



## Full wwPDB EM Validation Report ⓘ

Oct 7, 2024 – 09:06 AM EDT

PDB ID : 8GZ3  
EMDB ID : EMD-34389  
Title : Structure of human phagocyte NADPH oxidase in the resting state  
Authors : Chen, L.; Liu, R.  
Deposited on : 2022-09-24  
Resolution : 3.30 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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

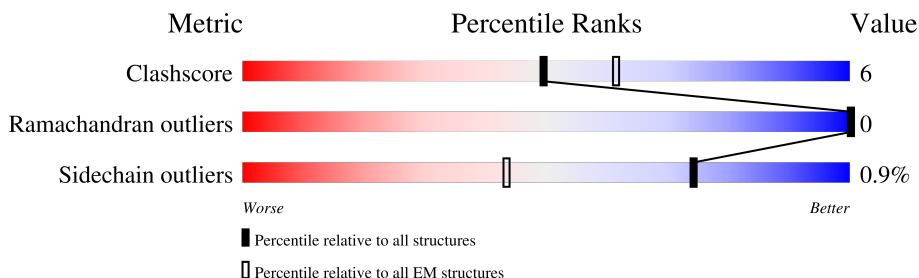
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
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  $\geq 3$ , 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	A	195	
2	B	570	
3	L	211	
4	H	215	
5	N	414	
6	C	3	

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 8542 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 Cytochrome b-245 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	134	Total	C	N	O	S	0	0
			1030	681	171	173	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	174	ALA	VAL	variant	UNP P13498

- Molecule 2 is a protein called Cytochrome b-245 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	529	Total	C	N	O	S	0	0
			4187	2753	702	709	23		

- Molecule 3 is a protein called 7D5 Fab light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	L	211	Total	C	N	O	0	0
			1055	633	211	211		

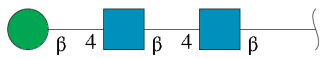
- Molecule 4 is a protein called 7D5 Fab heavy chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	214	Total	C	N	O	0	0
			1070	642	214	214		

- Molecule 5 is a protein called Green Fluorescent Protein, Anti-Fab (kappa) nanobody[TP1170] chimera.

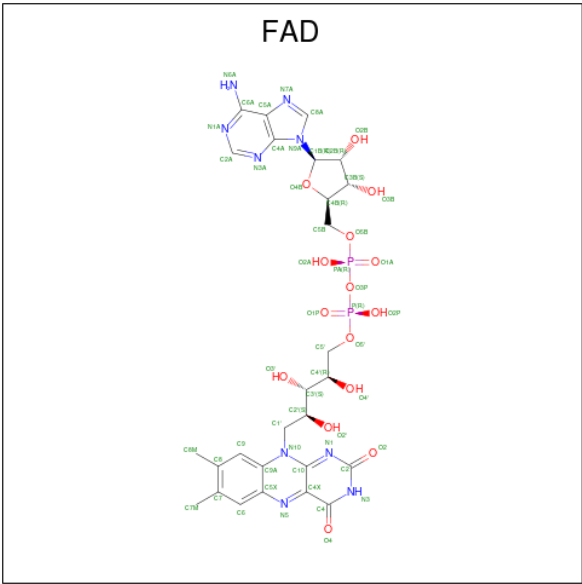
Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	126	Total	C	N	O	S	0	0
			945	596	165	179	5		

- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



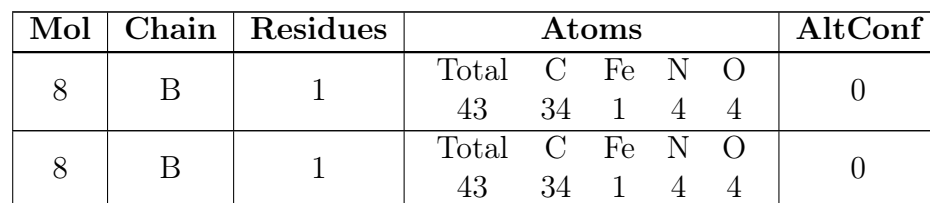
Mol	Chain	Residues	Atoms				AltConf	Trace
6	C	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 7 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					AltConf
7	B	1	Total	C	N	O	P	0
			53	27	9	15	2	

