

Full wwPDB EM Validation Report (i)

Oct 16, 2024 – 12:44 AM JST

PDB ID : 8Y52

EMDB ID : EMD-38928

Title : Cryo-EM structure of the BA1-bound BRS3-Gq complex

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Deposited on : 2024-01-31

Resolution : 2.90 Å(reported)

This is a Full wwPDB EM Validation 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 (i) 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 (i)) were used in the production of this report:

EMDB validation analysis : FAILED

Mogul : 1.8.5 (274361), CSD as541be (2020)

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)

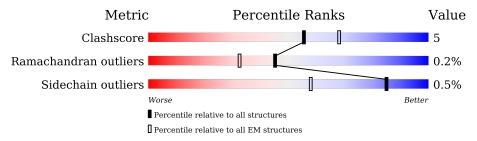
Validation Pipeline (wwPDB-VP) : 2.39

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 2.90 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 $(\# \mathrm{Entries})$	${ m EM\ structures} \ (\#{ m Entries})$
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	361	58%	7%	36	%	_	
2	В	345	83%			15% •		
3	G	71	70%		6%	24%	-	
4	R	361	73%		10%	17%	-	
5	X	9	33%	56%		11%	•	



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 7380 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(q) subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace	
1	A	232	Total 1908	C 1207	N 338	O 355	S 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	
2	В	338	Total 2592	C 1600	N 465	O 506	S 21	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	1	MET	-	initiating methionine	UNP P62873
В	2	GLY	-	expression tag	UNP P62873
В	3	SER	-	expression tag	UNP P62873
В	4	LEU	-	expression tag	UNP P62873
В	5	LEU	-	expression tag	UNP P62873
В	6	GLN	-	expression tag	UNP P62873

• Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

ľ	Mol	Chain	Residues	Atoms				AltConf	Trace	
	3	G	54	Total 407	C 253	N 71	O 80	S 3	0	0

• Molecule 4 is a protein called Bombesin receptor subtype-3.

Mol	Chain	Residues	Atoms				AltConf	Trace	
1	B	299	Total	С	N	О	S	0	0
4	11	299	2392	1589	385	405	13	0	U



• Molecule 5 is a protein called BA1.

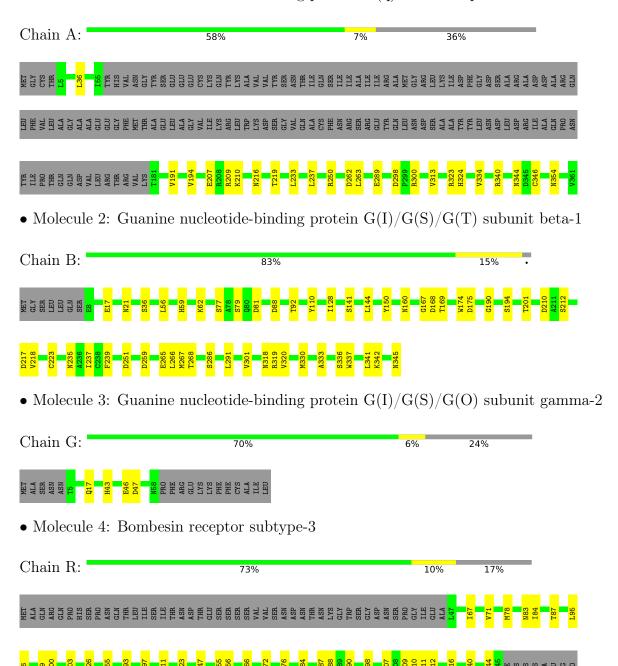
Mol	Chain	Residues	Atoms			AltConf	Trace	
5	X	9	Total 81	C 57	N 13	O 11	0	0



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(q) subunit alpha





GLU PRO PRO VAL ALA ASP THR SER

• Molecule 5: BA1

Chain X: 33% 56% 11%





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	675060	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 $(e^-/\text{Å}^2)$	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k 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: BAL, NLE, DPN

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		
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.23	0/1942	0.37	0/2614	
2	В	0.23	0/2638	0.43	0/3577	
3	G	0.24	0/411	0.37	0/555	
4	R	0.24	0/2454	0.36	0/3339	
5	X	0.90	0/58	0.99	0/77	
All	All	0.25	0/7503	0.40	0/10162	

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 (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	A	1908	0	1905	16	0
2	В	2592	0	2498	33	0
3	G	407	0	419	3	0
4	R	2392	0	2491	23	0
5	X	81	0	72	3	0
All	All	7380	0	7385	71	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 5.



