

# wwPDB EM Validation Summary Report (i)

#### Nov 20, 2022 – 09:50 am GMT

PDB ID : 6HUM EMDB ID : EMD-0281

Title : Structure of the photosynthetic complex I from Thermosynechococcus elonga-

tus

Authors: Schuller, J.M.; Schuller, S.K.; Kurisu, G.; Engel, B.D.; Nowaczyk, M.M.

Deposited on : 2018-10-09

Resolution : 3.34 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.dev43

Mogul : 1.8.4, CSD as541be (2020)

MolProbity : 4.02b-467 buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

MapQ: 1.9.9

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

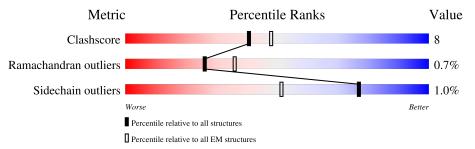
Validation Pipeline (wwPDB-VP) : 2.31.2

## 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 3.34 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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.

Mol	Chain	Length	Quality of chain		
1	A	372	7%	16%	• 5%
2	С	132	70%	16% •	14%
3	D	529	77%	15%	• 8%
4	Е	101	9%		13% •
5	В	515	75%	16%	• 8%
6	G	200	74%	10%	16%
7	J	168	<b>•</b> 69%	23%	• 7%
8	Р	42	88%		12%

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Mol	Chain	Length	Quality of chain	
9	Н	394	10%	14%
10	I	196	6% 88%	10% •
11	K	237	72% 14%	13%
12	L	76	79%	21%
13	F	656	84%	9% 7%
14	N	150	81%	15% • •
15	M	111	90%	8% ••
16	S	110	48% • 50%	
17	О	70	63% 30%	
18	Q	39	92%	8%



## 2 Entry composition (i)

There are 21 unique types of molecules in this entry. The entry contains 29521 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 NAD(P)H-quinone oxidoreductase subunit 1.

Mol	Chain	Residues		At	oms			AltConf	Trace
1	A	352	Total 2718	C 1833	N 421	O 454	S 10	0	0

• Molecule 2 is a protein called NAD(P)H-quinone oxidoreductase subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	С	114	Total 914	C 629	N 138	O 143	S 4	0	0

• Molecule 3 is a protein called NAD(P)H-quinone oxidoreductase chain 4 1.

Mol	Chain	Residues		At	oms			AltConf	Trace
3	D	488	Total 3706	C 2497	N 587	O 601	S 21	0	0

• Molecule 4 is a protein called NAD(P)H-quinone oxidoreductase subunit 4L.

Mol	Chain	Residues		At	oms	AltConf	Trace		
4	E	100	Total 769	_	N 126	O 133	S 4	0	0

• Molecule 5 is a protein called NAD(P)H-quinone oxidoreductase subunit 2.

Mol	Chain	Residues		At	AltConf	Trace			
5	В	475	Total 3541	C 2360	N 548	O 617	S 16	0	0

• Molecule 6 is a protein called NADH dehydrogenase subunit 6.

Mol	Chain	Residues		At	oms	AltConf	Trace		
6	G	168	Total 1262	C 844	N 196	O 218	S 4	0	0



• Molecule 7 is a protein called NAD(P)H-quinone oxidoreductase subunit J.

Mol	Chain	Residues		${f Atoms}$					Trace
7	т	156	Total	С	N	О	S	0	0
'	J	150	1278	817	218	238	5	U	U

• Molecule 8 is a protein called Proton-translocating NADH-quinone dehydrogenase subunit P NdhP.

Mo	Chain	Residues		${f Atoms}$					Trace
0	D	49	Total	С	N	О	S	0	0
0	Г	42	319	213	52	52	2	0	U

• Molecule 9 is a protein called NAD(P)H-quinone oxidoreductase subunit H.

Mol	Chain	Residues		${f Atoms}$					Trace
9	Н	393	Total 3153	C 2035	N 540	O 559	S 19	0	0

• Molecule 10 is a protein called NAD(P)H-quinone oxidoreductase subunit I.

Mol	Chain	Residues	Atoms				AltConf	Trace	
10	I	193	Total 1520	C 970	N 260	O 277	S 13	0	0

• Molecule 11 is a protein called NAD(P)H-quinone oxidoreductase subunit K.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	206	Total 1594	C 1024	N 276	O 281	S 13	0	0

• Molecule 12 is a protein called NAD(P)H-quinone oxidoreductase subunit L.