- Molecule 8 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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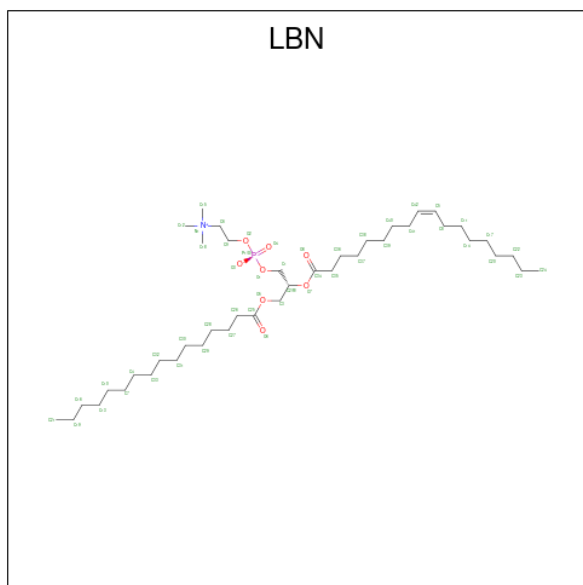
Mol	Chain	Residues	Atoms				AltConf
9	B	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms				AltConf
9	B	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 10 is 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (three-letter code: LBN) (formula:  $C_{42}H_{82}NO_8P$ ).



Mol	Chain	Residues	Atoms					AltConf
10	B	1	Total	C	N	O	P	0
			48	38	1	8	1	

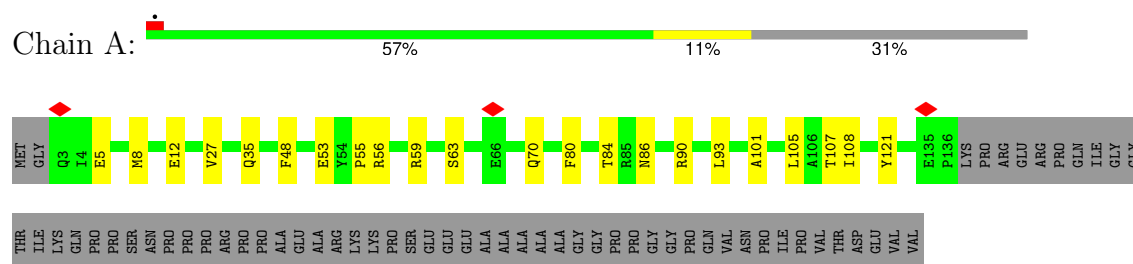
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		AltConf
11	B	1	Total	O	0
			1	1	

