wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:56 PM BST

PDB ID	:	4CG6
EMDB ID:	:	EMD-2512
Title	:	Cryo-em of the Sec61-complex bound to the 80s ribosome translating a membrane-inserting substrate
Authors	:	Gogala, M.; Becker, T.; Beatrix, B.; Barrio-Garcia, C.; Berninghausen, O.; Beckmann, R.
Deposited on	:	2013-11-21
Resolution	:	7.80 Å(reported)
Based on PDB ID	:	2WWB

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

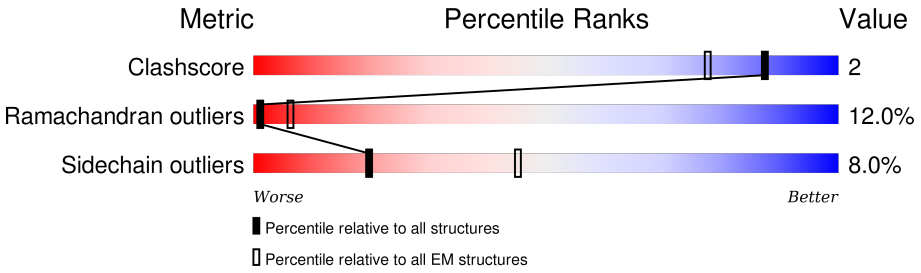
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

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 7.80 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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 >=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 <=5%

Mol	Chain	Length	Quality of chain
1	A	476	73% 15% 5% • 5%
2	B	68	81% 10% 9%
3	C	96	32% 5% 63%
4	D	17	94% 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4383 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 PROTEIN TRANSPORT PROTEIN SEC61 SUBUNIT ALPHA ISOFORM 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	452	3477	2275	560	619	23	0	0

- Molecule 2 is a protein called PROTEIN TRANSPORT PROTEIN SEC61 SUBUNIT GAMMA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	62	494	326	86	79	3	0	0

- Molecule 3 is a protein called PROTEIN TRANSPORT PROTEIN SEC61 SUBUNIT BETA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	36	281	188	44	47	2	0	0

- Molecule 4 is a protein called PEPTIDE.

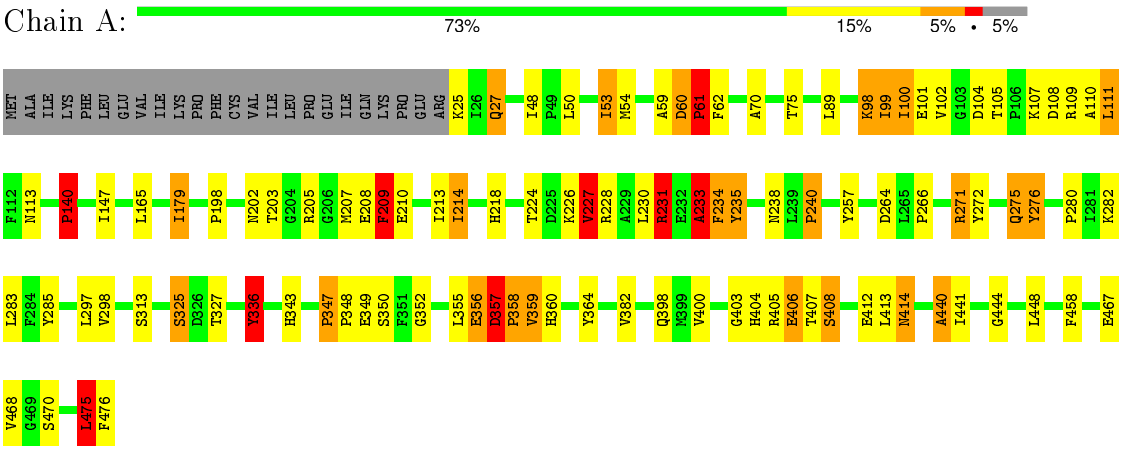
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	D	17	131	93	17	21	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

