

wwPDB EM Validation Summary Report (i)

Mar 12, 2024 – 06:53 PM JST

PDB ID	:	8H37
EMDB ID	:	EMD-34453
Title	:	Cryo-EM Structure of the KBTBD2-CUL3-Rbx1-p85a tetrameric complex
Authors	:	Hu, Y.; Mao, Q.; Chen, Z.; Sun, L.
Deposited on	:	2022-10-08
Resolution	:	7.52 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* 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 (1)) were used in the production of this report:

EMDB validation analysis	:	0.0.1.dev70
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 7.52 Å.

Ramachandran outliers

Sidechain outliers

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.



154571

154315

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 $<\!\!=\!5\%$
The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM
map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

4023

3826

Mol	Chain	Length	Quality of chain								
1	С	768	59%	27%	7% • 6%						
1	F	768	63%	26%	• 6%						
1	М	768	62%	27%	5% 6%						
1	Ο	768	61%	29%	• 6%						
2	D	108	5 1% 20%	7% •	18%						
2	Е	108	39% 32%	10% •	18%						
2	Q	108	48% 27%	6% •	18%						
2	R	108	• 34% 37%	10% •	18%						

Continued on next page...



Conti		i previous	page							
Mol	Chain	Length	Quality of chain							
3	А	623	58%	27%	6%	9%				
2	Р	693		2.10/		20/				
3	D	025	65%	24%	•	9%				
			<u>i</u>							
3	N	623	66%	23%	•	9%				
3	Р	623	69%	19%	•	11%				
			•							
4	G	724	14% 7% • 77%							
			•							
4	Н	724	17% 6% • 77%							
			5%							
4	I	724	16% 6% • 77%							
			5%							
4	J	724	16% 6% · 77%							

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2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 49321 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.

Mol	Chain	Residues		Α		AltConf	Trace		
1	1 C	720	Total	С	Ν	Ο	\mathbf{S}	0	0
1		120	5791	3633	1024	1095	39	0	0
1	F	790	Total	С	Ν	Ο	S	0	0
1	Г	720	5677	3558	1010	1073	36	0	0
1	М	720	Total	С	Ν	Ο	S	0	0
1	111	720	5672	3553	1008	1074	37	0	0
1 O	720	Total	С	Ν	Ο	S	0	0	
	0	720	5767	3620	1017	1091	39	0	0

• Molecule 1 is a protein called Cullin-3.

• Molecule 2 is a protein called E3 ubiquitin-protein ligase RBX1.

Mol	Chain	Residues		At	oms		AltConf	Trace	
0	F	80	Total	С	Ν	0	S	0	0
	Ľ	09	737	466	135	127	9	0	0
0	D	80	Total	С	Ν	0	S	0	0
	D	09	737	466	135	127	9	0	0
0	D	20	Total	С	Ν	0	S	0	0
	89	737	466	135	127	9	0	U	
2	0	80	Total	С	Ν	0	S	0	0
	Q	Q	89	737	466	135	127	9	

• Molecule 3 is a protein called Kelch repeat and BTB domain-containing protein 2.

Mol	Chain	Residues		At		AltConf	Trace		
3	2 1	567	Total	С	Ν	0	S	0	0
0	Л	507	4559	2918	750	853	38	0	0
3	В	564	Total	С	Ν	0	S	0	0
0	D	504	4510	2884	746	842	38	0	
2	N	564	Total	С	Ν	0	S	0	0
O IN	304	4510	2880	746	846	38	0	0	
3	D	557	Total	С	Ν	0	S	0	0
	Р	Р	557	4423	2833	725	831	34	0

There are 4 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
А	252	ASP	SER	engineered mutation	UNP Q8IY47
В	252	ASP	SER	engineered mutation	UNP Q8IY47
N	252	ASP	SER	engineered mutation	UNP Q8IY47
Р	252	ASP	SER	engineered mutation	UNP Q8IY47

• Molecule 4 is a protein called Phosphatidylinositol 3-kinase regulatory subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace		
4	4 0	169	Total	С	Ν	0	S	0	0		
4	G	108	1424	885	256	278	5	0			
4	4 H	П	TT	169	Total	С	Ν	0	S	0	0
4		108	1341	828	246	263	4	0	0		
4	т	169	Total	С	Ν	0	S	0	0		
4 1	108	1360	840	250	266	4	0	0			
4	4 I	I 169	Total	С	Ν	0	S	0	0		
4 J	J	100	1327	816	244	263	4	0	0		

• Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
5	Е	3	Total Zn 3 3	0
5	D	3	Total Zn 3 3	0
5	R	3	Total Zn 3 3	0
5	Q	3	Total Zn 3 3	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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

- Chain C: 59% 27% 7% • 6% PHE GGLY GGLY VAL LYS GGLV GGLY VAL CGLY VAL GGLY VAL GGLY VAL GGLY VAL ASN ASN • Molecule 1: Cullin-3
- Molecule 1: Cullin-3













• Molecule 1: Cullin-3





• Molecule 2: E3 ubiquitin-protein ligase RBX1





• Molecule 2: E3 ubiquitin-protein ligase RBX1

Chain R:	•	34%			37%	1	0% •	18%	
NET ALA ALA ALA ALA ALA ASP VAL	ASP THR PRO SER GLY THR	ASH SER GLY GLY LYS K20 K20	R21 F22 E23 K24 K25 K26	W27 N28 A29 V30 A31	L32 M33 V35 V35 D36 D36 D36 D36	V39 D40 N41 C42 A43	144 C45 R46 N47 H48 149	L52 C53 L54 L54	45 N59 Q60 S61 S62
A63 T64 S65 E66 A71 V72	N76 F79 I84	R86 W87 R91 Q92 V93	C94 P95 D97 N98 R99	E100 W101 E102 F103 Q104	4105 4017 4108 H108				
• Molecu	le 2: E3 ı	ıbiquitin	-protein	ligase F	RBX1				
Chain Q:		48%			27%	Ď	6% •	18%	-
MET ALA ALA ALA MET ASP VAL	ASP THR PRO SER GLY THR	SER SER GLY GLY CLYS K20 K20	R21 F22 623 W27 N28	A29 W35 D36 137	V38 D40 C41 C42 C42	M46 N47 M50 D51	I54 N59 E66	W72 G73 V74 184	101 101 101 101 101 101 101 101 101 101
R91 Q92 V93 C94 P95 L96 D97	N98 R99 E102 K105	1100 6107 H108							
• Molecu	le 3: Kelo	ch repeat	and BT	B doma	ain-conta	ining pi	otein 2		
Chain A:			58%			27%	(5% 9%	-
MET SER THR GLN ASP GLU	19 19 117	r 24 L29 V37 C44	H45 K46 S53 S54	R57 A58 M59 F60 M61	S67 R75 N76 A108	C109 0112 V113	K119 Y123 K126 K127	1128 E131 N132 C133	M170 D175 1178
L186 W201 R209	L225 S226 T229 D241	R243 8243 M253 F257 K258	P259 R260 M263 T264 K265	1270 F271 1272 E273	A274 S275 S276 E277 N278 N279 C280	2200 2281 1282 7283 8284 8285	V286 C287 Q291 A292	K297 L298 C299 S300 P301	L305 L305 H306 V308
G309 T310 V311 V311 T313 P314 P315	N316 D317 I318 Y319 I320	4326 V326 K328 ASN THR LYS	THR ASN HIS SER LYS THR	SER LYS LEU GLN THR	ALA F344 R345 T346 C349 E350	r351 W352 F353 Q356	4357 W360 K363	M366 L367 F368 V369 R370 T371	1371 8372 8374 1375 V376
C377 C378 Y381 1382 Y383 A384	C387 C387 D388 S389 C391 C391	C392 E393 L394 N395 R396 R397 T398	R401 Y402 D403 T404 E405	K406 D407 E408 W409 T410	N411 V412 A418 V426	1431 1431 1432 1436	Y442 F443 F444 R445 S446	D447 E451 M452 A453 M453	R455 Q456 T457 S458 R459 R459
A462 K470 F471 F472 Y473	1474 6475 6476 1477 HIS 11E	THR ASN SER GLY ILE ARG	LEU PRO SER GLY THR VAL	ASP GLY SER SER V497	1498 1499 E500 D503 V504 M505	K506 K506 K509 K510	M511 A512 A513 N514 N514 P515 P516	A517 K518 R519 Y520 S521	V525 V528 L534
C535 V536 F537 M538 R539 E540 T541	H5 42 L5 43 K5 48 T551	D555 L556 E557 L558 D559 R560	W561 S562 L563 I567	V571 L572 W573 D574 L575	G576 R577 D578 F579 R580 C581	T582 V583 <mark>G584</mark> K585 L586	S589 C590 L591 E592 E593 S594	K597 P598 P599	L602 F603 S604 T605 D606 GLY
THR GLU GLU PHE GLU LEU ASP	GLY GLU MET VAL ALA LEU LEU	PRO VAL							