Mol	Chain	Residues	Atoms				AltConf	Trace	
12	L	76	Total 609	C 417	N 93	O 97	S 2	0	0

• Molecule 13 is a protein called NADH dehydrogenase subunit 5.

Mol	Chain	Residues	Atoms				AltConf	Trace	
13	F	611	Total 4717	C 3148	N 736	O 796	S 37	0	0



• Molecule 14 is a protein called NAD(P)H-quinone oxidoreductase subunit N.

Mol	Chain	Residues	Atoms				AltConf	Trace	
14	N	147	Total	С	N	0	S	0	0
			1160	755	200	204	1		

• Molecule 15 is a protein called NAD(P)H-quinone oxidoreductase subunit M.

Mol	Chain	Residues	Atoms				AltConf	Trace	
15	M	110	Total 879	C 548	N 160	O 169	S 2	0	0

• Molecule 16 is a protein called Tlr0636 protein.

Mol	Chain	Residues	Atoms				AltConf	Trace	
16	S	55	Total 432	C 280	N 69	O 82	S 1	0	0

• Molecule 17 is a protein called NAD(P)H-quinone oxidoreductase subunit O.

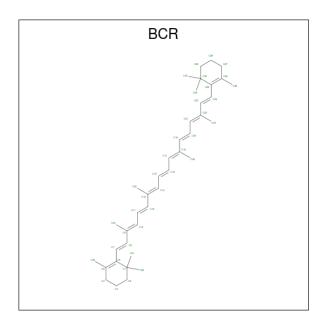
Mol	Chain	Residues	Atoms				AltConf	Trace
17	О	68	Total	C 240	N 01	O 98	0	0
			538	349	91	98		

• Molecule 18 is a protein called Proton-translocating NADH-quinone dehydrogenase subunit Q NdhQ.

Mol	Chain	Residues	Atoms				AltConf	Trace	
18	Q	39	Total 293	C 198	N 47	O 46	S 2	0	0

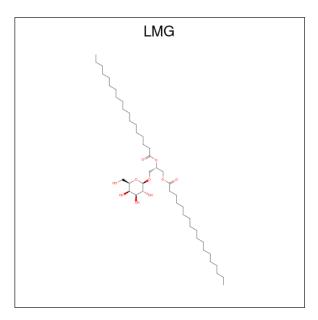
 $\bullet$  Molecule 19 is BETA-CAROTENE (three-letter code: BCR) (formula:  $\mathrm{C_{40}H_{56}}).$ 





Mol	Chain	Residues	Atoms	AltConf
19	D	1	Total C 40 40	0

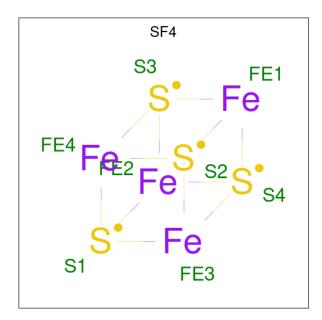
• Molecule 20 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



Mol	Chain	Residues	Atoms	AltConf
20	D	1	Total C O 55 45 10	0

 $\bullet$  Molecule 21 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe $_4$ S4).





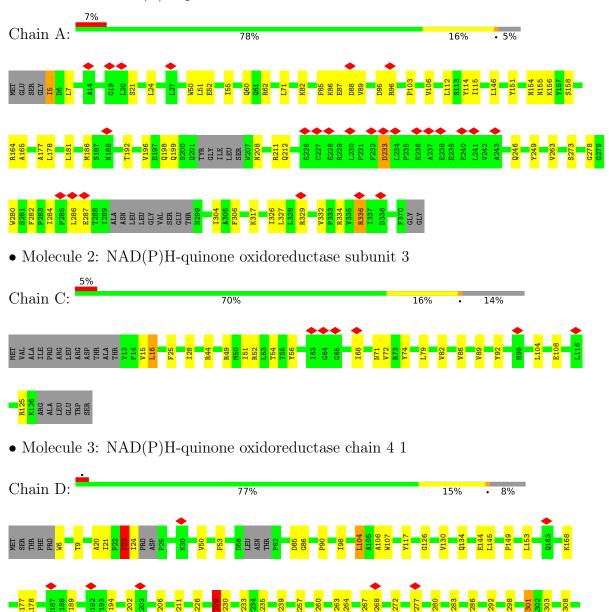
Mol	Chain	Residues	Atoms	AltConf
21	Ţ	1	Total Fe S	0
21	1	1	16 8 8	0
21	Т	1	Total Fe S	0
21	1	1	16 8 8	0
21	I/	1	Total Fe S	0
\ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \ \	K	1	8 4 4	0