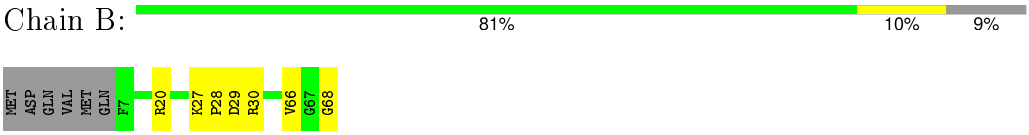
• Molecule 1: PROTEIN TRANSPORT PROTEIN SEC61 SUBUNIT ALPHA ISOFORM 1

Chain A:



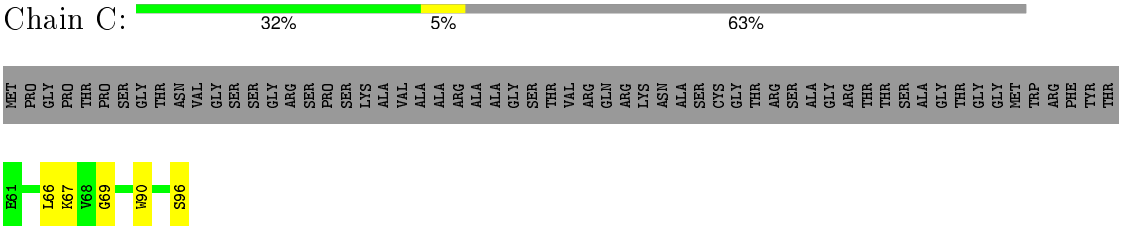
• Molecule 2: PROTEIN TRANSPORT PROTEIN SEC61 SUBUNIT GAMMA

Chain B:



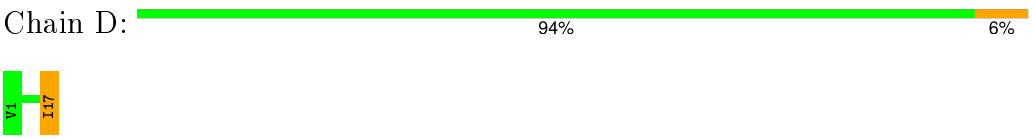
• Molecule 3: PROTEIN TRANSPORT PROTEIN SEC61 SUBUNIT BETA

Chain C:



• Molecule 4: PEPTIDE

Chain D:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	ON 3D-VOLUME (SPIDER)	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	Not provided	Depositor
Image detector	TVIPS TEMCAM-F416 (4K 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	#$\|Z\|>2$	RMSZ	#$\|Z\|>2$
1	A	0.93	1/3552 (0.0%)	1.20	26/4815 (0.5%)
2	B	1.15	1/504 (0.2%)	1.00	1/673 (0.1%)
3	C	1.12	1/289 (0.3%)	1.04	1/391 (0.3%)
4	D	1.69	2/133 (1.5%)	0.94	1/179 (0.6%)
All	All	1.00	5/4478 (0.1%)	1.17	29/6058 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	68	GLY	C-O	-14.50	1.00	1.23
3	C	96	SER	C-O	-12.08	1.00	1.23
4	D	17	ILE	C-OXT	-12.06	1.00	1.23
4	D	17	ILE	C-O	-12.06	1.00	1.23
1	A	476	PHE	C-O	-12.03	1.00	1.23

