



wwPDB EM Validation Summary Report ⓘ

Oct 7, 2024 – 04:42 AM EDT

PDB ID : 6XBY
EMDB ID : EMD-22122
Title : Cryo-EM structure of V-ATPase from bovine brain, state 2
Authors : Wang, R.; Li, X.
Deposited on : 2020-06-07
Resolution : 3.79 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

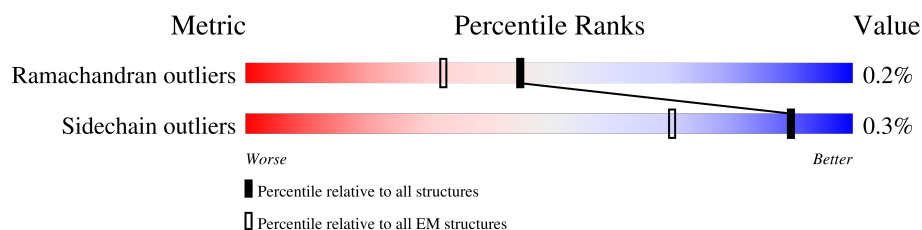
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.79 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.



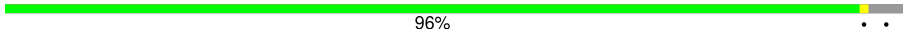
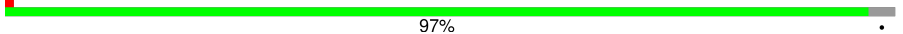












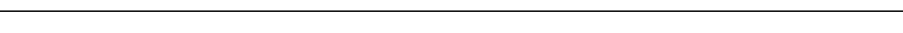
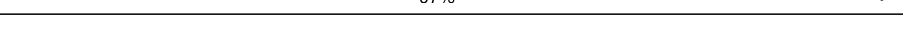
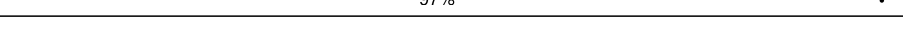
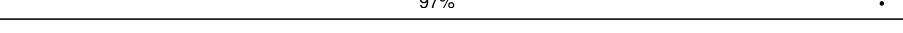
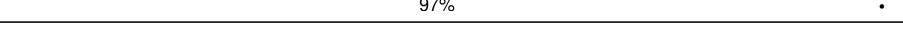
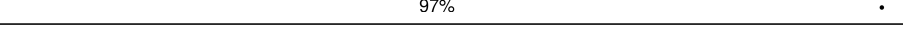

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$. 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	A	617	 96%
1	B	617	 93% 6%
1	C	617	 93% 6%
2	D	511	 88% 11%
2	E	511	 89% 11%
2	F	511	 88% 11%
3	G	382	 7% 90% 10%
4	H	247	 85% 14%
5	I	226	 12% 96%

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Mol	Chain	Length	Quality of chain
5	J	226	 96% ..
5	K	226	 97% .
6	L	119	 85% 15%
7	M	118	 19% 89% .. 8%
7	N	118	 92% 8%
7	O	118	 89% .. 8%
8	P	465	 79% 20%
9	a	838	 58% . 41%
10	b	205	 99% .
11	d	351	 95% .
12	c	155	 96% ..
12	g	155	 97% .
12	k	155	 97% .
12	l	155	 97% .
12	m	155	 97% .
12	n	155	 97% .
12	o	155	 97% .
12	p	155	 97% .
12	q	155	 97% .
13	s	468	 43% . 56%
14	r	351	 11% . 88%

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 57516 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 V-type proton ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	597	Total	C	N	O	S	0	0
			4628	2935	781	884	28		
1	B	577	Total	C	N	O	S	0	0
			4484	2847	756	853	28		
1	C	583	Total	C	N	O	S	0	0
			4530	2877	763	863	27		

- Molecule 2 is a protein called V-type proton ATPase subunit B, brain isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	457	Total	C	N	O	S	0	0
			3581	2268	615	678	20		
2	E	457	Total	C	N	O	S	0	0
			3576	2268	612	676	20		
2	F	454	Total	C	N	O	S	0	0
			3556	2256	609	671	20		

- Molecule 3 is a protein called V-type proton ATPase subunit C 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	343	Total	C	N	O	S	0	0
			1892	1162	359	369	2		

- Molecule 4 is a protein called V-type proton ATPase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	212	Total	C	N	O	S	0	0
			1708	1084	308	311	5		

- Molecule 5 is a protein called V-type proton ATPase subunit E 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	218	Total	C	N	O	S	0	0
			1573	980	293	294	6		
5	J	218	Total	C	N	O	S	0	0
			1577	983	294	294	6		
5	K	220	Total	C	N	O	S	0	0
			1583	986	295	296	6		

- Molecule 6 is a protein called V-type proton ATPase subunit F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	101	Total	C	N	O	S	0	0
			801	508	138	154	1		

- Molecule 7 is a protein called V-type proton ATPase subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	108	Total	C	N	O	S	0	0
			665	395	138	129	3		
7	N	108	Total	C	N	O	S	0	0
			661	393	138	127	3		
7	O	108	Total	C	N	O	S	0	0
			665	395	138	129	3		

- Molecule 8 is a protein called V-type proton ATPase subunit H.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	P	370	Total	C	N	O	0	0
			1837	1097	370	370		

- Molecule 9 is a protein called V-type proton ATPase subunit a.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	494	Total	C	N	O	S	0	0
			3917	2507	682	705	23		

- Molecule 10 is a protein called V-type proton ATPase 21 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	203	Total	C	N	O	S	0	0
			1498	993	237	258	10		

- Molecule 11 is a protein called V-type proton ATPase subunit d 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	d	336	Total	C	N	O	S	0	0
			2740	1771	447	508	14		

- Molecule 12 is a protein called V-type proton ATPase 16 kDa proteolipid subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	q	151	Total	C	N	O	S	0	0
			1073	703	173	189	8		
12	p	151	Total	C	N	O	S	0	0
			1073	703	173	189	8		
12	c	150	Total	C	N	O	S	0	0
			1064	697	171	188	8		
12	g	150	Total	C	N	O	S	0	0
			1064	697	171	188	8		
12	k	150	Total	C	N	O	S	0	0
			1064	697	171	188	8		
12	l	150	Total	C	N	O	S	0	0
			1064	697	171	188	8		
12	m	150	Total	C	N	O	S	0	0
			1064	697	171	188	8		
12	n	150	Total	C	N	O	S	0	0
			1064	697	171	188	8		
12	o	151	Total	C	N	O	S	0	0
			1073	703	173	189	8		

- Molecule 13 is a protein called V-type proton ATPase subunit S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	s	205	Total	C	N	O	S	0	0
			1668	1083	264	312	9		

- Molecule 14 is a protein called Renin receptor.

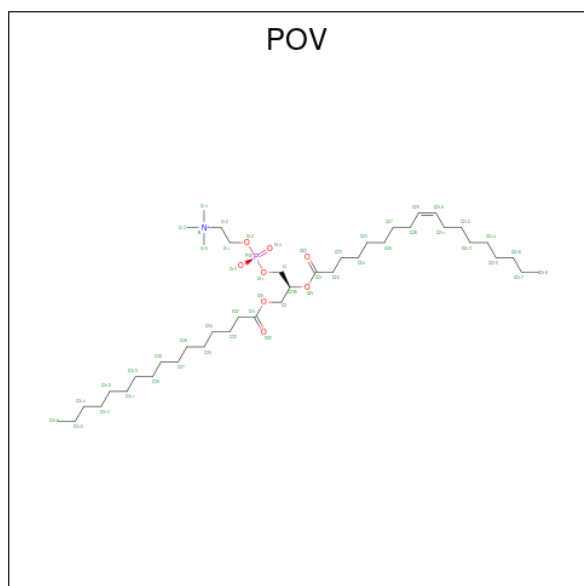
Mol	Chain	Residues	Atoms					AltConf	Trace
14	r	43	Total	C	N	O	S	0	0
			358	245	51	59	3		

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total	Mg	0
			1	1	

- # ADP

- Molecule 17 is (2S)-3-(hexadecanoyloxy)-2-[(9Z)-octadec-9-enoyloxy]propyl 2-(trimethylammonio)ethyl phosphate (three-letter code: POV) (formula: $C_{42}H_{82}NO_8P$).

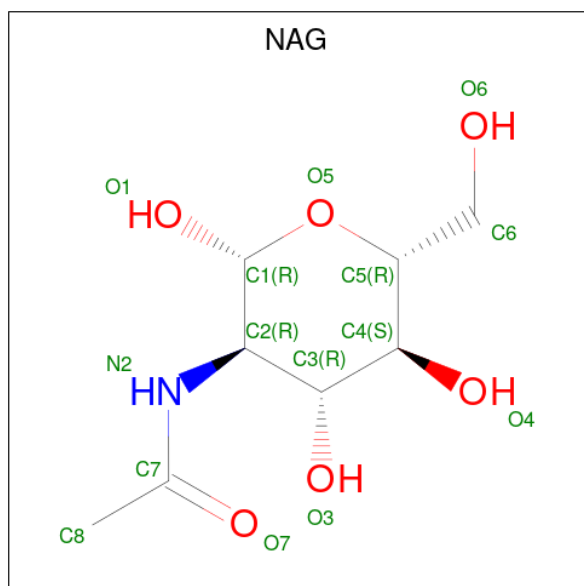


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Mol	Chain	Residues	Atoms					AltConf
17	l	1	Total	C	N	O	P	0
			42	32	1	8	1	
17	o	1	Total	C	N	O	P	0
			44	34	1	8	1	
17	s	1	Total	C	N	O	P	0
			46	36	1	8	1	
17	r	1	Total	C	N	O	P	0
			43	33	1	8	1	
17	r	1	Total	C	N	O	P	0
			42	32	1	8	1	
17	r	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 18 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
18	s	1	Total	C	N	O	0
			14	8	1	5	
18	s	1	Total	C	N	O	0
			14	8	1	5	
18	s	1	Total	C	N	O	0
			14	8	1	5	
18	s	1	Total	C	N	O	0
			14	8	1	5	
18	s	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
18	s	1	14	8	1	5	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.

