

wwPDB EM Validation Summary Report (i)

Nov 29, 2022 – 06:47 PM EST

PDB ID	:	8DJM
EMDB ID	:	EMD-27461
Title	:	HMGCR-UBIAD1 Complex State 1
Authors	:	Chen, H.; Qi, X.; Li, X.
Deposited on		
Resolution	:	3.23 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 (i)) were used in the production of this report:

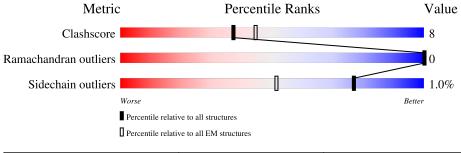
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.23 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	$egin{array}{c} { m Whole \ archive}\ (\#{ m Entries}) \end{array}$	${f EM} {f structures} \ (\#{f Entries})$		
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 $\geq=3, 2, 1$ 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 $\leq=5\%$ 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	А	364	6% 63%		·	35%					
2	В	301	•	90%			• 7%				
3	С	120	69%			14% •					
4	L	214	45%	5%	5	0%					
5	Н	232	• 50%	•	4	.9%					

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	Y01	А	401	Х	-	-	-
6	Y01	А	402	Х	-	-	-
6	Y01	А	403	Х	-	-	-
6	Y01	А	404	Х	-	-	-
6	Y01	В	401	Х	-	-	-
6	Y01	В	403	Х	-	-	-
7	AJP	А	405	Х	-	-	-
7	AJP	В	402	Х	-	Х	-



2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7032 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 3-hydroxy-3-methylglutaryl-coenzyme A reductase.

Mol	Chain	Residues	Atoms				AltConf	Trace	
1	А	237	Total 1871	C 1225	N 309	0 319	S 18	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	-7	MET	-	expression tag	UNP P00347
А	-6	ASP	-	expression tag	UNP P00347
А	-5	TYR	-	expression tag	UNP P00347
A	-4	LYS	-	expression tag	UNP P00347
А	-3	ASP	-	expression tag	UNP P00347
А	-2	ASP	-	expression tag	UNP P00347
А	-1	ASP	-	expression tag	UNP P00347
А	0	ASP	-	expression tag	UNP P00347
А	1	LYS	-	expression tag	UNP P00347
A	89	ARG	LYS	conflict	UNP P00347
А	248	ARG	LYS	conflict	UNP P00347

• Molecule 2 is a protein called UbiA prenyltransferase domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	В	281	Total 2152	C 1431	N 338	0 374	S 9	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	38	MET	-	initiating methionine	UNP G3IEF0
В	39	ALA	-	expression tag	UNP G3IEF0
В	40	SER	-	expression tag	UNP G3IEF0
В	102	SER	ASN	conflict	UNP G3IEF0

• Molecule 3 is a protein called Soluble cytochrome b562.



Mol	Chain	Residues	Atoms					AltConf	Trace
3	С	120	Total 944	$\begin{array}{c} \mathrm{C} \\ 585 \end{array}$	N 171	O 186	${ m S} { m 2}$	0	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	264	ALA	-	expression tag	UNP P0ABE7
С	265	ARG	-	expression tag	UNP P0ABE7
С	266	ARG	-	expression tag	UNP P0ABE7
С	267	LEU	-	expression tag	UNP P0ABE7
С	268	ALA	-	expression tag	UNP P0ABE7
С	273	TRP	MET	conflict	UNP P0ABE7
С	368	ILE	HIS	conflict	UNP P0ABE7
С	372	LEU	-	expression tag	UNP P0ABE7
С	373	GLU	-	expression tag	UNP P0ABE7
С	374	ARG	-	expression tag	UNP P0ABE7
С	375	ALA	-	expression tag	UNP P0ABE7
С	376	ARG	-	expression tag	UNP P0ABE7
С	377	SER	-	expression tag	UNP P0ABE7
С	378	THR	-	expression tag	UNP P0ABE7
С	379	LEU	-	expression tag	UNP P0ABE7
С	380	GLN	-	expression tag	UNP P0ABE7
С	381	LYS	-	expression tag	UNP P0ABE7
С	382	GLU	-	expression tag	UNP P0ABE7
С	383	VAL	-	expression tag	UNP P0ABE7

• Molecule 4 is a protein called Fab 15B2 Light Chain.