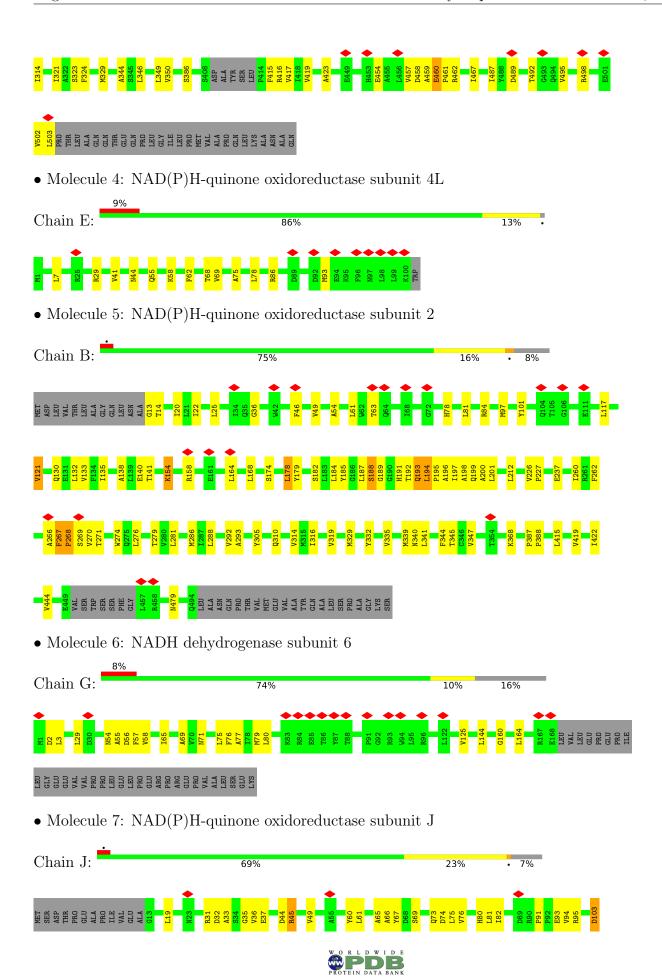
## 3 Residue-property plots (i)

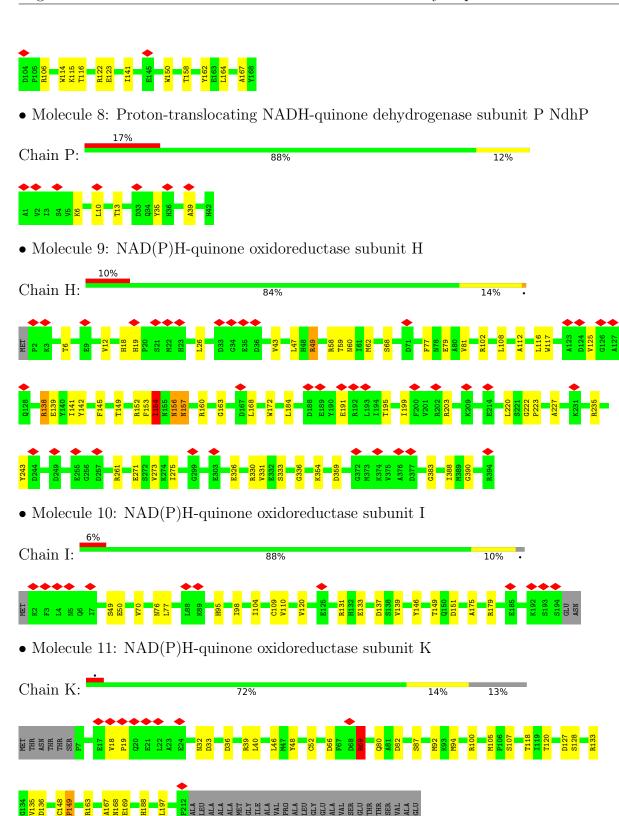
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

