D344 I345 K346 C347 R348 L349 A350 K351 S352 T353 I366 V370 R376 G377 T378 K383 E387 I400 F404 E412 K415 E423

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1252175	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	80	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (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	A	0.54	0/1890	0.56	0/2560
2	B	0.53	0/2619	0.64	0/3555
3	P	0.36	0/244	0.44	0/329
4	G	0.27	0/433	0.45	0/586
5	N	0.44	0/981	0.67	0/1329
6	R	0.40	0/3197	0.52	0/4365
All	All	0.47	0/9364	0.57	0/12724

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	1856	0	1751	47	0
2	B	2572	0	2462	39	0
3	P	238	0	219	2	0
4	G	427	0	435	11	0
5	N	961	0	930	17	0
6	R	3104	0	3014	45	0
All	All	9158	0	8811	152	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 8.

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PROTEIN DATA BANK

The worst 5 of 152 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:292:THR:O	1:A:292:THR:HG23	1.66	0.94
5:N:45:LEU:HB3	5:N:110:VAL:HG22	1.53	0.91
1:A:53:MET:HG3	1:A:189:PHE:HB2	1.61	0.82
1:A:53:MET:HG3	1:A:189:PHE:CB	2.12	0.79
2:B:130:GLU:OE1	2:B:132:ASN:HB2	1.82	0.79

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	A	234/356 (66%)	210 (90%)	20 (8%)	4 (2%)	7	6
2	B	336/338 (99%)	320 (95%)	16 (5%)	0	100	100
3	P	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
4	G	55/57 (96%)	54 (98%)	1 (2%)	0	100	100
5	N	124/126 (98%)	114 (92%)	9 (7%)	1 (1%)	16	21
6	R	382/394 (97%)	344 (90%)	33 (9%)	5 (1%)	10	10
All	All	1158/1300 (89%)	1068 (92%)	80 (7%)	10 (1%)	17	18

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	277	ASP
1	A	280	PRO
1	A	284	ARG
6	R	339	LEU
1	A	279	PHE

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	A	188/312 (60%)	156 (83%)	32 (17%)	1	1
2	B	275/281 (98%)	237 (86%)	38 (14%)	3	2
3	P	25/25 (100%)	20 (80%)	5 (20%)	1	0
4	G	44/46 (96%)	39 (89%)	5 (11%)	4	4
5	N	104/104 (100%)	81 (78%)	23 (22%)	1	0
6	R	327/354 (92%)	281 (86%)	46 (14%)	3	2
All	All	963/1122 (86%)	814 (84%)	149 (16%)	4	1

5 of 149 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	R	74	ASP
6	R	370	VAL
6	R	100	VAL
6	R	221	GLN
2	B	192	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	338	ASN
4	G	44	HIS
6	R	180	HIS
6	R	406	ASN

5.3.3   RNA ⓘ

There are no RNA molecules 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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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.