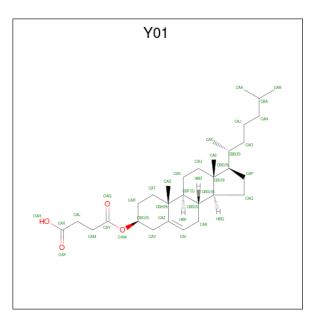
Mol	Chain	Residues	Atoms				AltConf	Trace	
4	L	106	Total 808	C 504	N 136	0 166	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0

• Molecule 5 is a protein called Fab 15B2 Heavy Chain.

Mol	Chain	Residues		At	oms			AltConf	Trace
5	Н	118	Total 930	C 587	N 160	0 178	${f S}{5}$	0	0

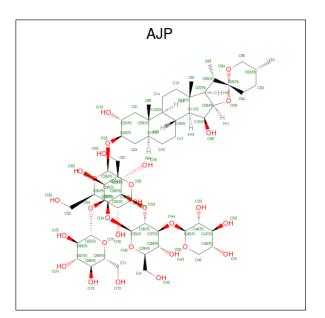
• Molecule 6 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).





Mol	Chain	Residues	Atoms	AltConf
6	А	1	Total C O 140 124 16	0
6	А	1	Total C O 140 124 16	0
6	А	1	Total C O 140 124 16	0
6	А	1	Total C O 140 124 16	0
6	В	1	Total C O 70 62 8	0
6	В	1	Total C O 70 62 8	0





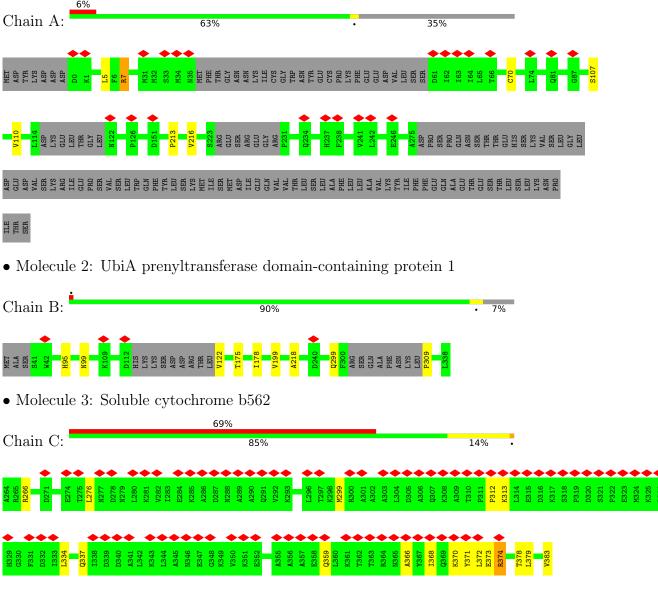
Mol	Chain	Residues	Atoms	AltConf
7	А	1	Total C O 74 50 24	0
7	В	1	Total C O 43 33 10	0



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: 3-hydroxy-3-methylglutaryl-coenzyme A reductase



• Molecule 4: Fab 15B2 Light Chain



Chain L:	45%	5%	50%
226 226 129 V32 V32 V38 V66 V66	DI OI MI13 P114 E124 LY S LY S ARG THR ALA ALA ALA	SER VAL PHE TLE PHE PRO PRO PRO PRO CLU CLU CLU CLU SER SER SER	GLY THR ALA SER VAL VAL CYS CYS CYS CYS CYS CYS ASN ASN ASN ASN ASN ASN ASN ASN ASN AS
GLN TRP LYS LYS VAL ASP ASP ASP ASN GLN GLN GLN GLY	SER GLU GLU GLU GLU GLU GLU GLU GLU GLU ASP SER LYS SER THR TTR	JER LEU SER SER THR LEU LEU LVS SER ALA ASP TYR GLU	LYS LYS LYS LYS LYR VAL ALA CUU VAL HIS CUU VAL LEU CLN CLN CLN CLN THR CLN THR THR THR THR THR
LYS PHE ASN ASN GLY GLY CYS			
• Molecule 5: Fa	b 15B2 Heavy Chain	L	
Chain H:	50%		49%
E20	SER ALA SER SER SER LY GLY GLY SER SER VAL PHE PRO LEU LEU SER SER SER SER SER SER SER SER SER SER	SER LYS SER THR SER GLY GLY ALA ALA ALA LEU CYS	VAL VAL LYS ASP ASP ASP PHE PHC PHC PHC PHC PHC ALU SER ALA ALA ALA LEU THR ASN SER ALA
SER GLY VAL HIS HHE PHE PRO ALA VAL LEU GLN SER	SER GLY LEU TYR SER SER SER SER VAL VAL VAL THR VAL SER SER	SEK LEU GLY THR GLN THR GLN THR CVS CVS ASN VAL ASN HIS LYS	PR0 ASN THR ASN LYS VAL ASP CVS SER ASP CYS SER ASP THR HIS
HIS HIS HIS HIS HIS			