• Molecule 1: NAD(P)H-quinone oxidoreductase subunit 1









• Molecule 12: NAD(P)H-quinone oxidoreductase subunit L

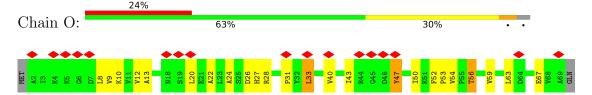
Chain L: 79% 21%



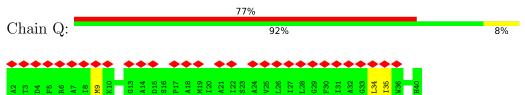




• Molecule 17: NAD(P)H-quinone oxidoreductase subunit O



 $\bullet$  Molecule 18: Proton-translocating NADH-quinone dehydrogenase subunit Q NdhQ





# 4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	133485	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 $(e^-/\text{Å}^2)$	49.93	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.659	Depositor
Minimum map value	-0.230	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	405.0, 405.0, 405.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	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: SF4, BCR, LMG

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		Bond angles	
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.37	0/2788	0.60	0/3812	
2	С	0.37	0/942	0.65	0/1285	
3	D	0.38	0/3805	0.58	2/5189 (0.0%)	
4	Е	0.35	0/777	0.57	0/1054	
5	В	0.38	0/3623	0.61	2/4947~(0.0%)	
6	G	0.35	0/1288	0.55	0/1765	
7	J	0.40	0/1314	0.72	3/1789~(0.2%)	
8	Р	0.39	0/328	0.59	0/447	
9	Н	0.39	0/3236	0.65	0/4389	
10	I	0.41	0/1558	0.60	0/2116	
11	K	0.40	0/1636	0.65	0/2228	
12	L	0.36	0/629	0.62	0/860	
13	F	0.33	0/4852	0.58	1/6603 (0.0%)	
14	N	0.35	0/1192	0.66	1/1621 (0.1%)	
15	M	0.35	0/895	0.72	2/1214 (0.2%)	
16	S	0.34	0/441	0.55	0/601	
17	О	0.45	0/550	1.26	12/748 (1.6%)	
18	Q	0.27	0/301	0.48	0/409	
All	All	0.37	0/30155	0.63	23/41077 (0.1%)	

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
2	С	0	1
3	D	0	2
5	В	0	1
11	K	0	3
17	O	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
All	All	0	9

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
3	D	23	PHE	O-C-N	-8.40	109.25	122.70
17	О	22	ALA	C-N-CA	7.50	140.45	121.70
17	О	50	ILE	CG1-CB-CG2	6.86	126.49	111.40
17	О	40	VAL	CG1-CB-CG2	6.79	121.77	110.90
17	О	9	VAL	CG1-CB-CG2	6.78	121.75	110.90

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	В	387	PRO	Peptide
2	С	16	LEU	Peptide
3	D	23	PHE	Mainchain
3	D	301	ASN	Peptide
11	K	18	VAL	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	2718	0	2838	47	0
2	С	914	0	945	24	0
3	D	3706	0	3835	66	0
4	Е	769	0	827	17	0
5	В	3541	0	3650	119	0
6	G	1262	0	1334	17	0
7	J	1278	0	1233	48	0
8	Р	319	0	319	4	0
9	Н	3153	0	3116	51	0
10	I	1520	0	1467	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	1594	0	1627	34	0
12	L	609	0	625	12	0
13	F	4717	0	4784	46	0
14	N	1160	0	1171	21	0
15	M	879	0	859	8	0
16	S	432	0	430	2	0
17	О	538	0	549	15	0
18	Q	293	0	299	3	0
19	D	40	0	56	0	0
20	D	55	0	86	2	0
21	I	16	0	0	1	0
21	K	8	0	0	0	0
All	All	29521	0	30050	447	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.