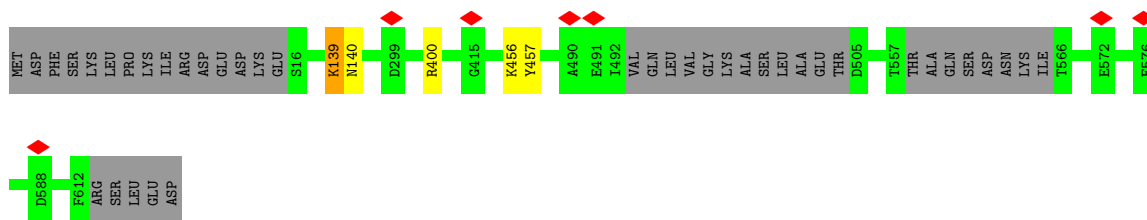
- Molecule 1: V-type proton ATPase catalytic subunit A

Chain A:  96%



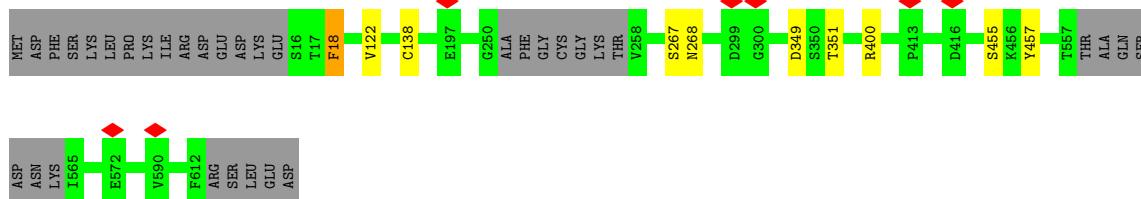
- Molecule 1: V-type proton ATPase catalytic subunit A

Chain B:  93% 6%




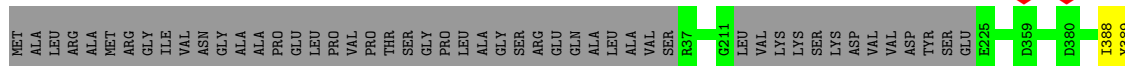
- Molecule 1: V-type proton ATPase catalytic subunit A

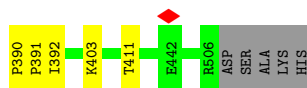
Chain C:  93% 6%



- Molecule 2: V-type proton ATPase subunit B, brain isoform

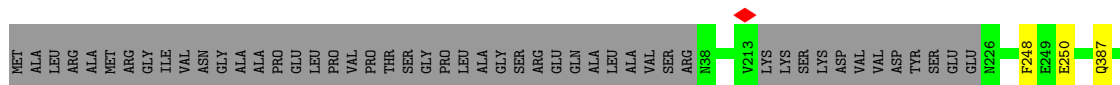
Chain D:  88% 11%





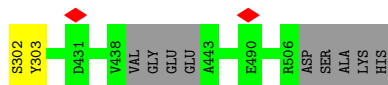
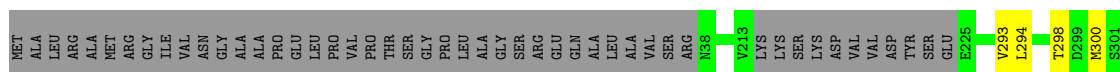
- Molecule 2: V-type proton ATPase subunit B, brain isoform

Chain E: 89% 11%



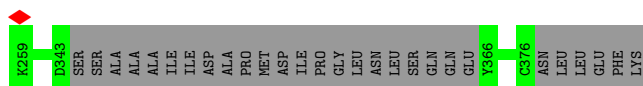
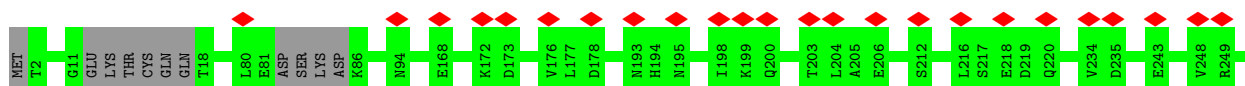
- Molecule 2: V-type proton ATPase subunit B, brain isoform

Chain F: 88% 11%



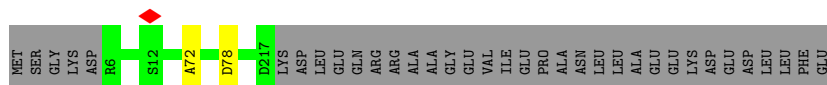
- Molecule 3: V-type proton ATPase subunit C 1

Chain G: 7% 90% 10%



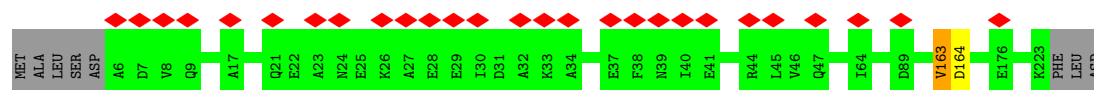
- Molecule 4: V-type proton ATPase subunit D

Chain H: 85% 14%



- Molecule 5: V-type proton ATPase subunit E 1

Chain I: 12% 96%



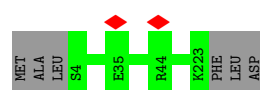
- Molecule 5: V-type proton ATPase subunit E 1

Chain J: 96%



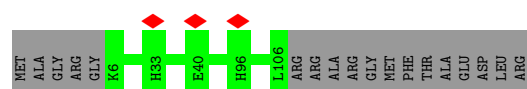
- Molecule 5: V-type proton ATPase subunit E 1

Chain K: 97%



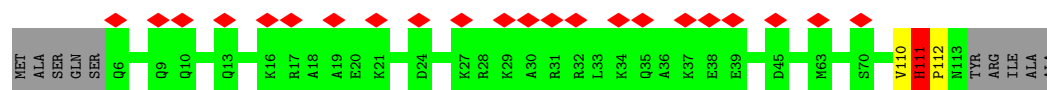
- Molecule 6: V-type proton ATPase subunit F

Chain L: 85%



- Molecule 7: V-type proton ATPase subunit G

Chain M: 19% 89% 8%



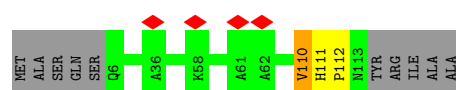
- Molecule 7: V-type proton ATPase subunit G

Chain N: 92% 8%



- Molecule 7: V-type proton ATPase subunit G

Chain O: 89% 8%



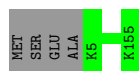
- Molecule 8: V-type proton ATPase subunit H

Chain q:  97% .



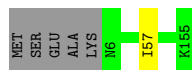
- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

Chain p:  97% .



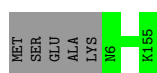
- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

Chain c:  96% . .



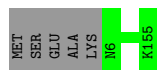
- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

Chain g:  97% .



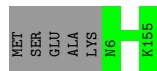
- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

Chain k:  97% .



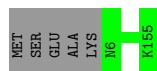
- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

Chain l:  97% .



- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

Chain m:  97% .



- Molecule 12: V-type proton ATPase 16 kDa proteolipid subunit

MET
SER
GLU
ALA
LYS
N6
K155

- Chain o: 97%

MET
SER
GLU
ALA
K5
K155

- Chain s:  43% . 56%

[illegible]

- Chain r:  11% 88%

L320	LEU	ASP	GLU	TRP	MET
G335	ILE	LEU	THR	PRO	ALA
	ASP	LEU	PRO	GLY	VAL
	ALA	PHE	VAL	LEU	LEU
	ASP	LEU	VAL	ALA	VAL
	SER	SER	LEU	VAL	VAL
	ILE	LYS	GLN	GLY	PHE
	ILE	PHE	LEU	LEU	ASN
	TYR	ALA	ALA	LEU	SER
	ARG	ASP	VAL	PHE	PHE
	MET	ASP	LEU	SER	LEU
THR	MET	ARG	GLU	VAL	
ASN	TYR	ASP	GLU	PRO	
GLN	ASN	ILE	ARG	ASP	
LYS	LEU	SER	VAL	ALA	
ILE	TYR	SER	TYR	THR	
ARG	GLY	LEU	MET	GLY	
MET	GLY	LEU	VAL	ASN	
ASP	ASN	SER	GLY	GLU	
	ALA	ARG	VAL	PHE	
	VAL	HIS	LYS	MET	
	VAL	LYS	ASN	VAL	
	GLU	HIS	SER	ILE	
	LEU	LEU	VAL	LEU	
	VAL	ALA	PHE	ARG	
	THR	LYS	GLU	SER	
	VAL	ASP	ASP	PRO	
	ARG	HIS	LEU	ALA	
	SER	SER	SER	SER	
	SER	PRO	VAL	VAL	
	PHE	PRO	VAL	VAL	
	ASP	ASP	THR	PHE	
	THR	LEU	LEU	ARG	
	SER	TYR	ARG	ASN	
	LEU	SER	GLN	GLY	
	VAL	LEU	LEU	ASN	
	ARG	GLU	ARG	TRP	
	LYS	LEU	ASN	PRO	
	THR	ALA	ARG	ILE	
	ARG	GLY	LEU	PRO	
	ASN	LEU	PHE	GLY	
	ILE	ASP	GLN	ASN	
	LEU	GLU	GLU	ARG	
	GLU	ILE	ASN	ILE	
	THR	GLY	SER	PRO	
	LYS	LYS	VAL	PHE	
	GLN	HIS	LEU	VAL	
	VAL	TYR	THR	ALA	
	LYS	GLY	SER	ALA	
	ASP	GLU	LEU	SER	
	PRO	SER	PRO	MET	
	THR	THR	ASN	GLY	
	THR	GLN	SER	PHE	
	T293	PHE	LEU	SER	
	Y304	ARG	SER	LYS	
	I316	ASP	ARG	VAL	
	G317	ALA	ASN	GLU	
	I318	SER	ASN	PHE	
	I319	LYS	GLU	LEU	
	I320	ILE	VAL	SER	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41821	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	29.395	Depositor
Minimum map value	-15.945	Depositor
Average map value	0.017	Depositor
Map value standard deviation	1.102	Depositor
Recommended contour level	4	Depositor
Map size (\AA)	424.83002, 424.83002, 424.83002	wwPDB
Map dimensions	510, 510, 510	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.833, 0.833, 0.833	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, POV, ADP, MG