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	215396	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 $(e^-/\text{\AA}^2)$	8.5	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.411	Depositor
Minimum map value	-3.072	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.081	Depositor
Recommended contour level	0.395	Depositor
Map size (Å)	269.44, 269.44, 269.44	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.842, 0.842, 0.842	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: Y01, AJP

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	Bo	nd lengths	Bo	ond angles
IVIOI	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.42	0/1909	0.56	1/2583~(0.0%)
2	В	0.42	0/2204	0.55	0/3005
3	С	0.41	0/954	0.57	0/1283
4	L	0.60	2/826~(0.2%)	0.80	3/1121~(0.3%)
5	Н	0.36	0/953	0.55	0/1285
All	All	0.44	2/6846~(0.0%)	0.59	4/9277~(0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	Observed(Å)	Ideal(Å)
4	L	113	TRP	C-N	8.58	1.50	1.34
4	L	114	PRO	N-CA	7.48	1.59	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	L	113	TRP	CB-CA-C	-12.45	85.50	110.40
4	L	26	SER	C-N-CD	8.29	145.80	128.40
4	L	26	SER	N-CA-C	6.66	128.99	111.00
1	А	7	ARG	NE-CZ-NH2	5.52	123.06	120.30

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	1871	0	1927	3	0
2	В	2152	0	2225	11	0
3	С	944	0	960	26	0
4	L	808	0	769	3	0
5	Н	930	0	892	1	0
6	А	140	0	189	31	0
6	В	70	0	94	10	0
7	А	74	0	0	20	0
7	В	43	0	0	21	0
All	All	7032	0	7056	116	0

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

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 116 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)
6:A:402:Y01:CBF	6:A:402:Y01:CBH	1.74	1.61
6:A:401:Y01:CBF	6:A:401:Y01:CBH	1.74	1.60
6:A:403:Y01:CBH	6:A:403:Y01:CBF	1.75	1.59
6:B:401:Y01:CBF	6:B:401:Y01:CBH	1.74	1.59
6:A:404:Y01:CBH	6:A:404:Y01:CBF	1.74	1.59

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	ntiles
1	А	229/364~(63%)	221 (96%)	8 (4%)	0	100	100
2	В	275/301~(91%)	268 (98%)	7(2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentile	es
3	\mathbf{C}	118/120~(98%)	113~(96%)	5(4%)	0	100 100)
4	L	104/214~(49%)	98~(94%)	6~(6%)	0	100 100)
5	Н	116/232~(50%)	111 (96%)	5(4%)	0	100 100)
All	All	842/1231 (68%)	811 (96%)	31 (4%)	0	100 100)

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There are no Ramachandran outliers to report.

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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	А	209/328~(64%)	207~(99%)	2(1%)	76 88		
2	В	230/248~(93%)	228~(99%)	2(1%)	78 89		
3	С	98/98~(100%)	97~(99%)	1 (1%)	76 88		
4	L	92/189~(49%)	91~(99%)	1 (1%)	73 87		
5	Н	100/200~(50%)	99~(99%)	1 (1%)	76 88		
All	All	729/1063~(69%)	722~(99%)	7 (1%)	77 88		

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	В	175	THR
3	С	374	ARG
5	Н	121	ASP
4	L	101	ASP
2	В	122	VAL

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such side chains are listed below:

Mol	Chain	Res	Type
3	С	380	GLN
4	L	25	GLN

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Mol	Chain	Res	Type
3	С	272	ASN
3	С	277	ASN
3	С	279	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)

8 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).

Mol	Turne	Chain	Res	Link	В	ond leng	gths	Bo	nd angle	es
INIOI	Type	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
6	Y01	А	403	-	38,38,38	4.70	17 (44%)	57,57,57	2.20	13 (22%)
6	Y01	В	401	-	38,38,38	4.80	18 (47%)	57,57,57	2.48	19 (33%)
7	AJP	В	402	-	49,49,95	9.44	35 (71%)	74,80,149	2.16	24 (32%)
6	Y01	А	401	-	38,38,38	4.73	18 (47%)	57,57,57	2.02	16 (28%)
7	AJP	А	405	-	83,83,95	7.28	43 (51%)	125,131,149	1.72	28 (22%)
6	Y01	А	404	-	38,38,38	4.71	17 (44%)	57,57,57	1.93	19 (33%)
6	Y01	А	402	-	38,38,38	4.70	17 (44%)	57,57,57	2.06	16 (28%)
6	Y01	В	403	-	38,38,38	4.72	17 (44%)	57,57,57	2.03	17 (29%)