• Molecule 4: Phosphatidylinositol 3-kinase regulatory subunit alpha











PRO VAL TYR ALA GLN GLN ARG ARG



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	239068	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	45	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.603	Depositor
Minimum map value	-0.001	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.001	Depositor
Map size (Å)	511.488, 511.488, 511.488	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles $(^{\circ})$	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.664, 2.664, 2.664	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: ZN

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).

Mal	Mol Chain		Bond lengths		angles
			# Z > 5	RMSZ	# Z > 5
1	С	0.45	0/5879	0.52	0/7905
1	F	0.42	0/5760	0.50	0/7752
1	М	0.53	0/5753	0.53	0/7743
1	0	0.42	0/5854	0.51	0/7873
2	D	0.54	0/759	0.62	0/1029
2	Е	0.56	0/759	0.67	0/1029
2	Q	0.58	0/759	0.61	0/1029
2	R	0.54	0/759	0.65	0/1029
3	А	0.52	0/4667	0.52	0/6335
3	В	0.35	0/4616	0.43	0/6268
3	N	0.33	0/4616	0.43	0/6266
3	Р	0.35	0/4527	0.45	0/6151
4	G	0.38	0/1443	0.46	0/1926
4	Н	0.41	0/1356	0.48	0/1813
4	Ι	0.42	0/1376	0.47	0/1839
4	J	0.38	0/1342	0.46	0/1797
All	All	0.44	0/50225	0.50	0/67784

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	С	5791	0	5773	203	0
1	F	5677	0	5575	135	0
1	М	5672	0	5583	146	0
1	0	5767	0	5730	142	0
2	D	737	0	686	23	0
2	Ε	737	0	686	43	0
2	Q	737	0	686	16	0
2	R	737	0	686	54	0
3	А	4559	0	4441	107	0
3	В	4510	0	4385	113	0
3	N	4510	0	4373	126	0
3	Р	4423	0	4245	107	0
4	G	1424	0	1387	34	0
4	Н	1341	0	1243	22	0
4	Ι	1360	0	1276	28	0
4	J	1327	0	1203	25	0
5	D	3	0	0	0	0
5	Е	3	0	0	0	0
5	Q	3	0	0	0	0
5	R	3	0	0	0	0
All	All	49321	0	47958	1198	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 12.

The worst 5 of 1198 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)
3:B:154:ARG:HD3	3:B:357:GLN:NE2	1.43	1.33
3:N:154:ARG:HD3	3:N:357:GLN:NE2	1.43	1.30
1:M:531:ALA:HB3	2:R:27:TRP:CZ3	1.76	1.20
3:N:298:LEU:HD23	3:N:591:LEU:HD21	1.26	1.18
3:N:14:ALA:HB2	3:P:18:LEU:HD22	1.21	1.15

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	Perce	entiles
1	С	716/768~(93%)	628 (88%)	80 (11%)	8 (1%)	14	52
1	F	716/768~(93%)	633~(88%)	72 (10%)	11 (2%)	10	46
1	М	716/768~(93%)	648 (90%)	62 (9%)	6 (1%)	19	60
1	Ο	716/768~(93%)	646 (90%)	64 (9%)	6 (1%)	19	60
2	D	87/108 (81%)	60 (69%)	17 (20%)	10 (12%)	0	6
2	Е	87/108 (81%)	57~(66%)	18 (21%)	12 (14%)	0	4
2	Q	87/108 (81%)	62 (71%)	19 (22%)	6 (7%)	1	15
2	R	87/108~(81%)	57~(66%)	20 (23%)	10 (12%)	0	6
3	А	561/623~(90%)	480 (86%)	76 (14%)	5 (1%)	17	57
3	В	558/623~(90%)	510 (91%)	44 (8%)	4 (1%)	22	63
3	Ν	558/623~(90%)	512 (92%)	42 (8%)	4 (1%)	22	63
3	Р	547/623~(88%)	505~(92%)	40 (7%)	2 (0%)	34	72
4	G	166/724~(23%)	156 (94%)	10 (6%)	0	100	100
4	Н	166/724~(23%)	156 (94%)	10 (6%)	0	100	100
4	Ι	166/724~(23%)	156 (94%)	8 (5%)	2 (1%)	13	50
4	J	166/724~(23%)	155 (93%)	11 (7%)	0	100	100
All	All	6100/8892~(69%)	5421 (89%)	593 (10%)	86 (1%)	15	46

