Full wwPDB EM Validation Report

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PDB ID	:	9IK9 / pdb_00009ik9
EMDB ID	:	EMD-60651
Title	:	Cryo-EM Structure of SST analogs bond SSTR1-Gi complex
Authors	:	Wong, T.S.; Zeng, Z.C.; Xiong, T.T.; Gan, S.Y.; Du, Y.
Deposited on	:	2024-06-26
Resolution	:	3.37 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 ⓘ 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	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	FAILED
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)	:	2.43.1

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 3.37 Å.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	4J2	F	1	-	X	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 17031 atoms, of which 8426 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(i) subunit alpha-1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	217	3261	1065	1597	286	301	12	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	H	N	O	S		
2	B	336	4915	1564	2391	450	491	19	0	0

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-21	MET	-	initiating methionine	UNP P62873
B	-20	HIS	-	expression tag	UNP P62873
B	-19	HIS	-	expression tag	UNP P62873
B	-18	HIS	-	expression tag	UNP P62873
B	-17	HIS	-	expression tag	UNP P62873
B	-16	HIS	-	expression tag	UNP P62873
B	-15	HIS	-	expression tag	UNP P62873
B	-14	HIS	-	expression tag	UNP P62873
B	-13	HIS	-	expression tag	UNP P62873
B	-12	HIS	-	expression tag	UNP P62873
B	-11	HIS	-	expression tag	UNP P62873
B	-10	LEU	-	expression tag	UNP P62873
B	-9	GLU	-	expression tag	UNP P62873
B	-8	VAL	-	expression tag	UNP P62873
B	-7	LEU	-	expression tag	UNP P62873
B	-6	PHE	-	expression tag	UNP P62873
B	-5	GLN	-	expression tag	UNP P62873
B	-4	GLY	-	expression tag	UNP P62873
B	-3	PRO	-	expression tag	UNP P62873
B	-2	GLY	-	expression tag	UNP P62873

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	SER	-	expression tag	UNP P62873
B	0	SER	-	expression tag	UNP P62873
B	1	GLY	-	expression tag	UNP P62873
B	341	VAL	-	expression tag	UNP P62873
B	342	SER	-	expression tag	UNP P62873
B	343	GLY	-	expression tag	UNP P62873
B	344	TRP	-	expression tag	UNP P62873
B	345	ARG	-	expression tag	UNP P62873
B	346	LEU	-	expression tag	UNP P62873
B	347	PHE	-	expression tag	UNP P62873
B	348	LYS	-	expression tag	UNP P62873
B	349	LYS	-	expression tag	UNP P62873
B	350	ILE	-	expression tag	UNP P62873
B	351	SER	-	expression tag	UNP P62873

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	53	Total	C	H	N	O	S	0	0
			749	241	372	66	67	3		

- Molecule 4 is a protein called scFv16.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	E	232	Total	C	H	N	O	S	0	0
			3416	1116	1668	295	328	9		

- Molecule 5 is a protein called Somatostatin receptor type 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	D	283	Total	C	H	N	O	S	0	0
			4543	1467	2328	361	363	24		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	392	LEU	-	expression tag	UNP P30872
D	393	GLU	-	expression tag	UNP P30872

- Molecule 6 is a protein (with D amino acids) called (4J2)(DCY)(DTY)(DTR)K(DVA)(DCY)(ALO)(NH2).

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	9	Total	C	H	N	O	S	0	1
			147	54	70	11	10	2		

MolProbity failed to run properly - this section is therefore empty.

3 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	217201	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	53.6	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

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4.3.2 Protein sidechains

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4.3.3 RNA

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4.4 Non-standard residues in protein, DNA, RNA chains

7 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	DCY	F	2	6	4,5,6	0.54	0	1,5,7	1.76	0
6	ALO	F	8	6	5,6,7	0.68	0	6,7,9	1.55	2 (33%)
6	DCY	F	7	6	4,5,6	0.88	0	1,5,7	1.74	0
6	DVA	F	6	6	4,6,7	0.48	0	6,7,9	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	DTR	F	4	6	13,15,16	1.79	4 (30%)	13,20,22	1.94	5 (38%)
6	DTY	F	3	6	11,12,13	4.40	6 (54%)	12,15,17	1.41	1 (8%)
6	4J2	F	1	6	15,16,17	7.99	10 (66%)	18,21,23	5.12	16 (88%)