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	Y01	А	403	-	1/1/12/13	11/19/77/77	0/4/4/4
6	Y01	В	401	-	1/1/12/13	9/19/77/77	0/4/4/4
7	AJP	В	402	-	16/16/19/38	2/6/121/220	0/7/7/11
6	Y01	А	401	-	1/1/12/13	7/19/77/77	0/4/4/4
7	AJP	А	405	-	29/29/33/38	9/22/194/220	0/10/10/11
6	Y01	А	404	-	1/1/12/13	7/19/77/77	0/4/4/4
6	Y01	А	402	-	1/1/12/13	10/19/77/77	0/4/4/4
6	Y01	В	403	-	1/1/12/13	9/19/77/77	0/4/4/4

The worst 5 of 182 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	В	402	AJP	C07-C08	27.69	2.01	1.53
7	А	405	AJP	C07-C08	27.37	2.00	1.53
7	А	405	AJP	O09-C08	-26.04	1.00	1.43
7	В	402	AJP	O09-C08	-25.94	1.00	1.43
7	В	402	AJP	O84-C05	-24.00	1.05	1.42

The worst 5 of 152 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
6	В	401	Y01	CBF-CBD-CBG	7.32	118.89	109.09
6	В	401	Y01	CAU-CBI-CBE	6.07	125.66	116.57
7	А	405	AJP	C24-C23-C22	6.03	117.40	111.00
6	А	403	Y01	CBH-CAZ-CAI	-6.01	113.70	122.90
7	В	402	AJP	C24-C23-C22	5.99	117.36	111.00

5 of 51 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	А	401	Y01	CBD
6	А	402	Y01	CBD
6	А	403	Y01	CBD
6	А	404	Y01	CBD
6	В	401	Y01	CBD

5 of 64 torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
6	А	401	Y01	CAR-CBC-OAW-CAY
6	А	402	Y01	CAO-CBB-CBE-CAP
6	А	402	Y01	CAC-CBB-CBE-CBI
6	А	402	Y01	OAG-CAY-OAW-CBC
6	А	402	Y01	CAM-CAY-OAW-CBC

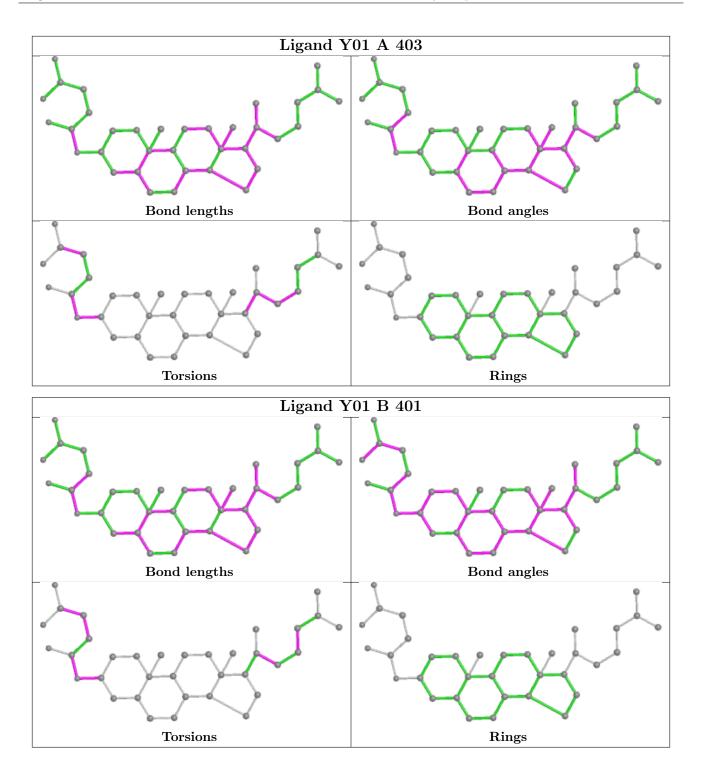
There are no ring outliers.