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 > 5$	RMSZ	# $ Z > 5$
1	A	0.37	2/4724 (0.0%)	0.53	1/6398 (0.0%)
1	B	0.34	1/4578 (0.0%)	0.51	1/6197 (0.0%)
1	C	0.41	4/4623 (0.1%)	0.57	3/6260 (0.0%)
2	D	0.36	0/3652	0.58	3/4949 (0.1%)
2	E	0.41	2/3647 (0.1%)	0.58	2/4944 (0.0%)
2	F	0.54	6/3626 (0.2%)	0.60	2/4914 (0.0%)
3	G	0.23	0/1906	0.43	0/2644
4	H	0.25	0/1726	0.69	3/2309 (0.1%)
5	I	0.34	0/1584	0.58	1/2144 (0.0%)
5	J	0.30	0/1588	0.54	1/2148 (0.0%)
5	K	0.26	0/1594	0.45	0/2158
6	L	0.25	0/814	0.50	0/1103
7	M	0.65	1/667 (0.1%)	0.63	3/912 (0.3%)
7	N	0.23	0/663	0.45	0/907
7	O	0.37	0/667	0.75	5/912 (0.5%)
8	P	0.23	0/1835	0.40	0/2558
9	a	0.28	0/3995	0.55	0/5401
10	b	0.43	1/1532 (0.1%)	0.52	0/2083
11	d	0.28	0/2801	0.54	1/3788 (0.0%)
12	c	0.28	0/1079	0.49	0/1459
12	g	0.26	0/1079	0.45	0/1459
12	k	0.26	0/1079	0.44	0/1459
12	l	0.26	0/1079	0.45	0/1459
12	m	0.28	0/1079	0.47	0/1459
12	n	0.27	0/1079	0.45	0/1459
12	o	0.27	0/1088	0.47	0/1470
12	p	0.28	0/1088	0.46	0/1470
12	q	0.26	0/1088	0.45	0/1470
13	s	0.46	0/1720	0.69	3/2341 (0.1%)
14	r	1.07	3/370 (0.8%)	1.04	3/508 (0.6%)
All	All	0.36	20/58050 (0.0%)	0.54	32/78742 (0.0%)

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	B	0	1
1	C	0	2
2	D	0	1
2	E	0	1
9	a	0	2
All	All	0	7

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	112	PRO	N-CD	14.04	1.67	1.47
10	b	22	VAL	C-N	9.64	1.50	1.33
1	C	457	TYR	CB-CG	-8.18	1.39	1.51
14	r	319	ALA	C-O	-8.17	1.07	1.23
14	r	319	ALA	CA-C	-7.71	1.32	1.52

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	72	ALA	N-CA-C	15.45	152.72	111.00
4	H	72	ALA	CB-CA-C	-14.11	88.94	110.10
2	F	294	LEU	CB-CG-CD2	-10.12	93.81	111.00
14	r	320	LEU	CB-CG-CD2	9.52	127.18	111.00
14	r	318	LEU	CB-CG-CD2	-8.99	95.71	111.00

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	139	LYS	Peptide
1	C	267	SER	Peptide
1	C	455	SER	Mainchain
2	D	411	THR	Peptide
2	E	387	GLN	Peptide

5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	595/617 (96%)	565 (95%)	29 (5%)	1 (0%)	44	74
1	B	571/617 (92%)	533 (93%)	37 (6%)	1 (0%)	44	74
1	C	577/617 (94%)	539 (93%)	37 (6%)	1 (0%)	44	74
2	D	453/511 (89%)	422 (93%)	31 (7%)	0	100	100
2	E	453/511 (89%)	416 (92%)	37 (8%)	0	100	100
2	F	448/511 (88%)	418 (93%)	29 (6%)	1 (0%)	44	74
3	G	335/382 (88%)	315 (94%)	20 (6%)	0	100	100
4	H	210/247 (85%)	199 (95%)	11 (5%)	0	100	100
5	I	216/226 (96%)	207 (96%)	8 (4%)	1 (0%)	25	58
5	J	216/226 (96%)	209 (97%)	7 (3%)	0	100	100
5	K	218/226 (96%)	209 (96%)	9 (4%)	0	100	100
6	L	99/119 (83%)	89 (90%)	10 (10%)	0	100	100
7	M	106/118 (90%)	102 (96%)	3 (3%)	1 (1%)	14	45
7	N	106/118 (90%)	99 (93%)	7 (7%)	0	100	100
7	O	106/118 (90%)	99 (93%)	6 (6%)	1 (1%)	14	45
8	P	366/465 (79%)	340 (93%)	25 (7%)	1 (0%)	37	69
9	a	486/838 (58%)	444 (91%)	39 (8%)	3 (1%)	22	55
10	b	201/205 (98%)	193 (96%)	8 (4%)	0	100	100
11	d	330/351 (94%)	309 (94%)	20 (6%)	1 (0%)	37	69
12	c	148/155 (96%)	145 (98%)	3 (2%)	0	100	100
12	g	148/155 (96%)	147 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	k	148/155 (96%)	146 (99%)	2 (1%)	0	100	100
12	l	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
12	m	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
12	n	148/155 (96%)	147 (99%)	1 (1%)	0	100	100
12	o	149/155 (96%)	147 (99%)	2 (1%)	0	100	100
12	p	149/155 (96%)	148 (99%)	1 (1%)	0	100	100
12	q	149/155 (96%)	148 (99%)	1 (1%)	0	100	100
13	s	203/468 (43%)	172 (85%)	31 (15%)	0	100	100
14	r	41/351 (12%)	39 (95%)	2 (5%)	0	100	100
All	All	7671/9237 (83%)	7240 (94%)	419 (6%)	12 (0%)	45	74

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	140	ASN
5	I	163	VAL
7	M	111	HIS
2	F	300	MET
7	O	110	VAL

5.3.2 Protein sidechains ⓘ

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	504/524 (96%)	503 (100%)	1 (0%)	92	94
1	B	488/524 (93%)	486 (100%)	2 (0%)	89	91
1	C	494/524 (94%)	490 (99%)	4 (1%)	79	84
2	D	390/432 (90%)	387 (99%)	3 (1%)	79	84
2	E	390/432 (90%)	389 (100%)	1 (0%)	91	92
2	F	388/432 (90%)	387 (100%)	1 (0%)	91	92
3	G	52/344 (15%)	52 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	183/212 (86%)	183 (100%)	0	100	100
5	I	141/198 (71%)	140 (99%)	1 (1%)	81	86
5	J	142/198 (72%)	141 (99%)	1 (1%)	81	86
5	K	141/198 (71%)	141 (100%)	0	100	100
6	L	88/100 (88%)	88 (100%)	0	100	100
7	M	38/97 (39%)	37 (97%)	1 (3%)	41	61
7	N	37/97 (38%)	37 (100%)	0	100	100
7	O	38/97 (39%)	38 (100%)	0	100	100
9	a	410/744 (55%)	409 (100%)	1 (0%)	92	94
10	b	156/158 (99%)	156 (100%)	0	100	100
11	d	294/306 (96%)	293 (100%)	1 (0%)	91	92
12	c	106/110 (96%)	105 (99%)	1 (1%)	75	82
12	g	106/110 (96%)	106 (100%)	0	100	100
12	k	106/110 (96%)	106 (100%)	0	100	100
12	l	106/110 (96%)	106 (100%)	0	100	100
12	m	106/110 (96%)	106 (100%)	0	100	100
12	n	106/110 (96%)	106 (100%)	0	100	100
12	o	107/110 (97%)	107 (100%)	0	100	100
12	p	107/110 (97%)	107 (100%)	0	100	100
12	q	107/110 (97%)	107 (100%)	0	100	100
13	s	184/398 (46%)	184 (100%)	0	100	100
14	r	39/315 (12%)	38 (97%)	1 (3%)	41	61
All	All	5554/7320 (76%)	5535 (100%)	19 (0%)	90	92