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	336	TYR	CB-CG-CD1	7.71	125.63	121.00
1	A	336	TYR	CB-CG-CD2	-7.09	116.75	121.00
1	A	405	ARG	C-N-CA	6.92	139.00	121.70
1	A	60	ASP	N-CA-CB	6.61	122.49	110.60
1	A	364	TYR	CB-CG-CD2	-6.53	117.08	121.00
1	A	140	PRO	CA-N-CD	-6.52	102.37	111.50
2	B	68	GLY	CA-C-O	-6.44	109.00	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	325	SER	N-CA-CB	6.28	119.92	110.50
1	A	227	VAL	CB-CA-C	6.22	123.22	111.40
1	A	364	TYR	CB-CG-CD1	6.14	124.69	121.00
1	A	240	PRO	CA-N-CD	-5.92	103.22	111.50
1	A	235	TYR	CB-CA-C	5.80	122.01	110.40
1	A	233	ALA	N-CA-CB	5.79	118.21	110.10
1	A	234	PHE	CB-CG-CD1	5.69	124.78	120.80
1	A	111	LEU	N-CA-CB	5.39	121.19	110.40
1	A	271	ARG	N-CA-CB	5.32	120.18	110.60
1	A	475	LEU	N-CA-CB	5.29	120.99	110.40
3	C	96	SER	CA-C-O	-5.29	108.99	120.10
1	A	61	PRO	CA-N-CD	-5.29	104.10	111.50
4	D	17	ILE	CA-C-O	-5.28	109.01	120.10
1	A	209	PHE	CB-CG-CD1	5.28	124.50	120.80
1	A	476	PHE	CA-C-O	-5.28	109.02	120.10
1	A	257	TYR	CB-CG-CD2	-5.21	117.88	121.00
1	A	104	ASP	C-N-CA	5.19	134.68	121.70
1	A	336	TYR	CB-CA-C	5.17	120.75	110.40
1	A	179	ILE	N-CA-CB	5.07	122.47	110.80
1	A	408	SER	N-CA-C	-5.06	97.34	111.00
1	A	240	PRO	N-CA-C	5.03	125.17	112.10
1	A	27	GLN	N-CA-CB	5.01	119.62	110.60

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	203	THR	Peptide
1	A	272	TYR	Peptide
1	A	276	TYR	Sidechain
1	A	313	SER	Peptide
1	A	403	GLY	Peptide
1	A	406	GLU	Peptide
1	A	414	ASN	Peptide
1	A	440	ALA	Peptide

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	3477	0	3575	19	0
2	B	494	0	527	0	0
3	C	281	0	294	1	0
4	D	131	0	147	2	0
All	All	4383	0	4543	22	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 2.

All (22) 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:358:PRO:O	1:A:359:VAL:HG23	1.52	1.10
1:A:356:GLU:O	1:A:358:PRO:HD3	1.64	0.96
1:A:358:PRO:O	1:A:359:VAL:CG2	2.30	0.77
1:A:356:GLU:O	1:A:358:PRO:CD	2.33	0.76
4:D:17:ILE:OXT	4:D:17:ILE:HG22	1.92	0.68
1:A:357:ASP:O	1:A:359:VAL:N	2.30	0.65
1:A:99:ILE:HG23	1:A:100:ILE:H	1.64	0.63
1:A:343:HIS:CE1	1:A:360:HIS:HE1	2.17	0.62
4:D:17:ILE:OXT	4:D:17:ILE:CG2	2.49	0.60
1:A:448:LEU:H	1:A:448:LEU:HD22	1.67	0.59
1:A:358:PRO:O	1:A:359:VAL:CB	2.57	0.52
1:A:231:ARG:HG2	1:A:233:ALA:H	1.75	0.51
1:A:357:ASP:O	1:A:358:PRO:C	2.48	0.49
1:A:227:VAL:HG12	1:A:228:ARG:H	1.79	0.48
1:A:355:LEU:C	1:A:357:ASP:H	2.18	0.47
1:A:343:HIS:CE1	1:A:360:HIS:CE1	2.99	0.47
3:C:66:LEU:H	3:C:66:LEU:HD23	1.82	0.45
1:A:347:PRO:HG3	1:A:355:LEU:HD23	1.98	0.45
1:A:214:ILE:H	1:A:214:ILE:HD13	1.83	0.44
1:A:347:PRO:HB2	1:A:348:PRO:HD2	2.01	0.43
1:A:352:GLY:O	1:A:355:LEU:HD11	2.18	0.43
1:A:440:ALA:HB3	1:A:444:GLY:C	2.42	0.40