7 monomers are involved in 82 short contacts:

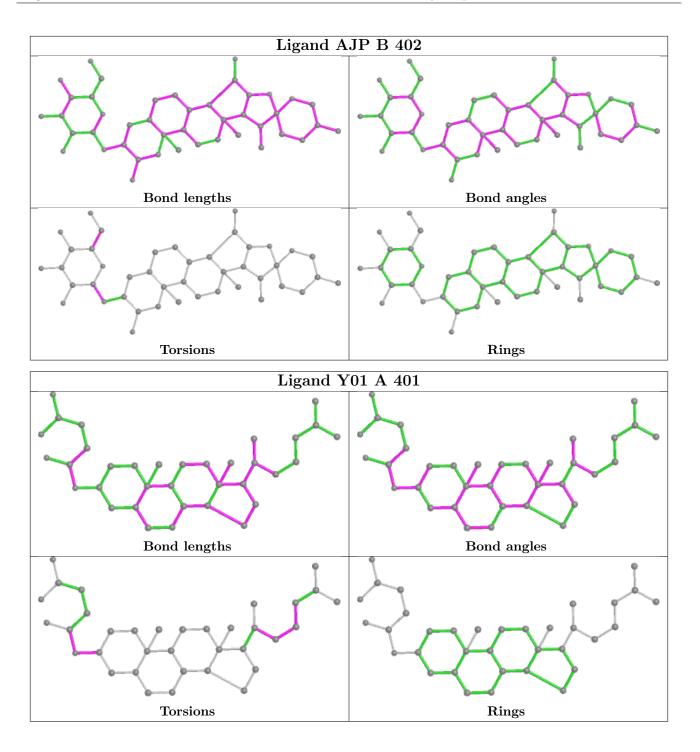
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	А	403	Y01	7	0
6	В	401	Y01	10	0
7	В	402	AJP	21	0
6	А	401	Y01	9	0
7	А	405	AJP	20	0
6	А	404	Y01	7	0
6	А	402	Y01	8	0

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 sufficient The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