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	M	111	HIS
12	c	57	ILE
14	r	304	TYR
11	d	276	LEU
2	D	391	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
12	m	92	GLN
12	n	78	ASN
5	J	149	GLN
5	J	77	ASN
12	n	92	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
18	NAG	s	507	-	14,14,15	0.27	0	19,19,21	0.33	0
17	POV	r	401	-	42,42,51	1.08	4 (9%)	48,50,59	0.96	2 (4%)
17	POV	s	501	-	45,45,51	1.06	3 (6%)	51,53,59	1.01	2 (3%)
18	NAG	s	503	13	14,14,15	0.33	0	17,19,21	0.51	0
16	ADP	D	601	15	24,29,29	1.22	2 (8%)	29,45,45	1.26	3 (10%)
17	POV	o	201	-	43,43,51	1.06	4 (9%)	49,51,59	0.90	2 (4%)
17	POV	b	301	-	43,43,51	2.29	11 (25%)	49,51,59	2.00	17 (34%)
17	POV	l	201	-	41,41,51	1.09	4 (9%)	47,49,59	0.89	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	NAG	s	506	13	14,14,15	0.41	0	17,19,21	0.35	0
17	POV	r	403	-	41,41,51	1.07	4 (9%)	47,49,59	0.92	2 (4%)
18	NAG	s	504	13	14,14,15	0.25	0	17,19,21	0.69	1 (5%)
17	POV	r	402	-	41,41,51	1.09	4 (9%)	47,49,59	0.97	2 (4%)
18	NAG	s	502	13	14,14,15	0.35	0	17,19,21	0.39	0
18	NAG	s	505	13	14,14,15	0.66	1 (7%)	17,19,21	0.72	1 (5%)

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
18	NAG	s	507	-	-	1/6/22/26	0/1/1/1
17	POV	r	401	-	-	25/46/46/55	-
17	POV	s	501	-	-	26/49/49/55	-
18	NAG	s	503	13	-	3/6/23/26	0/1/1/1
16	ADP	D	601	15	-	4/12/32/32	0/3/3/3
17	POV	o	201	-	-	23/47/47/55	-
17	POV	b	301	-	-	24/47/47/55	-
17	POV	l	201	-	-	22/45/45/55	-
18	NAG	s	506	13	-	1/6/23/26	0/1/1/1
17	POV	r	403	-	-	26/45/45/55	-
18	NAG	s	504	13	-	1/6/23/26	0/1/1/1
17	POV	r	402	-	-	16/45/45/55	-
18	NAG	s	502	13	-	2/6/23/26	0/1/1/1
18	NAG	s	505	13	-	0/6/23/26	0/1/1/1

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	b	301	POV	O21-C2	-6.50	1.31	1.46
17	b	301	POV	O31-C3	-5.96	1.31	1.45
17	b	301	POV	C12-N	-4.86	1.36	1.51
17	b	301	POV	C13-N	-4.58	1.36	1.50
17	b	301	POV	C15-N	-3.61	1.39	1.50

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	D	601	ADP	N3-C2-N1	-4.80	122.15	128.67
17	b	301	POV	C2-O21-C21	-4.80	106.31	117.80
17	s	501	POV	O21-C21-C22	4.40	121.00	111.48
17	r	402	POV	O21-C21-C22	4.28	120.74	111.48
17	r	401	POV	O21-C21-C22	4.01	120.16	111.48

There are no chirality outliers.

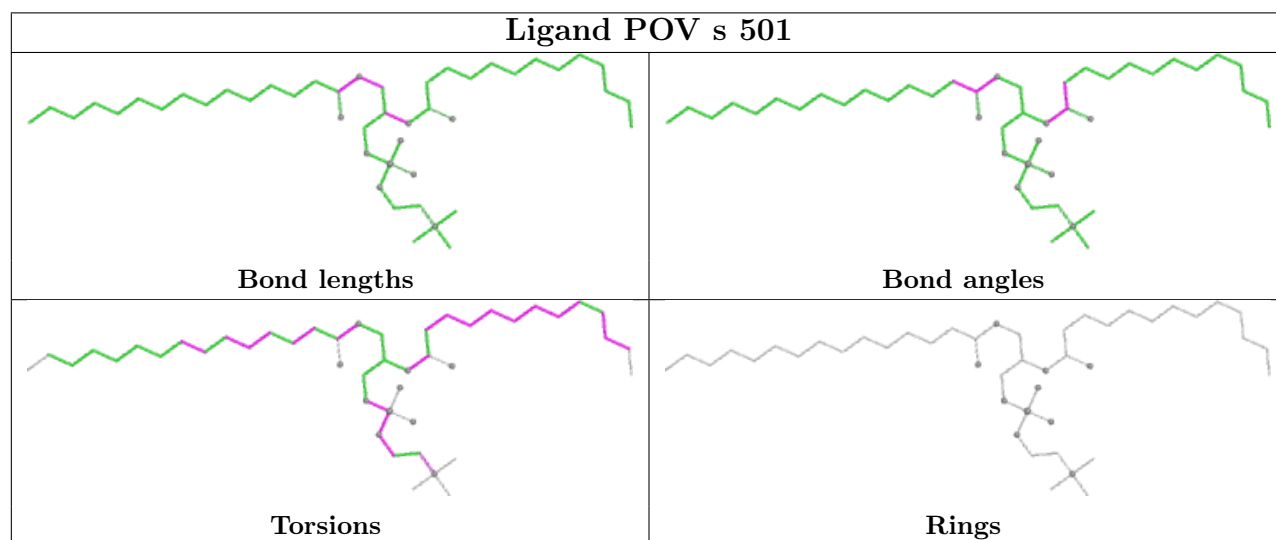
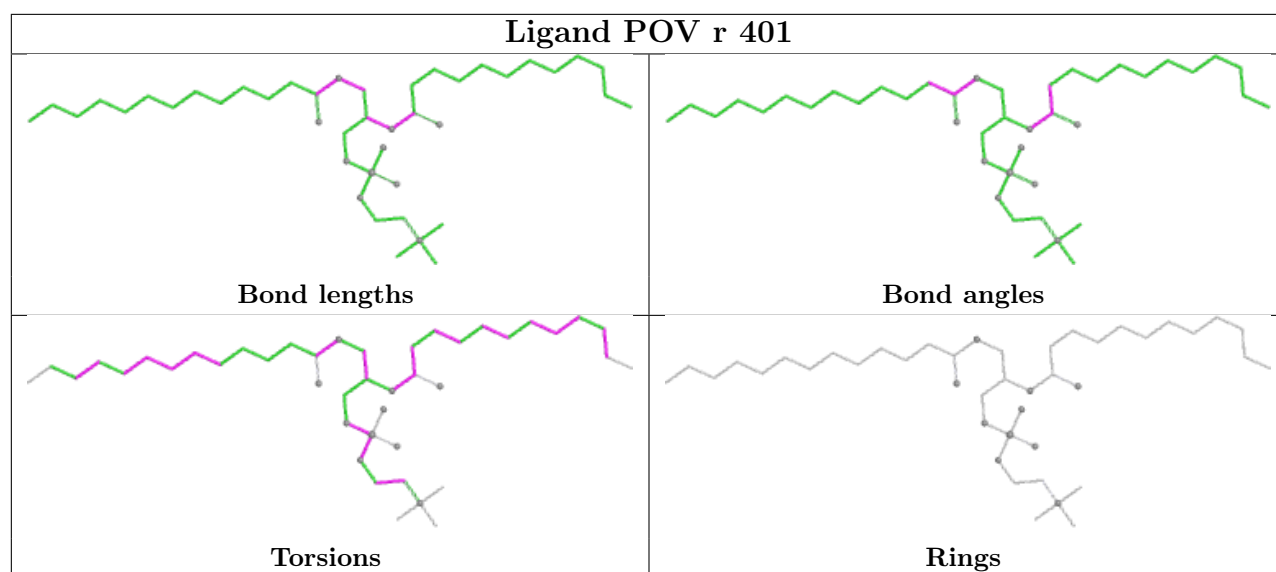
5 of 174 torsion outliers are listed below:

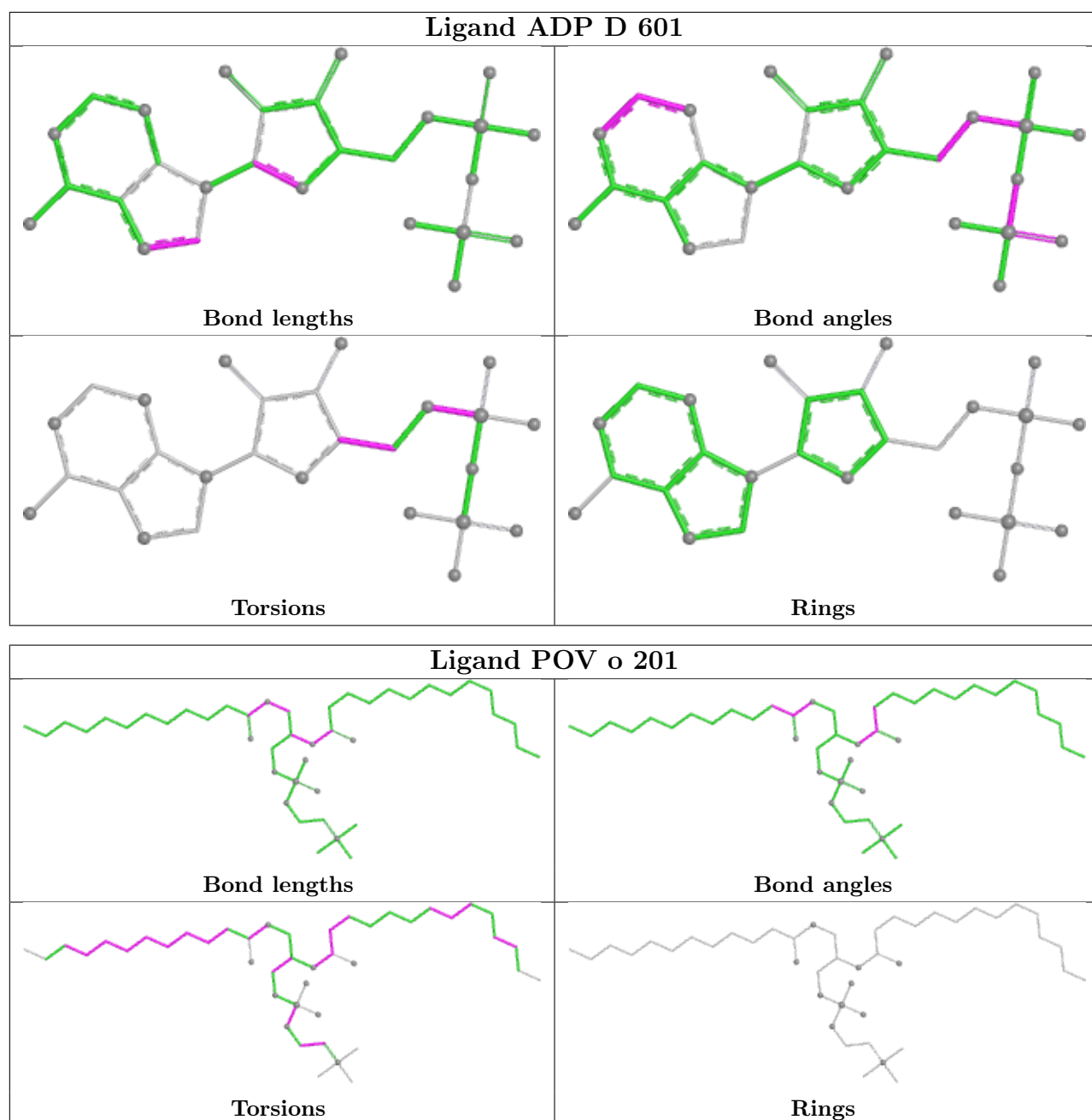
Mol	Chain	Res	Type	Atoms
16	D	601	ADP	C5'-O5'-PA-O2A
16	D	601	ADP	C5'-O5'-PA-O3A
17	b	301	POV	C11-O12-P-O11
17	b	301	POV	C11-O12-P-O14
17	l	201	POV	O12-C11-C12-N