The worst 5 of 447 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$
5:B:194:LEU:CB	5:B:266:ALA:HB2	1.35	1.55
5:B:194:LEU:HB3	5:B:266:ALA:CB	1.04	1.49
5:B:194:LEU:CB	5:B:266:ALA:CB	1.87	1.41
3:D:233:THR:CG2	13:F:610:ASP:OD1	1.68	1.39
7:J:103:ASP:OD2	17:O:20:LEU:CG	1.74	1.35

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	A	346/372 (93%)	308 (89%)	36 (10%)	2 (1%)	25	60
2	С	112/132 (85%)	99 (88%)	13 (12%)	0	100	100
3	D	480/529 (91%)	437 (91%)	36 (8%)	7 (2%)	10	40
4	Е	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
5	В	471/515 (92%)	423 (90%)	39 (8%)	9 (2%)	8	36
6	G	166/200 (83%)	156 (94%)	10 (6%)	0	100	100
7	J	154/168 (92%)	121 (79%)	33 (21%)	0	100	100
8	Р	40/42 (95%)	32 (80%)	8 (20%)	0	100	100
9	Н	391/394 (99%)	333 (85%)	57 (15%)	1 (0%)	41	72
10	I	191/196 (97%)	168 (88%)	22 (12%)	1 (0%)	29	63
11	K	204/237 (86%)	174 (85%)	28 (14%)	2 (1%)	15	49
12	L	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
13	F	603/656 (92%)	535 (89%)	67 (11%)	1 (0%)	47	78
14	N	145/150 (97%)	121 (83%)	24 (17%)	0	100	100
15	M	108/111 (97%)	87 (81%)	21 (19%)	0	100	100
16	S	53/110 (48%)	49 (92%)	4 (8%)	0	100	100
17	О	66/70 (94%)	47 (71%)	17 (26%)	2 (3%)	4	27
18	Q	37/39 (95%)	33 (89%)	4 (11%)	0	100	100
All	All	3739/4098 (91%)	3285 (88%)	429 (12%)	25 (1%)	26	57

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	В	187	LEU
5	В	194	LEU
5	В	267	PHE
9	Н	154	ILE
13	F	581	TYR

#### 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	284/302 (94%)	282 (99%)	2 (1%)	84	91
2	$\mathbf{C}$	93/109 (85%)	93 (100%)	0	100	100
3	D	370/424 (87%)	368 (100%)	2 (0%)	88	93
4	E	81/82 (99%)	81 (100%)	0	100	100
5	В	367/413 (89%)	363 (99%)	4 (1%)	73	86
6	G	134/166 (81%)	133 (99%)	1 (1%)	84	91
7	J	138/148 (93%)	136 (99%)	2 (1%)	67	83
8	Р	32/34 (94%)	32 (100%)	0	100	100
9	Н	331/338 (98%)	323 (98%)	8 (2%)	49	75
10	I	162/172 (94%)	162 (100%)	0	100	100
11	K	174/196 (89%)	172 (99%)	2 (1%)	73	86
12	L	63/63 (100%)	63 (100%)	0	100	100
13	F	487/527 (92%)	483 (99%)	4 (1%)	81	90
14	N	119/120 (99%)	117 (98%)	2 (2%)	60	80
15	M	95/96 (99%)	92 (97%)	3 (3%)	39	69
16	S	48/97 (50%)	48 (100%)	0	100	100
17	О	57/59 (97%)	56 (98%)	1 (2%)	59	79
18	Q	27/28 (96%)	27 (100%)	0	100	100
All	All	3062/3374 (91%)	3031 (99%)	31 (1%)	77	87

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	Н	154	ILE
		104	122
15	M	1	MET
9	H	261	ARG
15	M	59	ASN
13	F	596	ARG

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such side chains are listed below:

Mol	Chain	Res	Type
9	Н	18	HIS
9	Н	155	ASN
11	K	104	GLN
9	Н	157	ASN

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Mol	Chain	Res	Type
7	J	73	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)

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)

5 ligands 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).

Mal	Trmo	Chain	Dag	T inle	Bond lengths			Bond angles		
Mol	Type	Chain	Res	Link	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	SF4	I	202	10	0,12,12	-	-	-		
21	SF4	K	501	11	0,12,12	-	-	-		
20	LMG	D	602	-	55,55,55	0.80	2 (3%)	63,63,63	1.33	7 (11%)
21	SF4	I	201	10	0,12,12	-	-	-		
19	BCR	D	601	-	41,41,41	1.09	2 (4%)	56,56,56	1.48	9 (16%)

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
21	SF4	I	202	10	-	-	0/6/5/5
21	SF4	K	501	11	-	-	0/6/5/5
20	LMG	D	602	-	-	15/50/70/70	0/1/1/1
21	SF4	I	201	10	-	-	0/6/5/5
19	BCR	D	601	-	-	21/29/63/63	0/2/2/2