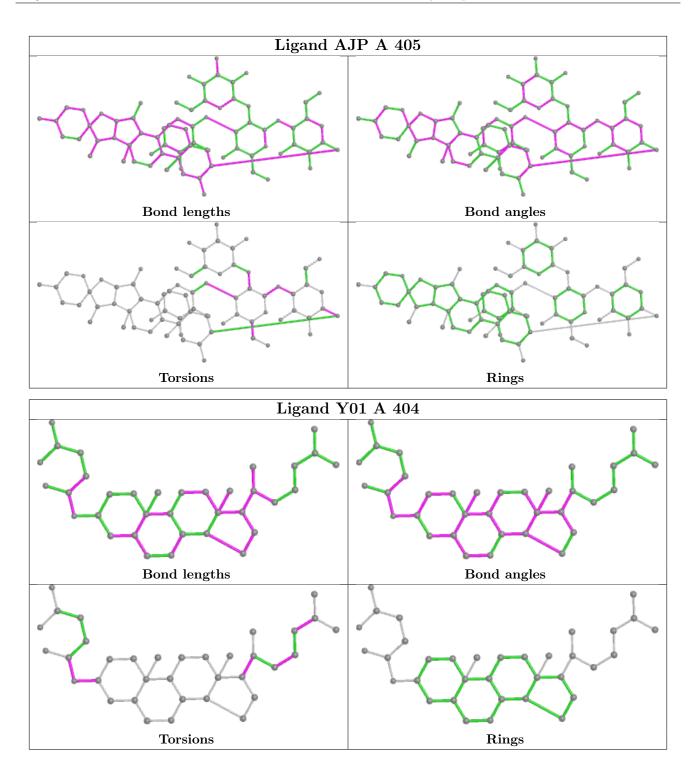




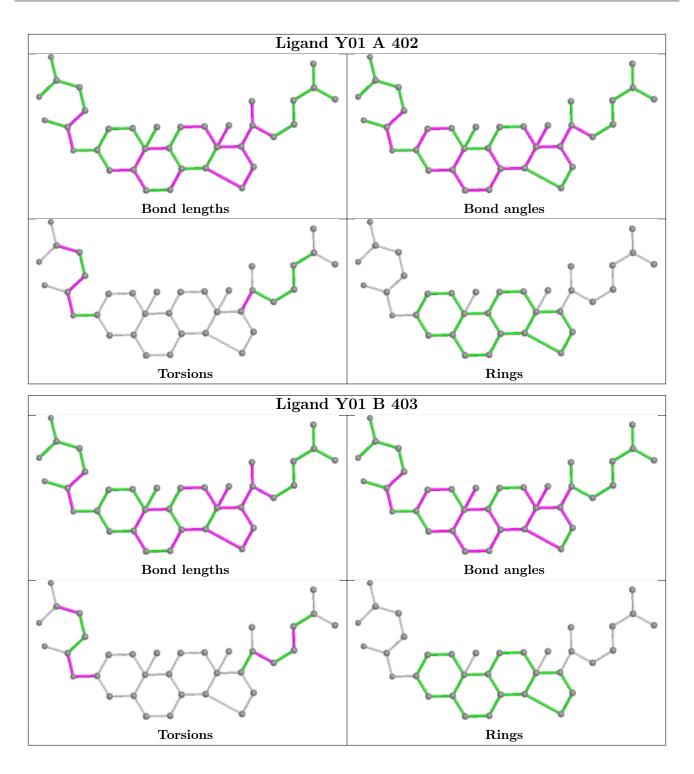












5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



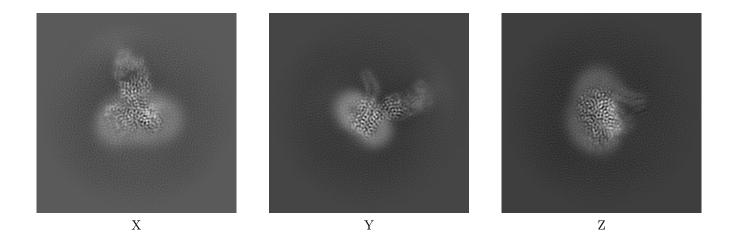
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-27461. These allow visual inspection of the internal detail of the map and identification of artifacts.

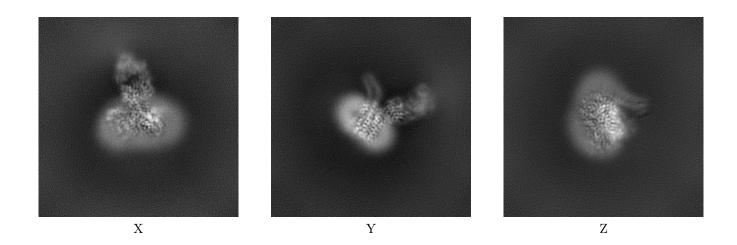
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

6.1.1 Primary map



6.1.2 Raw map

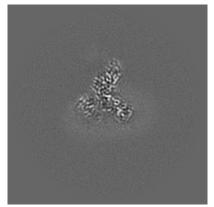


The images above show the map projected in three orthogonal directions.

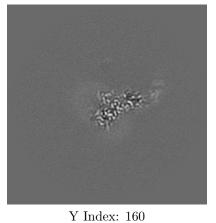


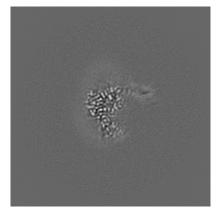
6.2 Central slices (i)

6.2.1 Primary map



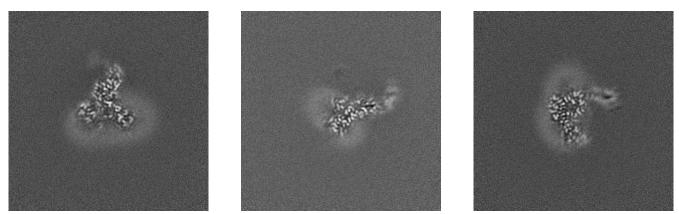
X Index: 160





Z Index: 160

6.2.2 Raw map



X Index: 160

Y Index: 160

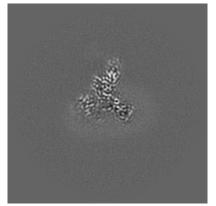


The images above show central slices of the map in three orthogonal directions.

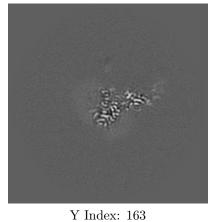


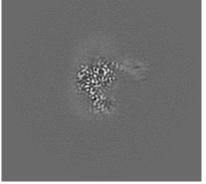
6.3 Largest variance slices (i)

6.3.1 Primary map



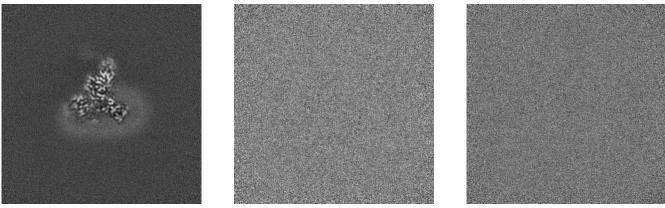
X Index: 159





Z Index: 157

6.3.2 Raw map



X Index: 159

Y Index: 0

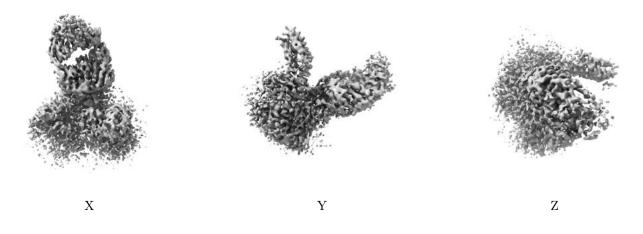


The images above show the largest variance slices of the map in three orthogonal directions.