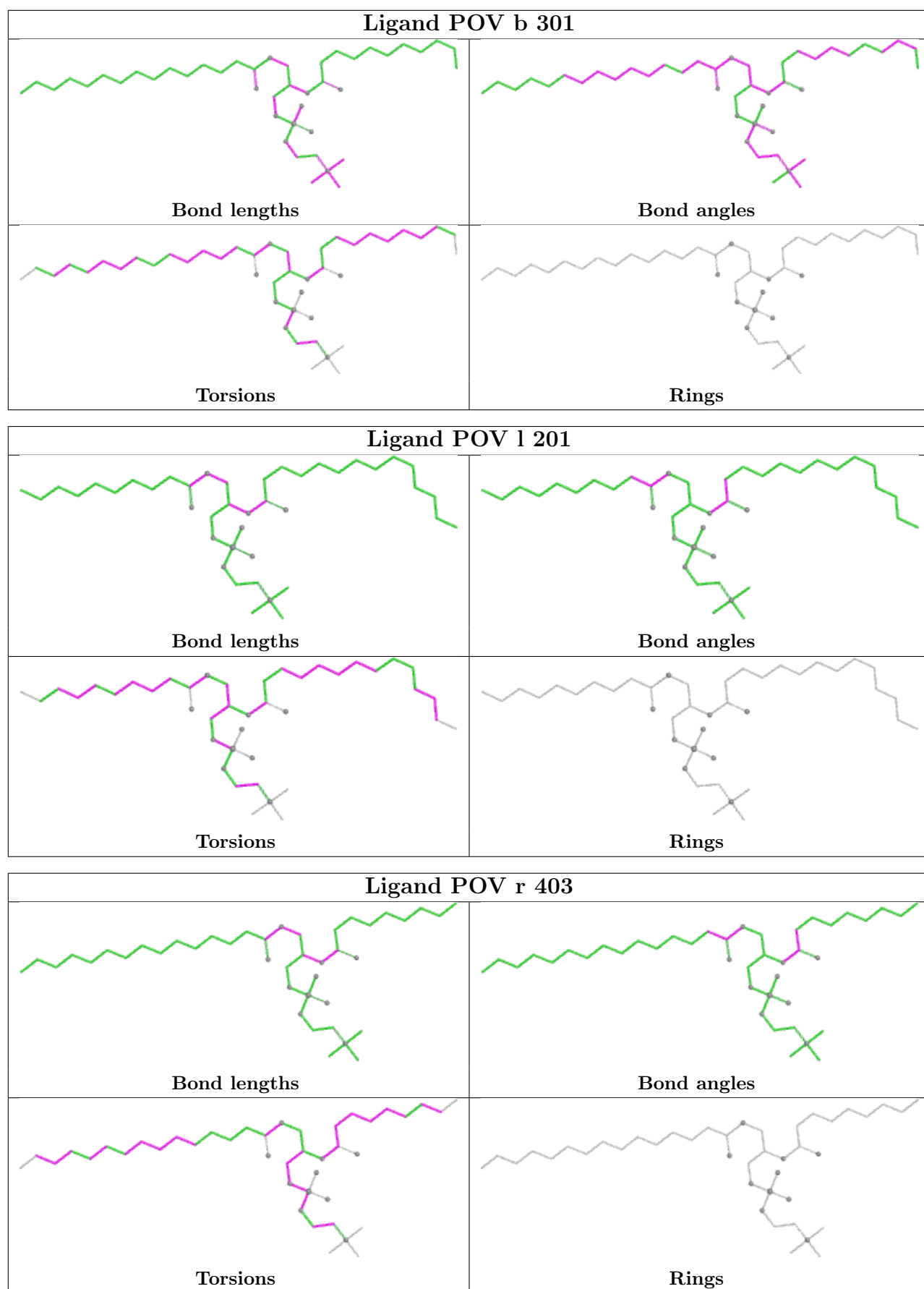
There are no ring outliers.

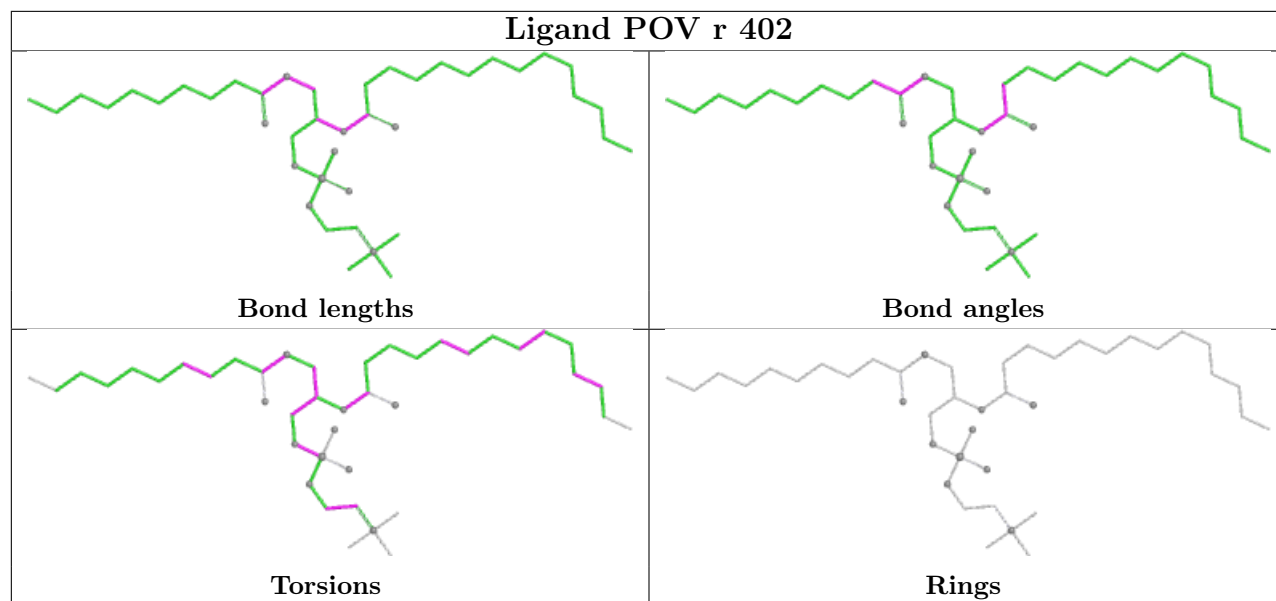
No monomer is involved in short contacts.

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 than 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.

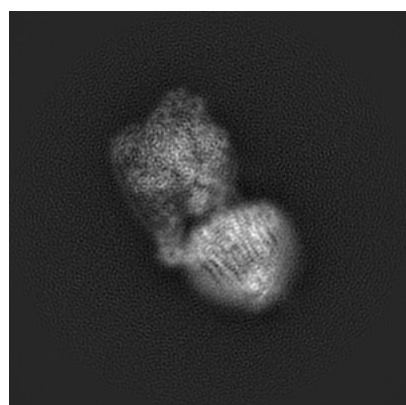
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22122. These allow visual inspection of the internal detail of the map and identification of artifacts.