#### All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\operatorname{Observed}(\text{\AA})$	$Ideal(\AA)$
19	D	601	BCR	C1-C6	-3.52	1.48	1.53
20	D	602	LMG	C4-C5	2.73	1.58	1.53
20	D	602	LMG	O7-C8	-2.34	1.40	1.46
19	D	601	BCR	C30-C25	-2.12	1.50	1.53

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$Observed(^o)$	$Ideal(^{o})$
19	D	601	BCR	C24-C23-C22	-4.23	119.84	126.23
19	D	601	BCR	C11-C10-C9	-3.73	121.98	127.31
20	D	602	LMG	O6-C5-C4	3.48	116.02	109.69
19	D	601	BCR	C15-C16-C17	-2.87	117.59	123.47
19	D	601	BCR	C33-C5-C6	-2.78	121.41	124.53

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	D	601	BCR	C1-C6-C7-C8
19	D	601	BCR	C6-C7-C8-C9
19	D	601	BCR	C11-C10-C9-C8
19	D	601	BCR	C11-C10-C9-C34
19	D	601	BCR	C10-C11-C12-C13

There are no ring outliers.

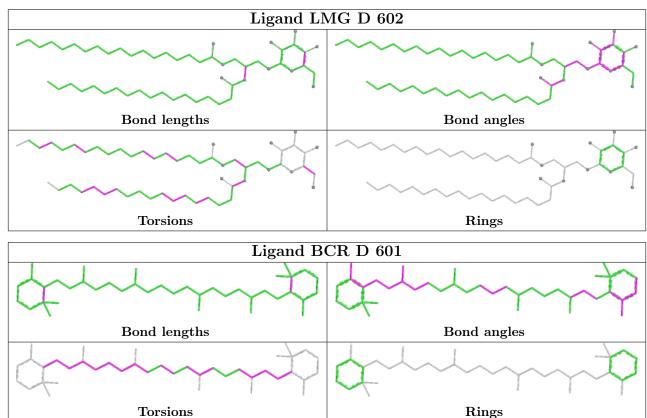
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	D	602	LMG	2	0
21	I	201	SF4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In



addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



### 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.



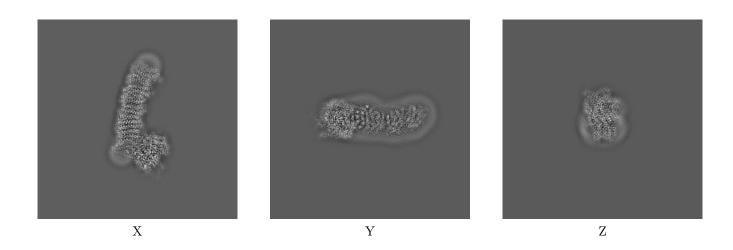
## 6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-0281. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

## 6.1 Orthogonal projections (i)

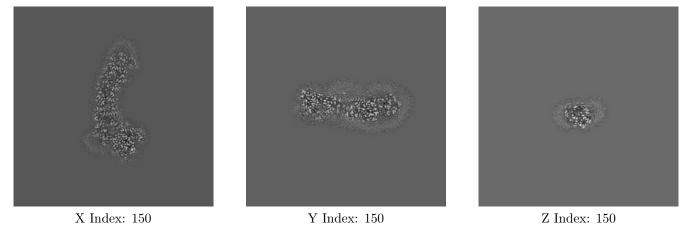
#### 6.1.1 Primary map



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

### 6.2 Central slices (i)

#### 6.2.1 Primary map

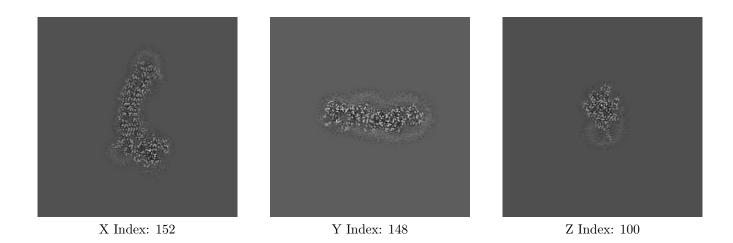




The images above show central slices of the map in three orthogonal directions.