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
6	DCY	F	2	6	-	1/1/4/6	-
6	ALO	F	8	6	-	5/5/6/8	-
6	DCY	F	7	6	-	1/1/4/6	-
6	DVA	F	6	6	-	0/5/6/8	-
6	DTR	F	4	6	-	1/4/6/8	0/2/2/2
6	DTY	F	3	6	-	2/5/6/8	0/1/1/1
6	4J2	F	1	6	-	2/5/6/8	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	1	4J2	CD1-CG	-15.33	1.05	1.38
6	F	1	4J2	CZ3-CZ2	11.96	1.64	1.36
6	F	1	4J2	CE3-CE2	-11.79	1.13	1.41
6	F	1	4J2	CE1-CD1	-11.14	1.13	1.36
6	F	1	4J2	CD2-CE2	8.43	1.61	1.42
6	F	3	DTY	CE1-CD1	8.42	1.54	1.38
6	F	1	4J2	CE4-CE3	-8.32	1.17	1.36
6	F	1	4J2	CE2-CZ1	8.27	1.61	1.42
6	F	1	4J2	CZ2-CZ1	7.86	1.61	1.41
6	F	3	DTY	CE2-CZ	7.15	1.52	1.38
6	F	3	DTY	CD2-CG	6.44	1.52	1.38
6	F	1	4J2	CD2-CG	-5.95	1.23	1.37
6	F	3	DTY	CE1-CZ	-3.87	1.31	1.38
6	F	3	DTY	CD1-CG	-3.77	1.30	1.38
6	F	3	DTY	CE2-CD2	-3.70	1.32	1.38
6	F	4	DTR	CD1-NE1	-3.34	1.29	1.36
6	F	4	DTR	CZ2-CE2	-2.94	1.36	1.41
6	F	4	DTR	CD2-CE2	2.11	1.48	1.42
6	F	4	DTR	CZ3-CE3	2.05	1.41	1.36
6	F	1	4J2	CB-CG	2.02	1.56	1.51

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	1	4J2	CZ2-CZ1-CE1	9.83	146.18	123.19
6	F	1	4J2	CD2-CE2-CZ1	-7.60	108.13	118.96
6	F	1	4J2	CZ2-CZ1-CE2	-7.27	105.89	118.92
6	F	1	4J2	CE1-CZ1-CE2	-6.12	107.94	118.92
6	F	1	4J2	CD1-CE1-CZ1	5.72	129.68	120.82
6	F	1	4J2	CD1-CG-CD2	5.57	129.66	118.85
6	F	1	4J2	CZ3-CE4-CE3	5.42	128.03	120.44
6	F	1	4J2	CE3-CE2-CZ1	5.34	128.48	118.92
6	F	1	4J2	CE4-CE3-CE2	5.15	128.50	120.44
6	F	1	4J2	CE4-CZ3-CZ2	-4.30	114.41	120.44
6	F	4	DTR	CB-CG-CD2	-4.06	119.92	126.25
6	F	3	DTY	CG-CB-CA	-3.86	106.28	114.10
6	F	1	4J2	CZ3-CZ2-CZ1	-3.69	114.68	120.44
6	F	1	4J2	CE1-CD1-CG	3.68	128.71	121.14
6	F	8	ALO	CB-CA-C	-3.07	106.87	111.77
6	F	1	4J2	CG-CB-CA	-2.99	108.04	114.10
6	F	4	DTR	CD2-CE2-NE1	-2.98	101.31	107.92
6	F	1	4J2	CB-CG-CD2	-2.90	114.20	120.57
6	F	1	4J2	CG-CD2-CE2	-2.71	115.89	121.22
6	F	4	DTR	CE3-CD2-CG	2.51	139.02	134.42
6	F	1	4J2	CB-CG-CD1	-2.40	116.14	120.91
6	F	4	DTR	CZ2-CE2-NE1	2.29	137.14	130.80
6	F	4	DTR	CG-CB-CA	2.22	117.96	114.53
6	F	8	ALO	O-C-CA	-2.08	119.31	124.78

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	1	4J2	N-CA-CB-CG
6	F	1	4J2	C-CA-CB-CG
6	F	7	DCY	N-CA-CB-SG
6	F	8	ALO	N-CA-CB-CG2
6	F	8	ALO	C-CA-CB-CG2
6	F	8	ALO	C-CA-CB-OG1
6	F	3	DTY	C-CA-CB-CG
6	F	2	DCY	N-CA-CB-SG
6	F	3	DTY	N-CA-CB-CG
6	F	4	DTR	CA-CB-CG-CD1
6	F	8	ALO	N-CA-CB-OG1
6	F	8	ALO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

4.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

4.6 Ligand geometry (i)

There are no ligands in this entry.

4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.