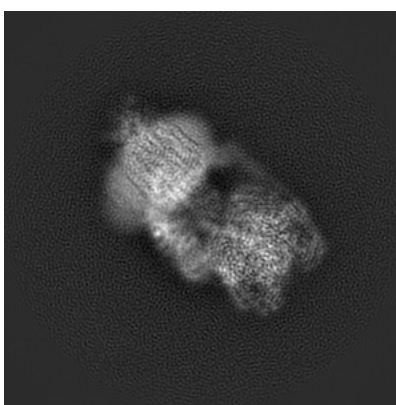
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

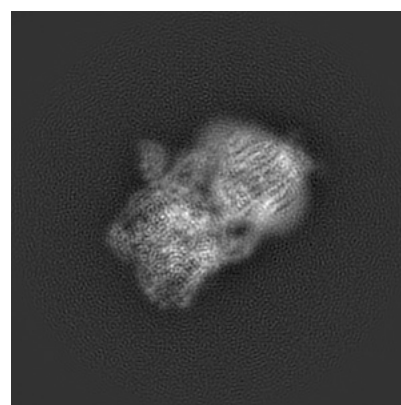
6.1.1 Primary map



X



Y

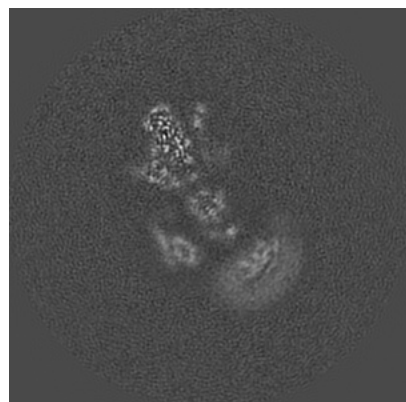


Z

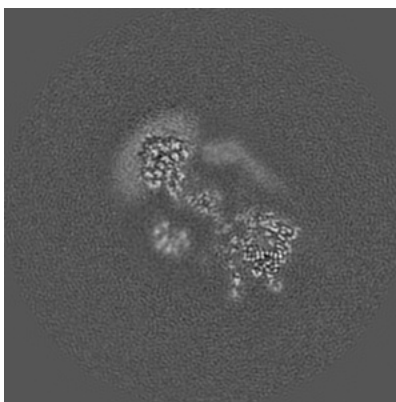
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

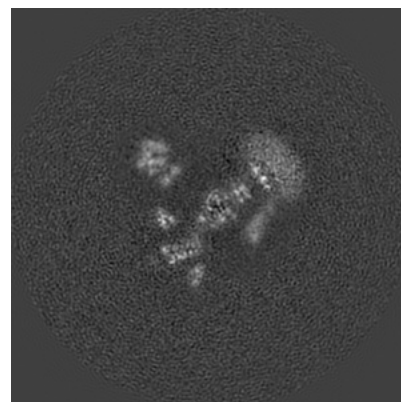
6.2.1 Primary map



X Index: 255



Y Index: 255

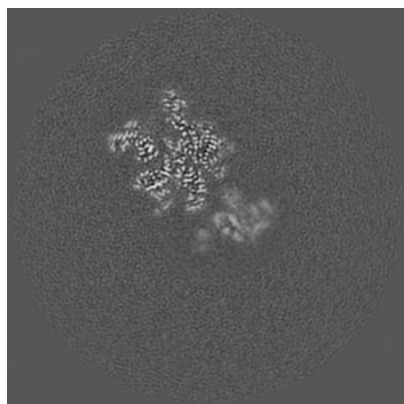


Z Index: 255

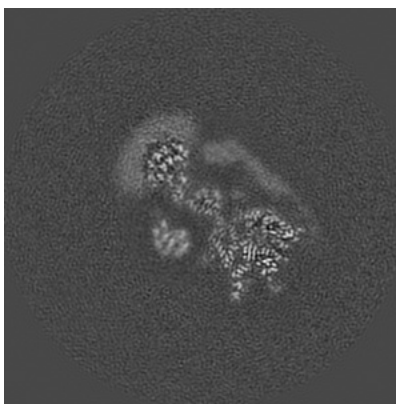
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

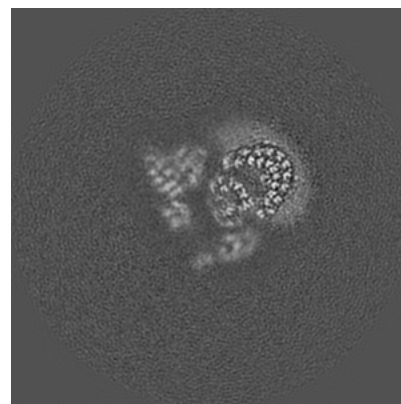
6.3.1 Primary map



X Index: 194



Y Index: 251

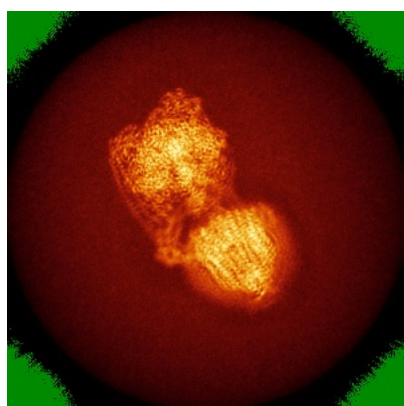


Z Index: 224

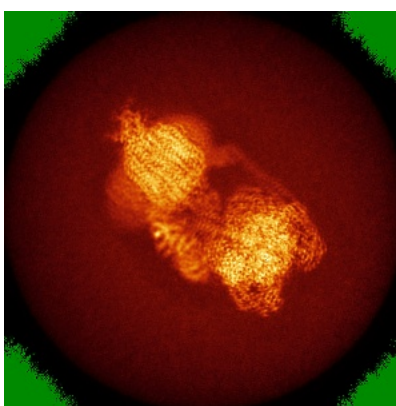
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

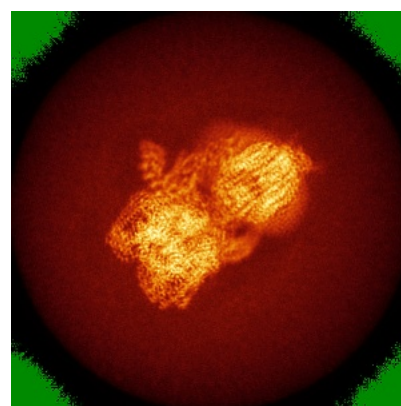
6.4.1 Primary map



X



Y

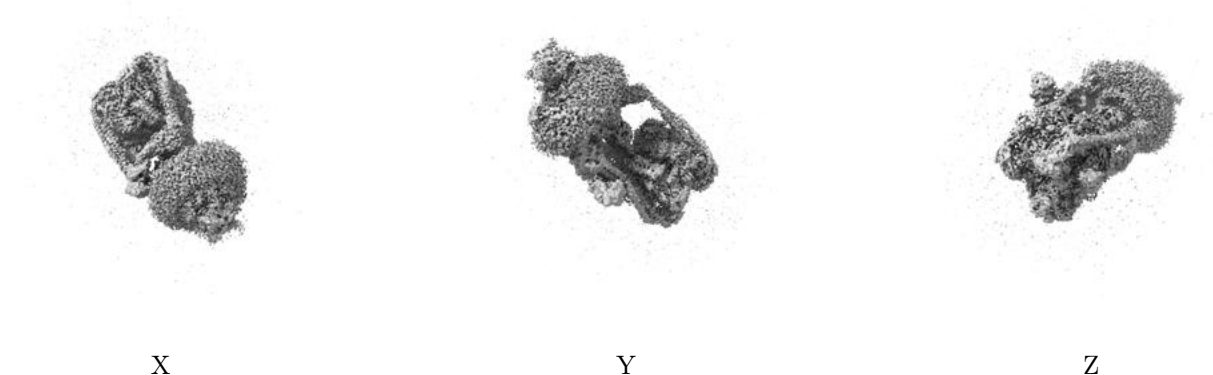


Z

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

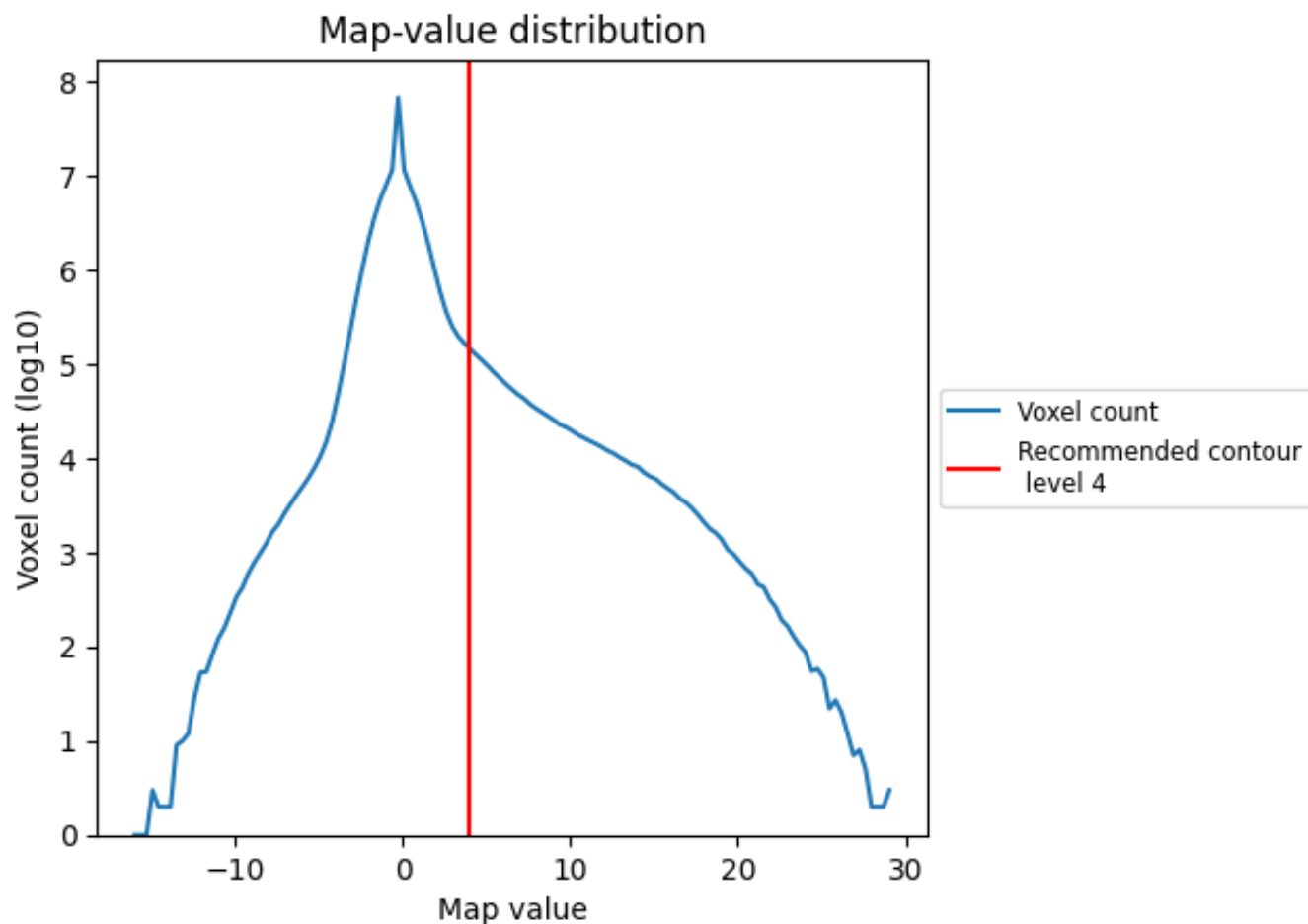
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