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 0.395. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

6.5 Mask visualisation (i)

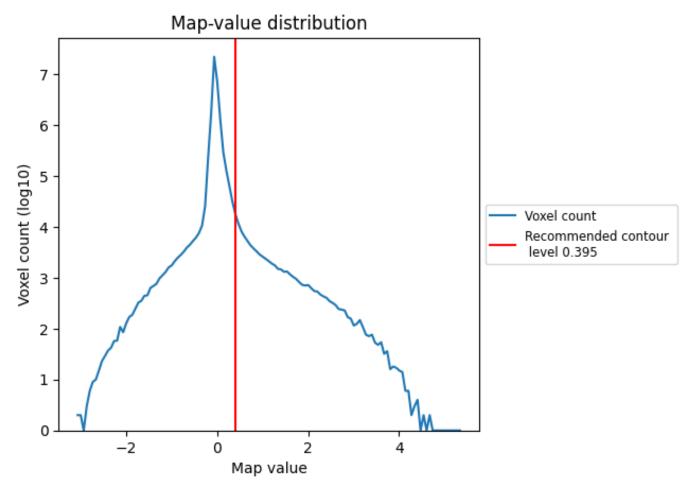
This section was not generated. No masks/segmentation were deposited.



7 Map analysis (i)

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

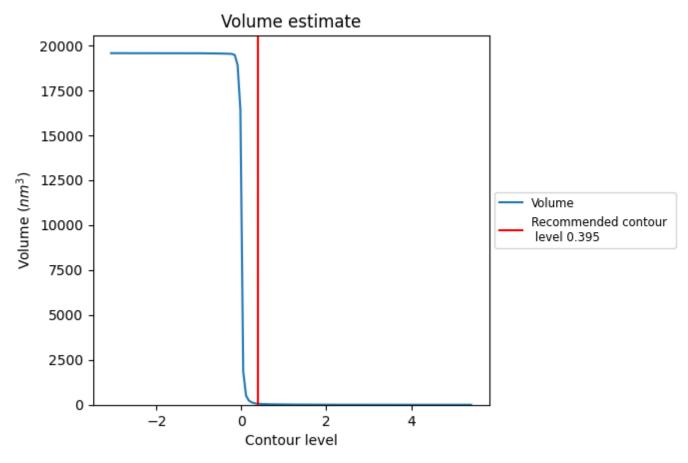
7.1 Map-value distribution (i)



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)

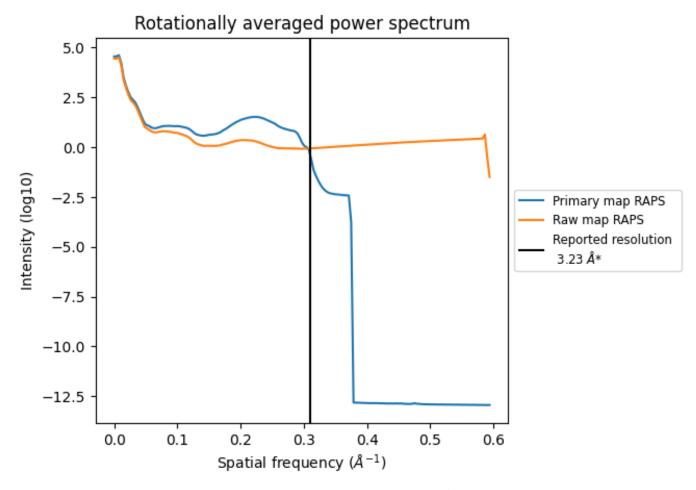


The volume at the recommended contour level is 56 $\rm nm^3;$ this corresponds to an approximate mass of 51 kDa.