5 of 86 Ramachandran outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
1	С	88	LYS
1	С	268	LEU
1	F	526	PRO
2	D	40	ASP
2	Q	40	ASP



5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Perce	entiles
1	\mathbf{C}	635/693~(92%)	527~(83%)	108 (17%)	2	12
1	F	603/693~(87%)	502~(83%)	101 (17%)	2	12
1	М	604/693~(87%)	506 (84%)	98~(16%)	2	13
1	Ο	628/693~(91%)	525 (84%)	103 (16%)	2	12
2	D	78/90~(87%)	55 (70%)	23~(30%)	0	2
2	Ε	78/90~(87%)	61~(78%)	17 (22%)	1	6
2	Q	78/90~(87%)	52~(67%)	26 (33%)	0	2
2	R	78/90~(87%)	63 (81%)	15 (19%)	1	8
3	А	504/560~(90%)	379~(75%)	125~(25%)	0	3
3	В	495/560~(88%)	461 (93%)	34 (7%)	15	40
3	Ν	496/560~(89%)	464 (94%)	32~(6%)	17	42
3	Р	477/560~(85%)	445~(93%)	32 (7%)	16	41
4	G	151/654~(23%)	123~(82%)	28 (18%)	1	9
4	Н	129/654~(20%)	111 (86%)	18 (14%)	3	17
4	Ι	134/654~(20%)	115 (86%)	19 (14%)	3	16
4	J	125/654~(19%)	106 (85%)	19 (15%)	3	14
All	All	5293/7988~(66%)	4495 (85%)	798 (15%)	6	14

5 of 798 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	R	102	GLU
3	А	470	LYS
2	Q	74	VAL
2	R	99	ARG
3	А	308	VAL

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 116 such side chains are listed below:



Mol	Chain	Res	Type
1	0	618	GLN
4	J	564	ASN
2	R	41	ASN
4	J	457	GLN
4	Ι	564	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.



6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-34453. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map



6.1.2 Raw map



The images above show the map projected in three orthogonal directions.



6.2 Central slices (i)

6.2.1 Primary map



X Index: 96



Y Index: 96



Z Index: 96

6.2.2 Raw map



X Index: 96

Y Index: 96

Z Index: 96

The images above show central slices of the map in three orthogonal directions.



6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 102



Y Index: 106



Z Index: 68

6.3.2 Raw map



X Index: 102

Y Index: 108



The images above show the largest variance slices of the map in three orthogonal directions.



6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



6.4.2 Raw map



The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.001. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.



7.2 Volume estimate (i)



The volume at the recommended contour level is 108428 nm^3 ; this corresponds to an approximate mass of 97946 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.



7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.133 ${\rm \AA}^{-1}$



8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.133 $\mathrm{\AA^{-1}}$



8.2 Resolution estimates (i)

$\mathbf{Bosolution} \text{ ostimato } (\mathbf{\hat{\lambda}})$	Estim	Estimation criterion (FSC cut-off)			
Resolution estimate (A)	0.143	0.5	Half-bit		
Reported by author	7.52	-	-		
Author-provided FSC curve	-	-	-		
Unmasked-calculated*	8.58	10.89	8.79		

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.58 differs from the reported value 7.52 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-34453 and PDB model 8H37. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.001 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.



9.2 Q-score mapped to coordinate model (i)



The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model (i)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.001).



9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.



9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.001) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score	
All	0.9740	0.0570	
А	0.9950	0.0600	
В	0.9880	0.0440	1 0
С	0.9930	0.1050	
D	0.9200	0.0200	
Е	0.9710	0.0270	
F	0.9950	0.0940	
G	0.9610	0.0420	
Н	0.9320	0.0330	
Ι	0.7700	-0.0150	
J	0.8140	-0.0430	
М	0.9860	0.0840	0.0
N	0.9800	0.0250	<0.0
0	0.9870	0.0720	
Р	0.9890	0.0280]
Q	0.9810	0.0150	
R	0.9490	-0.0020	