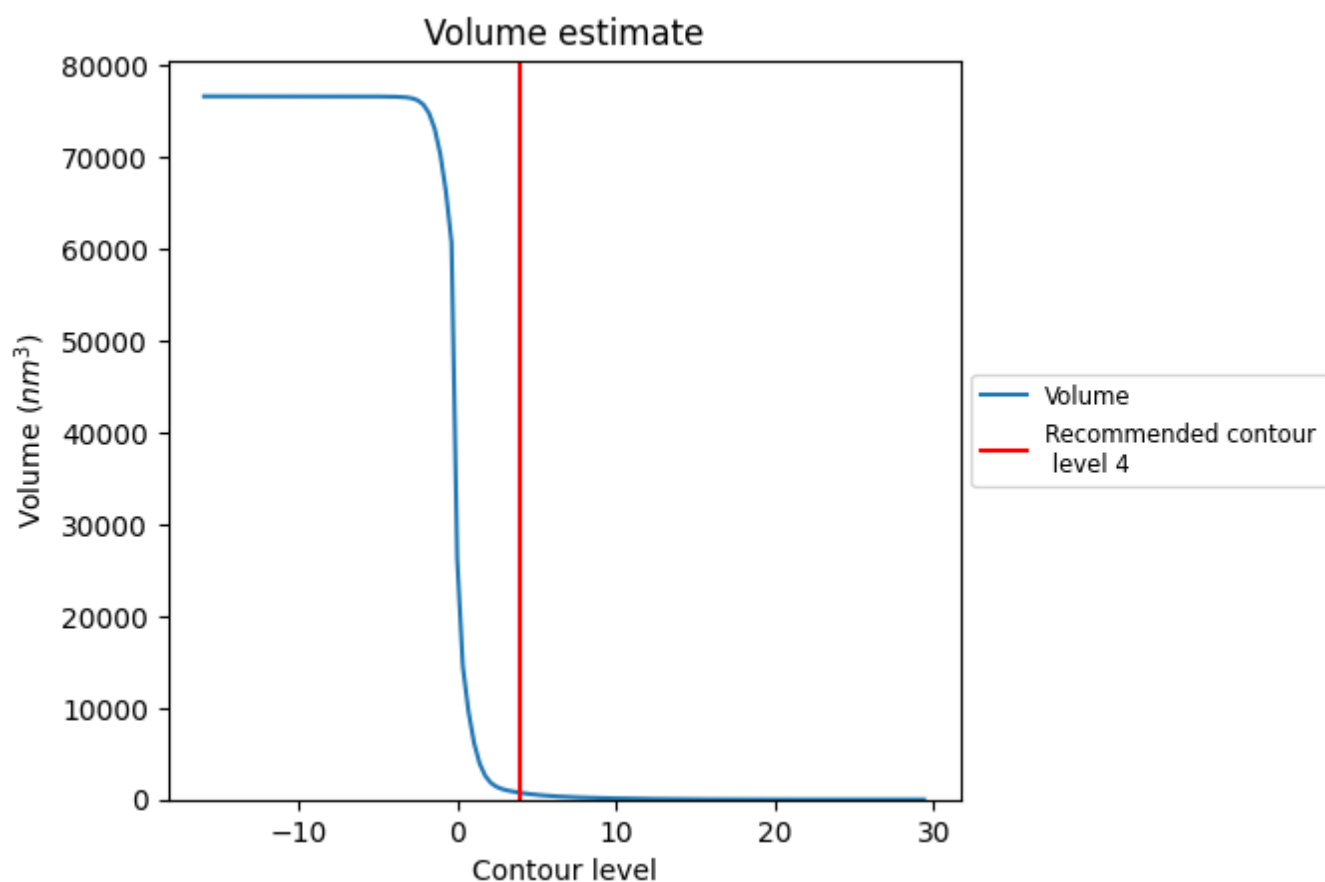
This section contains the results of statistical analysis of the map.

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.

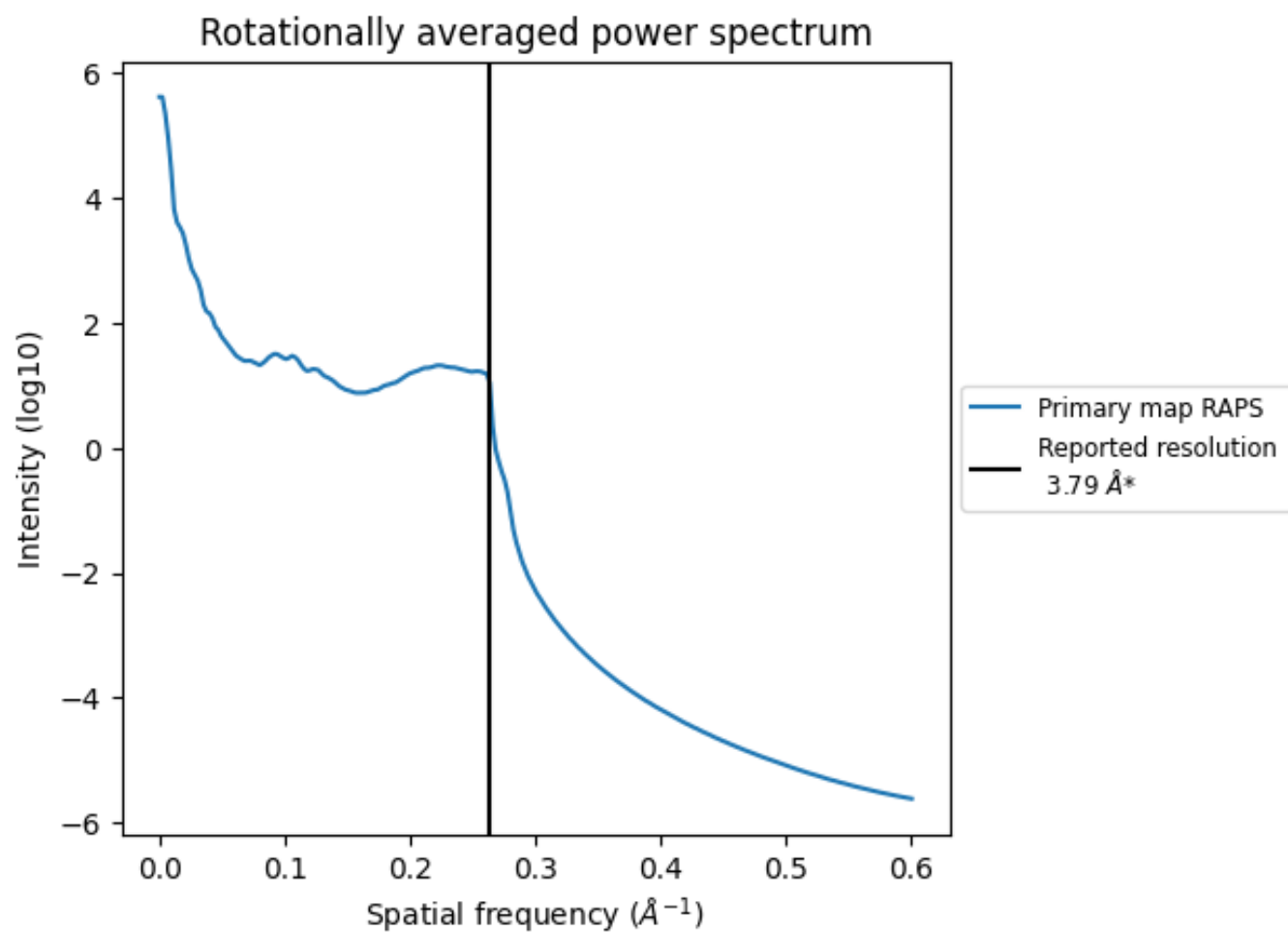
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 729 nm³; this corresponds to an approximate mass of 659 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.264 Å⁻¹