### 6.3 Largest variance slices (i)

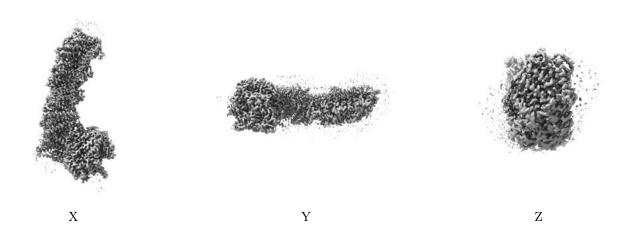
#### 6.3.1 Primary map



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

## 6.4 Orthogonal surface views (i)

#### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



## 6.5 Mask visualisation (i)

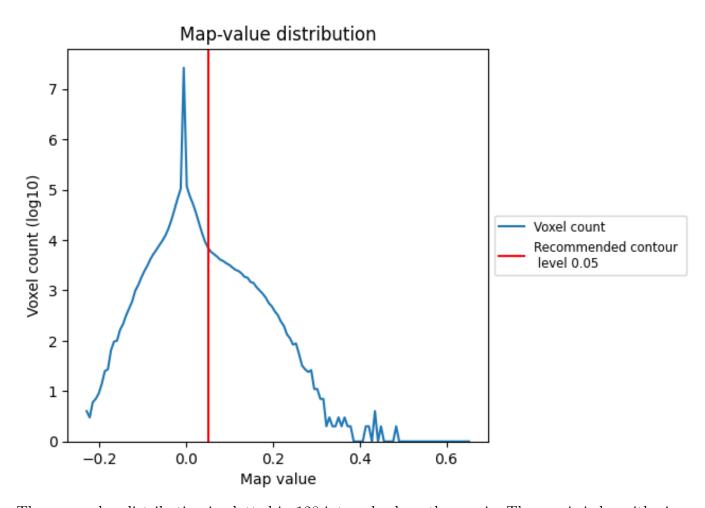
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis (i)

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

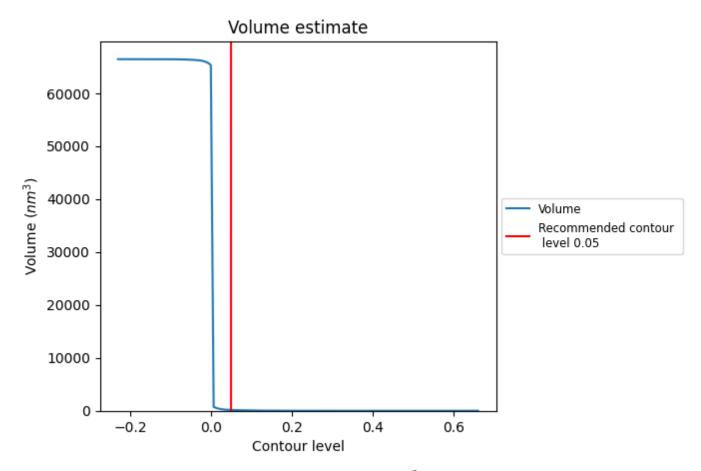
## 7.1 Map-value distribution (i)



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)

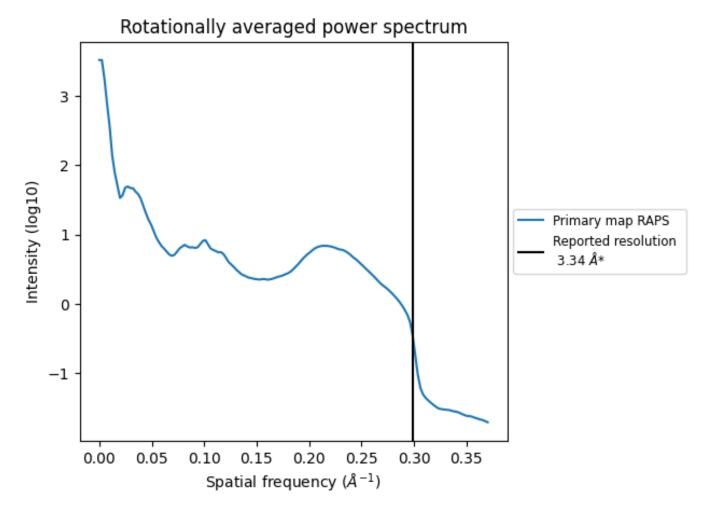


The volume at the recommended contour level is  $150~\mathrm{nm}^3$ ; this corresponds to an approximate mass of  $135~\mathrm{kDa}$ .