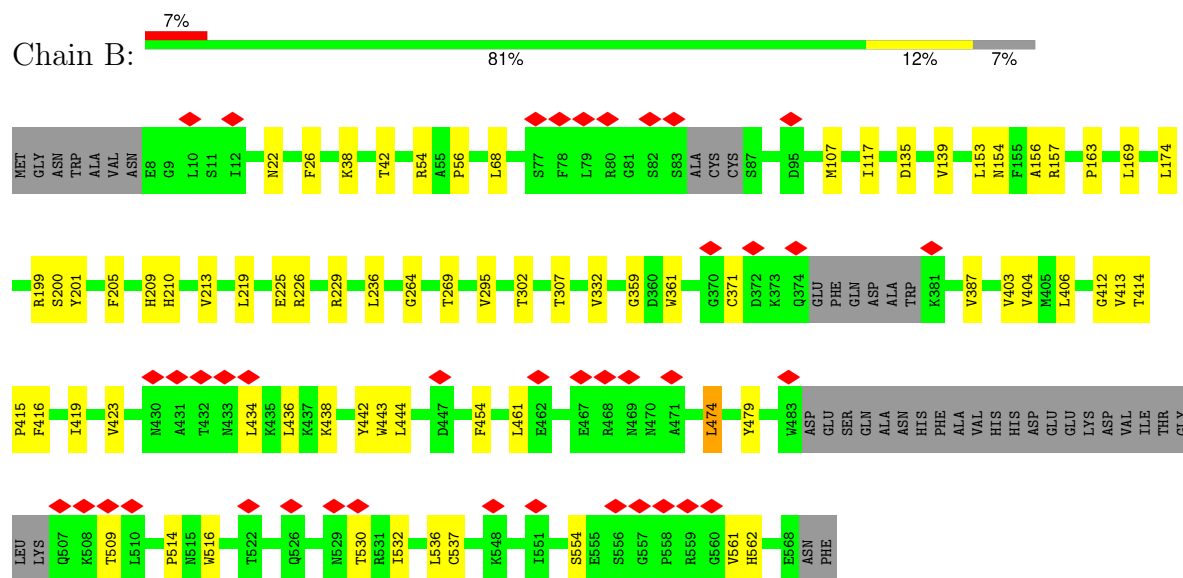
### 3 Residue-property plots

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.

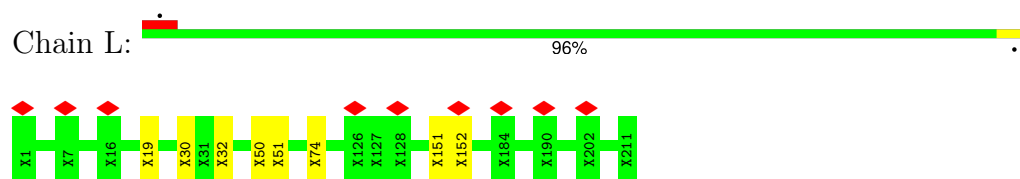
#### • Molecule 1: Cytochrome b-245 light chain



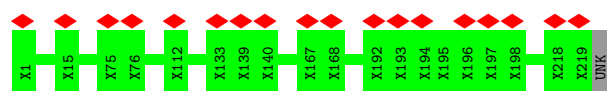
#### • Molecule 2: Cytochrome b-245 heavy chain



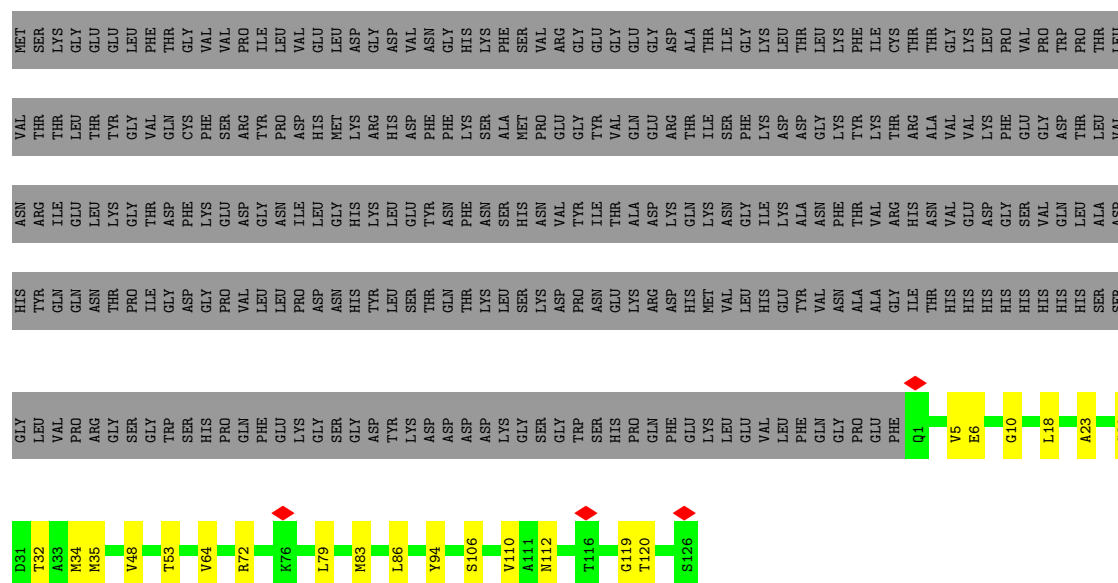
#### • Molecule 3: 7D5 Fab light chain



#### • Molecule 4: 7D5 Fab heavy chain



- Chain N: 