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)



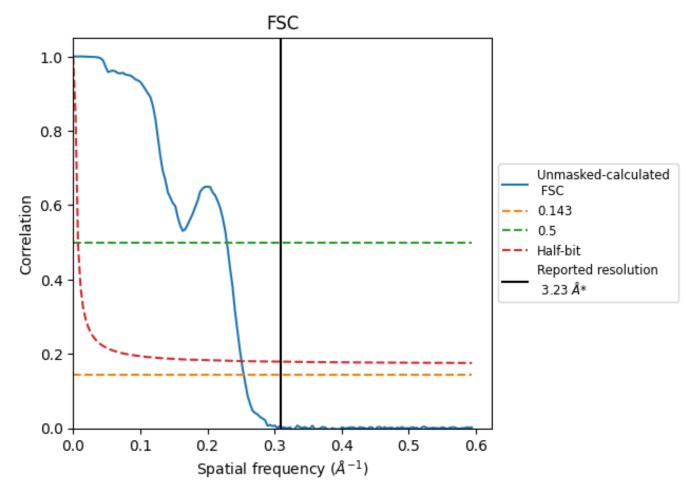
*Reported resolution corresponds to spatial frequency of 0.310 \AA^{-1}



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 0.310 ${\rm \AA^{-1}}$



8.2 Resolution estimates (i)

Resolution estimate (Å)	Estim	Estimation criterion (FSC cut-off)			
Resolution estimate (A)	0.143	0.5	Half-bit		
Reported by author	3.23	-	-		
Author-provided FSC curve	-	-	-		
Unmasked-calculated*	3.94	4.37	3.99		

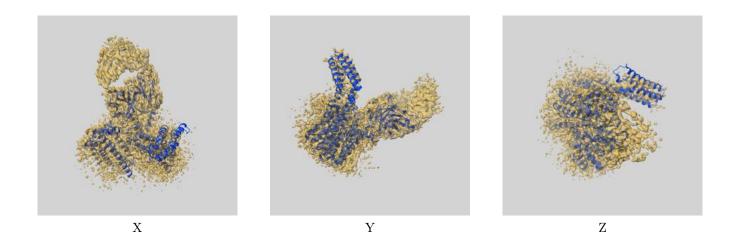
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.94 differs from the reported value 3.23 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-27461 and PDB model 8DJM. Per-residue inclusion information can be found in section 3 on page 8.

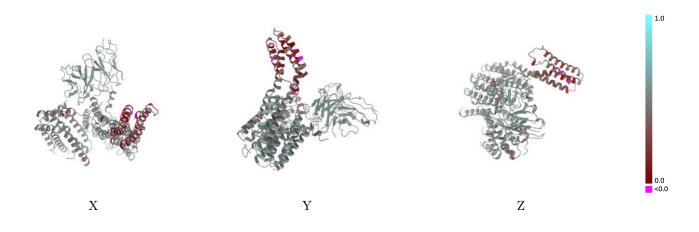
9.1 Map-model overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.395 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.

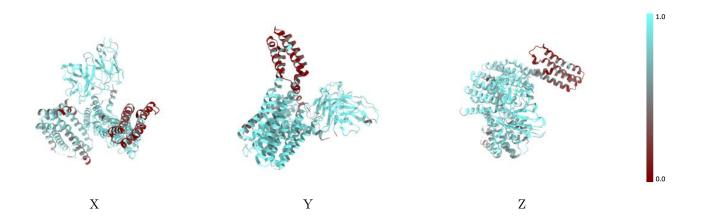


9.2 Q-score mapped to coordinate model (i)



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.

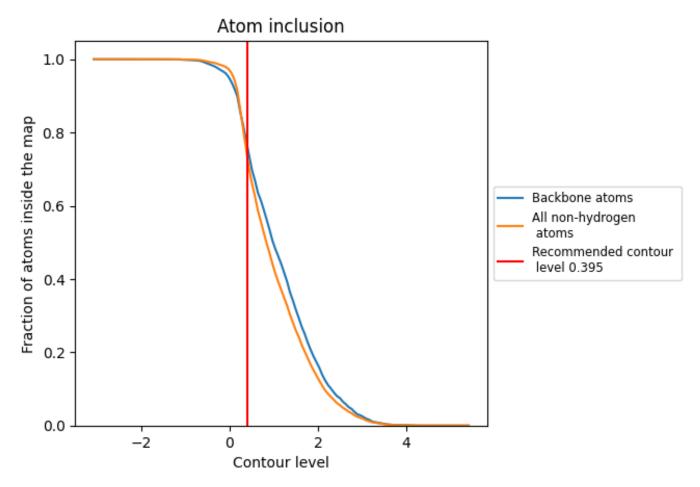
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.395).



9.4 Atom inclusion (i)



At the recommended contour level, 77% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.



1.0

0.0 <0.0

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.395) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7377	0.4680
А	0.7182	0.4640
В	0.8421	0.5110
С	0.3074	0.2600
Н	0.8779	0.5370
L	0.8382	0.5170