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	450/476 (94%)	344 (76%)	47 (10%)	59 (13%)	0 7
2	B	60/68 (88%)	54 (90%)	1 (2%)	5 (8%)	1 18
3	C	34/96 (35%)	29 (85%)	2 (6%)	3 (9%)	1 17
4	D	15/17 (88%)	15 (100%)	0	0	100 100
All	All	559/657 (85%)	442 (79%)	50 (9%)	67 (12%)	1 8

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	50	LEU
1	A	59	ALA
1	A	60	ASP
1	A	61	PRO
1	A	70	ALA
1	A	75	THR
1	A	98	LYS
1	A	99	ILE
1	A	100	ILE
1	A	102	VAL
1	A	105	THR
1	A	110	ALA
1	A	113	ASN
1	A	140	PRO
1	A	179	ILE
1	A	207	MET
1	A	209	PHE
1	A	227	VAL
1	A	233	ALA
1	A	238	ASN
1	A	240	PRO

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Mol	Chain	Res	Type
1	A	275	GLN
1	A	325	SER
1	A	327	THR
1	A	336	TYR
1	A	347	PRO
1	A	349	GLU
1	A	350	SER
1	A	357	ASP
1	A	358	PRO
1	A	359	VAL
1	A	398	GLN
1	A	400	VAL
1	A	406	GLU
1	A	408	SER
1	A	412	GLU
1	A	441	ILE
1	A	470	SER
1	A	475	LEU
2	B	30	ARG
1	A	101	GLU
1	A	107	LYS
1	A	111	LEU
1	A	271	ARG
2	B	27	LYS
2	B	66	VAL
3	C	67	LYS
3	C	69	GLY
1	A	108	ASP
1	A	109	ARG
1	A	147	ILE
1	A	231	ARG
1	A	280	PRO
1	A	467	GLU
2	B	29	ASP
1	A	53	ILE
1	A	266	PRO
3	C	90	TRP
1	A	62	PHE
1	A	224	THR
1	A	356	GLU
1	A	407	THR
1	A	382	VAL

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Mol	Chain	Res	Type
1	A	468	VAL
1	A	198	PRO
2	B	28	PRO

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	375/398 (94%)	338 (90%)	37 (10%)	10 39
2	B	53/59 (90%)	52 (98%)	1 (2%)	65 86
3	C	32/74 (43%)	32 (100%)	0	100 100
4	D	16/16 (100%)	16 (100%)	0	100 100
All	All	476/547 (87%)	438 (92%)	38 (8%)	20 50

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LYS
1	A	48	ILE
1	A	53	ILE
1	A	54	MET
1	A	61	PRO
1	A	89	LEU
1	A	98	LYS
1	A	140	PRO
1	A	165	LEU
1	A	202	ASN
1	A	205	ARG
1	A	208	GLU
1	A	209	PHE
1	A	210	GLU
1	A	213	ILE
1	A	214	ILE
1	A	218	HIS
1	A	226	LYS

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Mol	Chain	Res	Type
1	A	230	LEU
1	A	231	ARG
1	A	234	PHE
1	A	235	TYR
1	A	264	ASP
1	A	275	GLN
1	A	276	TYR
1	A	282	LYS
1	A	283	LEU
1	A	285	TYR
1	A	297	LEU
1	A	298	VAL
1	A	336	TYR
1	A	357	ASP
1	A	404	HIS
1	A	413	LEU
1	A	414	ASN
1	A	458	PHE
1	A	475	LEU
2	B	20	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	315	ASN
1	A	343	HIS
1	A	360	HIS
1	A	411	HIS
1	A	414	ASN
2	B	58	HIS

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

There are no carbohydrates 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.