- Chain C:  67% 100%





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	84035	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 ( $e^-/\text{\AA}^2$ )	37.6	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	11.911	Depositor
Minimum map value	-7.850	Depositor
Average map value	-0.007	Depositor
Map value standard deviation	0.191	Depositor
Recommended contour level	1.3	Depositor
Map size ( $\text{\AA}$ )	295.56, 295.56, 295.56	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.0555714, 1.0555714, 1.0555714	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: FAD, NAG, HEM, BMA, LBN

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	0.40	0/1058	0.60	0/1443
2	B	0.58	0/4304	0.68	0/5848
5	N	0.44	0/967	0.68	0/1313
All	All	0.54	0/6329	0.67	0/8604

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1030	0	1041	14	0
2	B	4187	0	4159	53	0
3	L	1055	0	225	4	0
4	H	1070	0	227	0	0
5	N	945	0	899	13	0
6	C	39	0	34	0	0
7	B	53	0	31	3	0
8	B	86	0	60	3	0
9	B	28	0	26	0	0
10	B	48	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	B	1	0	0	1	0
All	All	8542	0	6702	84	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 6.

All (84) 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)
2:B:406:LEU:HD23	2:B:416:PHE:CD1	1.59	1.36
2:B:42:THR:HG22	2:B:153:LEU:HD11	1.33	1.05
2:B:406:LEU:CD2	2:B:416:PHE:CD1	2.48	0.95
2:B:406:LEU:CD2	2:B:416:PHE:HD1	1.82	0.93
2:B:42:THR:CG2	2:B:153:LEU:HD11	2.06	0.86
2:B:406:LEU:HD23	2:B:416:PHE:HD1	1.09	0.83
2:B:413:VAL:HG11	2:B:454:PHE:CD2	2.15	0.82
7:B:601:FAD:H2'	7:B:601:FAD:N1	1.94	0.82
2:B:413:VAL:CG1	2:B:454:PHE:CE2	2.65	0.80
2:B:413:VAL:HG11	2:B:454:PHE:CE2	2.18	0.78
5:N:35:MET:SD	5:N:110:VAL:HG11	2.28	0.74
2:B:413:VAL:CG1	2:B:454:PHE:CZ	2.71	0.73
2:B:404:VAL:HG22	2:B:436:LEU:HD11	1.72	0.71
8:B:602:HEM:HHC	8:B:602:HEM:HBB2	1.77	0.65
2:B:42:THR:HG21	2:B:229:ARG:O	1.98	0.64
8:B:602:HEM:HBC2	8:B:602:HEM:HHD	1.83	0.60
8:B:603:HEM:HBB2	8:B:603:HEM:HHC	1.85	0.58
5:N:10:GLY:H	5:N:18:LEU:HD21	1.67	0.58
3:L:50:UNK:O	3:L:51:UNK:C	2.52	0.57
1:A:35:GLN:HG3	2:B:163:PRO:HD3	1.87	0.56
2:B:561:VAL:O	2:B:561:VAL:HG23	2.06	0.55
2:B:302:THR:HG22	2:B:371:CYS:SG	2.46	0.55
2:B:226:ARG:HB3	2:B:264:GLY:HA3	1.89	0.54