All (71) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

		Interatomic	Clash
Atom-1	Atom-2	distance (\mathring{A})	overlap (Å)
1:A:216:ASN:OD1	2:B:62:LYS:NZ	2.16	0.78
1:A:207:GLU:OE2	1:A:209:ARG:NH1	2.17	0.77
4:R:284:TRP:O	4:R:288:HIS:ND1	2.18	0.76
2:B:223:CYS:SG	3:G:17:GLN:NE2	2.59	0.75
2:B:286:SER:OG	3:G:47:ASP:OD2	2.06	0.74
4:R:78:MET:O	4:R:83:ASN:ND2	2.25	0.68
4:R:256:GLN:N	4:R:256:GLN:OE1	2.27	0.68
2:B:128:ILE:O	2:B:141:SER:OG	2.10	0.67
1:A:210:LYS:NZ	2:B:235:ASN:OD1	2.25	0.67
1:A:340:ARG:O	1:A:344:ASN:ND2	2.29	0.66
4:R:211:LYS:HG3	4:R:298:SER:OG	1.96	0.66
2:B:210:ASP:OD2	2:B:212:SER:OG	2.14	0.64
2:B:17:GLU:O	2:B:21:ASN:ND2	2.32	0.62
1:A:250:ARG:O	1:A:323:ARG:NH1	2.32	0.61
2:B:36:SER:OG	2:B:267:MET:SD	2.59	0.61
1:A:289:GLU:N	1:A:289:GLU:OE1	2.36	0.59
2:B:168:ASP:O	2:B:169:THR:OG1	2.18	0.58
2:B:79:SER:OG	2:B:81:ASP:OD1	2.16	0.56
4:R:223:LEU:HD13	4:R:223:LEU:O	2.07	0.55
2:B:150:TYR:O	2:B:167:GLY:N	2.40	0.55
3:G:43:HIS:ND1	3:G:46:GLU:OE2	2.40	0.54
2:B:56:LEU:HD12	2:B:341:LEU:HB3	1.90	0.53
5:X:1:DPN:C	5:X:3:TRP:H	2.23	0.51
2:B:59:HIS:NE2	2:B:77:SER:OG	2.43	0.50
4:R:193:ASP:O	4:R:197:ASN:N	2.41	0.50
2:B:160:ASN:ND2	2:B:175:ASP:OD1	2.45	0.50
4:R:310:ILE:HG23	4:R:311:PHE:N	2.27	0.50
2:B:318:ASN:OD1	2:B:319:ARG:N	2.41	0.49
4:R:71:VAL:HG22	4:R:344:GLN:HG3	1.94	0.49
1:A:36:LEU:HD21	1:A:346:CYS:SG	2.52	0.49
2:B:217:ASP:OD1	2:B:218:VAL:N	2.46	0.49
1:A:262:ASP:OD1	1:A:263:LEU:N	2.46	0.48
2:B:128:ILE:HD12	2:B:128:ILE:N	2.29	0.47
4:R:95:LEU:O	4:R:99:THR:N	2.47	0.47
1:A:191:VAL:O	1:A:194:VAL:HG12	2.14	0.47
2:B:291:LEU:HD12	2:B:291:LEU:N	2.30	0.46
2:B:265:GLU:OE2	2:B:268:THR:OG1	2.22	0.46
2:B:320:VAL:O	2:B:320:VAL:HG13	2.15	0.46
2:B:201:THR:O	2:B:201:THR:HG22	2.15	0.45
4:R:247:SER:OG	4:R:266:ARG:NH1	2.50	0.45