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)



<sup>\*</sup>Reported resolution corresponds to spatial frequency of 0.299  $\rm \AA^{-1}$ 



# 8 Fourier-Shell correlation (i)

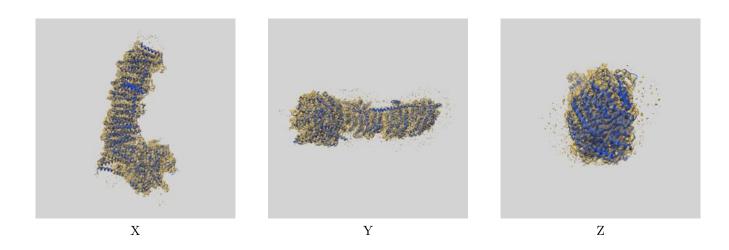
This section was not generated. No FSC curve or half-maps provided.



## 9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-0281 and PDB model 6HUM. Per-residue inclusion information can be found in section 3 on page 9.

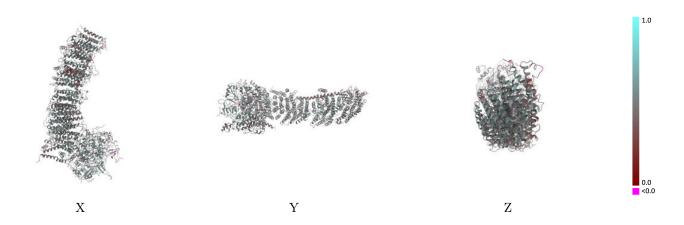
## 9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.05 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.

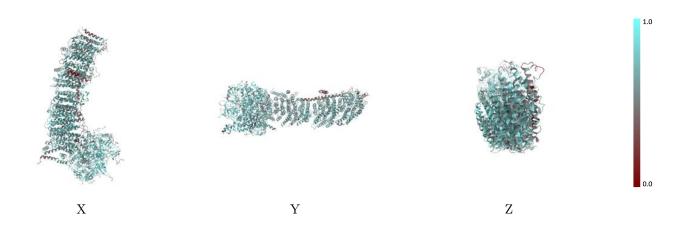


### 9.2 Q-score mapped to coordinate model (i)



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.

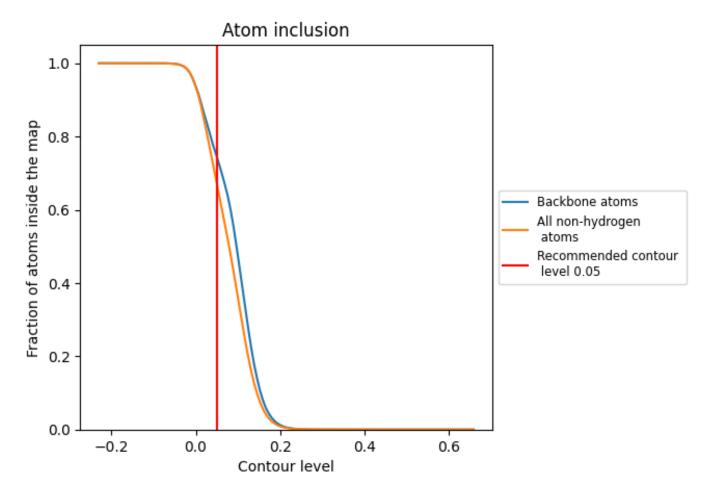
## 9.3 Atom inclusion mapped to coordinate model (i)



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 (0.05).



## 9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 67% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6715	0.4820
A	0.6629	0.4820
В	0.7012	0.4880
С	0.6801	0.4760
D	0.7018	0.4960
E	0.6618	0.4970
F	0.6088	0.4610
G	0.6514	0.4980
Н	0.6841	0.4840
I	0.7093	0.5050
J	0.7111	0.4740
K	0.7301	0.5060
L	0.5808	0.4550
M	0.7098	0.4850
N	0.7120	0.4910
О	0.6027	0.3740
Р	0.6635	0.4780
Q	0.2457	0.3980
S	0.7237	0.5200