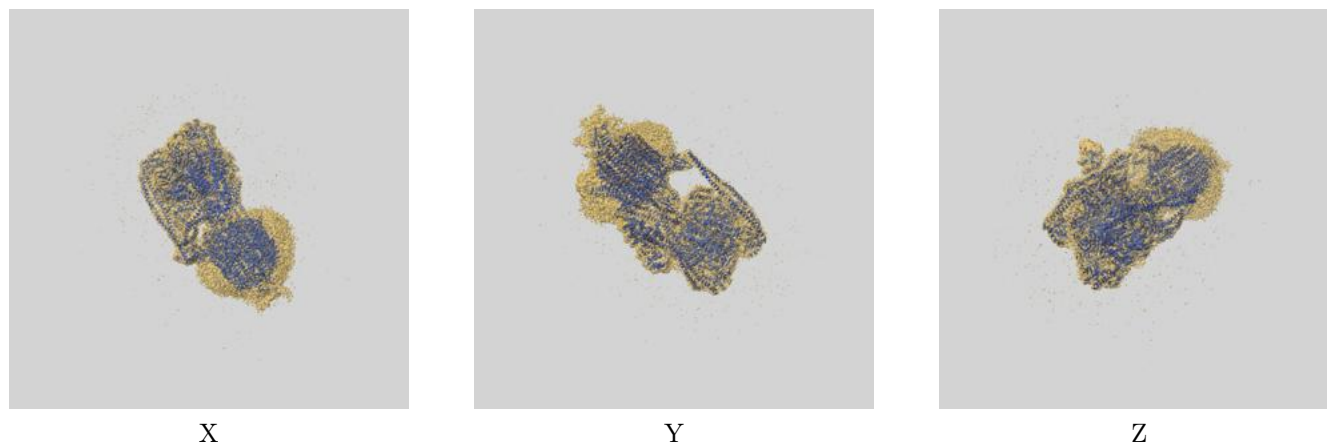
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

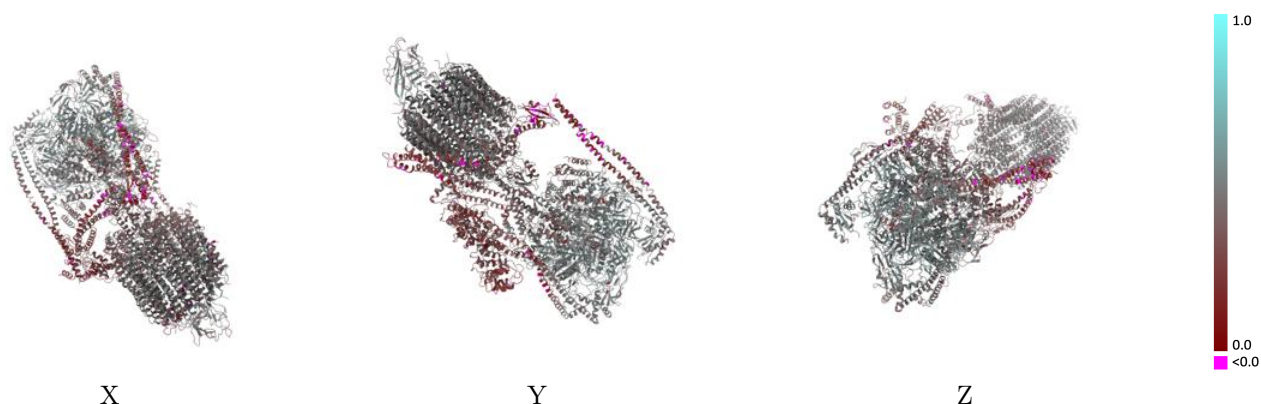
This section contains information regarding the fit between EMDB map EMD-22122 and PDB model 6XBY. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



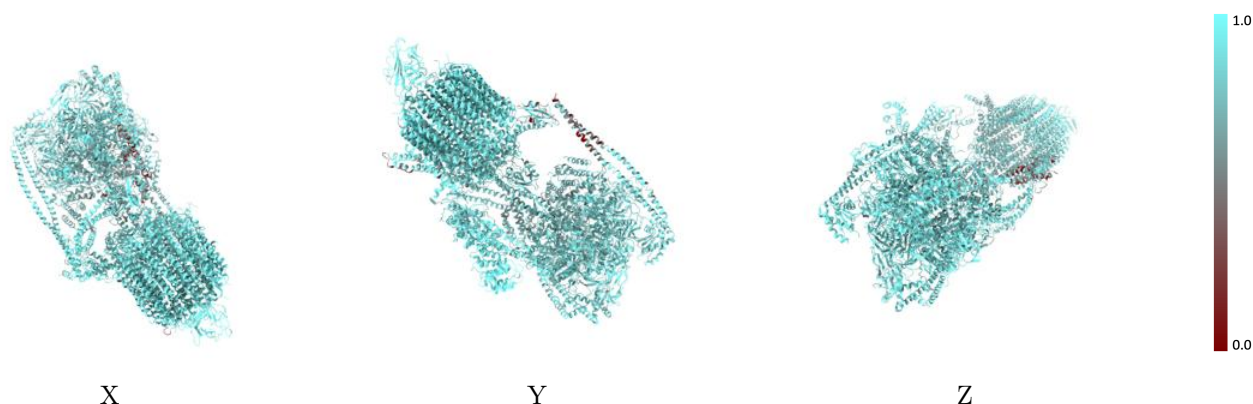
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



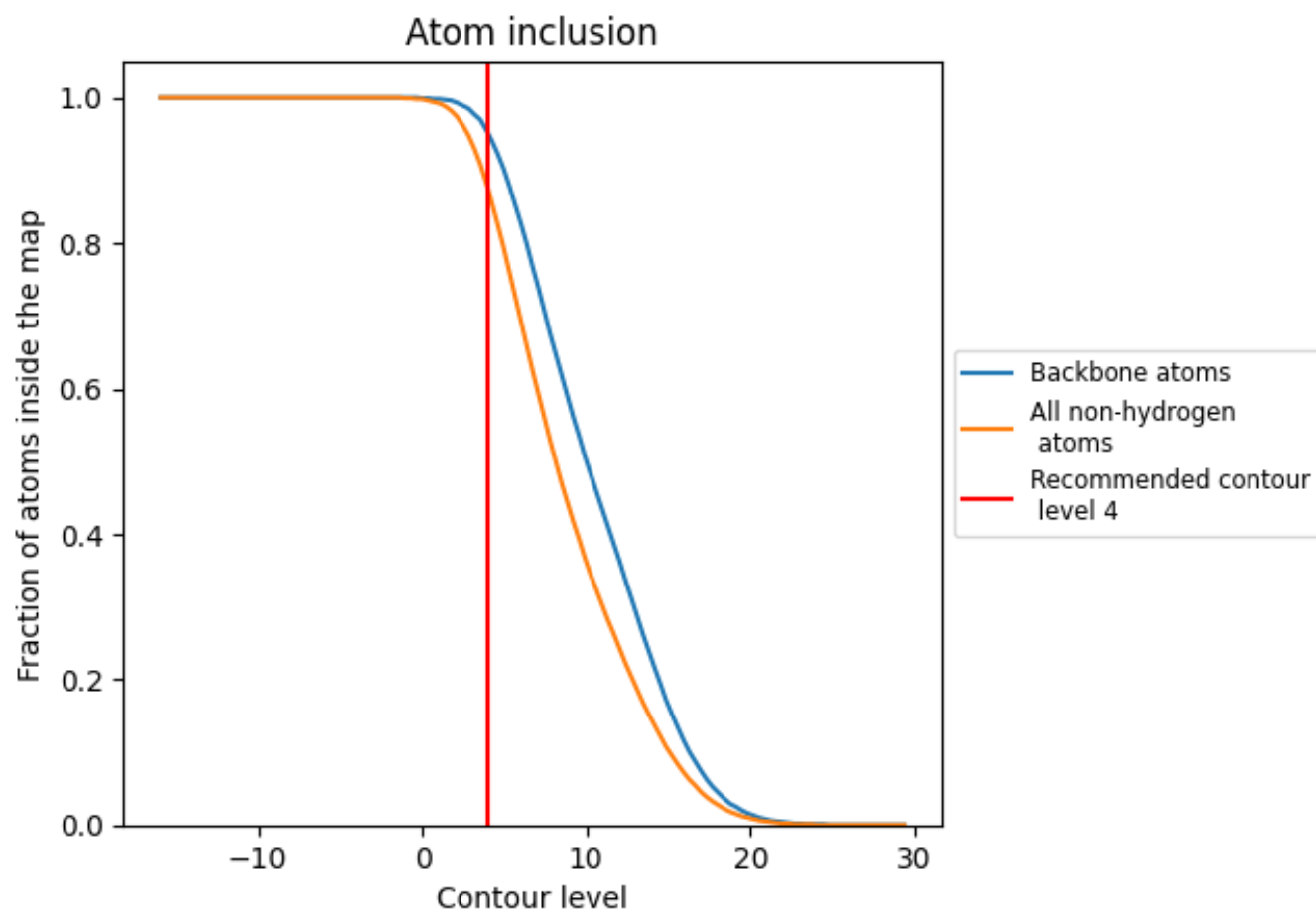
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4).































































9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8760	 0.4320
A	 0.8690	 0.4800
B	 0.8560	 0.4680
C	 0.8580	 0.4760
D	 0.8700	 0.4910
E	 0.8830	 0.5000
F	 0.8730	 0.4900
G	 0.8660	 0.2370
H	 0.8080	 0.4350
I	 0.8060	 0.3940
J	 0.8760	 0.4280
K	 0.8800	 0.4290
L	 0.7810	 0.3890
M	 0.7460	 0.3150
N	 0.9030	 0.3690
O	 0.8640	 0.3540
P	 0.9880	 0.3010
a	 0.8420	 0.2670
b	 0.9070	 0.4560
c	 0.9110	 0.4460
d	 0.8610	 0.4360
g	 0.9120	 0.4470
k	 0.9100	 0.4430
l	 0.9160	 0.4550
m	 0.9110	 0.4430
n	 0.9210	 0.4560
o	 0.9150	 0.4570
p	 0.9250	 0.4550
q	 0.9220	 0.4640
r	 0.9230	 0.4830
s	 0.9380	 0.4540