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A to ma 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	${ m distance}({ m \AA})$	overlap (Å)
2:B:92:THR:HG22	2:B:92:THR:O	2.16	0.45
2:B:194:SER:OG	2:B:237:ILE:HG22	2.16	0.45
2:B:341:LEU:HD23	2:B:342:LYS:N	2.31	0.45
2:B:88:ASP:O	2:B:92:THR:N	2.46	0.45
2:B:259:ASP:HB2	2:B:266:LEU:HD11	2.00	0.44
4:R:67:ILE:O	4:R:71:VAL:HG23	2.17	0.44
2:B:333:ALA:HB1	2:B:341:LEU:HD21	2.00	0.43
5:X:1:DPN:C	5:X:3:TRP:N	2.82	0.43
2:B:169:THR:HG22	2:B:190:GLY:C	2.38	0.43
2:B:235:ASN:ND2	2:B:251:ASP:OD1	2.45	0.43
2:B:144:LEU:HD13	2:B:174:TRP:CD2	2.54	0.43
2:B:336:SER:HG	2:B:337:TRP:H	1.67	0.43
5:X:5:VAL:HG23	5:X:5:VAL:O	2.18	0.43
4:R:290:LEU:HD21	4:R:312:THR:OG1	2.17	0.43
1:A:354:ASN:OD1	4:R:155:ARG:NH1	2.48	0.42
1:A:36:LEU:HD23	1:A:219:THR:HB	2.01	0.42
4:R:307:MET:O	4:R:310:ILE:HG22	2.20	0.42
1:A:233:LEU:O	1:A:237:LEU:HD13	2.20	0.42
2:B:291:LEU:HG	2:B:301:VAL:HG22	2.01	0.42
2:B:330:MET:O	2:B:345:ASN:ND2	2.52	0.42
4:R:84:ILE:O	4:R:87:THR:HG22	2.20	0.42
4:R:272:THR:O	4:R:276:LEU:HD13	2.20	0.42
4:R:309:PHE:O	4:R:312:THR:HG22	2.20	0.42
1:A:313:VAL:HG13	4:R:255:GLU:HG3	2.02	0.41
4:R:96:LEU:O	4:R:100:CYS:N	2.54	0.41
4:R:287:ASN:OD1	4:R:316:ARG:NH2	2.53	0.41
1:A:334:VAL:HG22	1:A:334:VAL:O	2.21	0.41
4:R:99:THR:HG21	4:R:126:ILE:HG23	2.02	0.41
4:R:99:THR:O	4:R:103:VAL:HG23	2.21	0.41
1:A:298:ASP:OD2	1:A:300:ARG:NE	2.50	0.40
1:A:313:VAL:HG11	4:R:256:GLN:OE1	2.21	0.40

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	Percer	ntiles
1	A	228/361 (63%)	226 (99%)	2 (1%)	0	100	100
2	В	336/345~(97%)	334 (99%)	2 (1%)	0	100	100
3	G	52/71 (73%)	52 (100%)	0	0	100	100
4	R	297/361 (82%)	287 (97%)	10 (3%)	0	100	100
5	X	6/9 (67%)	3 (50%)	1 (17%)	2 (33%)	0	0
All	All	919/1147 (80%)	902 (98%)	15 (2%)	2 (0%)	45	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	X	2	GLN
5	X	5	VAL

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	Perce	ntiles
1	A	210/316~(66%)	209 (100%)	1 (0%)	86	96
2	В	279/287 (97%)	277 (99%)	2 (1%)	81	94
3	G	43/58 (74%)	43 (100%)	0	100	100
4	R	270/325~(83%)	269 (100%)	1 (0%)	89	97
5	X	5/5 (100%)	5 (100%)	0	100	100
All	All	807/991 (81%)	803 (100%)	4 (0%)	85	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	324	HIS
2	В	110	TYR
2	В	239	PHE

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Mol	Chain	Res	Type
4	R	340	HIS

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

Mol	Chain	Res	Type
2	В	273	ASN
2	В	300	ASN
3	G	17	GLN
5	X	2	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)

3 non-standard protein/DNA/RNA residues 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	Trmo	Chain	Dag	Link	B	ond leng	gths	В	ond ang	gles
MIOI	Type	Chain	Res	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
5	NLE	X	9	5	7,8,8	0.90	1 (14%)	8,9,9	1.41	1 (12%)
5	BAL	X	6	5	4,4,5	1.63	1 (25%)	3,3,5	11.04	1 (33%)

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
5	NLE	X	9	5	-	2/8/8/8	-
5	BAL	X	6	5	-	0/1/2/3	-



All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(A)	$\operatorname{Ideal}(\text{\AA})$
5	X	6	BAL	CB-CA	-3.18	1.37	1.51
5	X	9	NLE	OXT-C	-2.27	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^{o})$
5	X	6	BAL	CB-CA-C	19.08	139.75	111.42
5	X	9	NLE	OXT-C-O	-3.40	116.38	124.09

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	X	9	NLE	N-CA-CB-CG
5	X	9	NLE	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

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.