2:B:302:THR:CG2	2:B:371:CYS:SG	2.97	0.53
2:B:413:VAL:HG12	2:B:454:PHE:CE1	2.44	0.53
2:B:54:ARG:HD2	11:B:701:HOH:O	2.09	0.52
2:B:403:VAL:HG13	2:B:438:LYS:HB3	1.91	0.52
2:B:413:VAL:HG21	2:B:443:TRP:CD1	2.44	0.52
3:L:30:UNK:C	3:L:32:UNK:N	2.71	0.51
3:L:151:UNK:O	3:L:152:UNK:CB	2.59	0.50
2:B:174:LEU:HD23	2:B:225:GLU:HG2	1.94	0.49
1:A:48:PHE:HE2	1:A:93:LEU:HD21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:GLU:OE2	1:A:56:ARG:NH2	2.40	0.48
1:A:27:VAL:HG21	2:B:117:ILE:HG23	1.96	0.47
1:A:84:THR:O	1:A:90:ARG:NH2	2.43	0.47
2:B:219:LEU:HG	2:B:269:THR:HG21	1.97	0.47
1:A:53:GLU:OE1	1:A:121:TYR:OH	2.33	0.46
2:B:413:VAL:HG21	2:B:443:TRP:NE1	2.31	0.46
2:B:199:ARG:NH1	2:B:200:SER:OG	2.47	0.46
5:N:6:GLU:HB3	5:N:120:THR:HG23	1.97	0.46
5:N:34:MET:HB3	5:N:79:LEU:HD22	1.97	0.46
3:L:19:UNK:O	3:L:74:UNK:HA	2.15	0.46
5:N:83:MET:HB3	5:N:86:LEU:HD21	1.98	0.46
1:A:55:PRO:HA	1:A:70:GLN:HG3	1.97	0.46
2:B:210:HIS:O	2:B:213:VAL:HG12	2.15	0.46
2:B:154:ASN:HB3	2:B:157:ARG:HH21	1.80	0.46
5:N:5:VAL:HG23	5:N:23:ALA:HB3	1.98	0.45
1:A:5:GLU:HB2	2:B:201:TYR:CZ	2.52	0.45
2:B:359:GLY:HA3	7:B:601:FAD:O2A	2.16	0.45
5:N:32:THR:O	5:N:72:ARG:NH2	2.31	0.45
2:B:332:VAL:HG11	2:B:361:TRP:HA	1.99	0.44
1:A:8:MET:HG3	2:B:201:TYR:CE2	2.51	0.44
5:N:48:VAL:HG13	5:N:64:VAL:HG11	1.99	0.44
2:B:295:VAL:HG21	2:B:387:VAL:H	1.82	0.44
2:B:403:VAL:HB	2:B:532:ILE:HG12	1.98	0.44
5:N:5:VAL:CG2	5:N:23:ALA:HB3	2.48	0.44
2:B:423:VAL:HG13	2:B:434:LEU:HD11	1.99	0.44
2:B:419:ILE:O	2:B:423:VAL:HG23	2.19	0.43
2:B:442:TYR:HD1	2:B:479:TYR:HE1	1.67	0.43
5:N:30:SER:O	5:N:53:THR:HB	2.18	0.43
2:B:413:VAL:HG13	2:B:454:PHE:CZ	2.50	0.43
2:B:554:SER:HB3	2:B:562:HIS:HA	2.01	0.43
1:A:59:ARG:NH2	1:A:63:SER:O	2.46	0.42
2:B:26:PHE:HE2	2:B:56:PRO:HG3	1.85	0.42
2:B:444:LEU:HD11	2:B:516:TRP:HZ2	1.84	0.42
5:N:112:ASN:OD1	5:N:112:ASN:N	2.49	0.42
7:B:601:FAD:H1'1	7:B:601:FAD:H9	1.73	0.42
1:A:5:GLU:HB2	2:B:201:TYR:CE1	2.54	0.42
1:A:80:PHE:HB2	1:A:84:THR:HG23	2.02	0.42
2:B:461:LEU:HD23	2:B:474:LEU:HG	2.01	0.42
5:N:106:SER:O	5:N:110:VAL:HG23	2.19	0.42
2:B:38:LYS:HA	2:B:236:LEU:HD11	2.01	0.42
2:B:135:ASP:O	2:B:139:VAL:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:536:LEU:HG	2:B:537:CYS:N	2.30	0.42
1:A:101:ALA:O	1:A:107:THR:OG1	2.32	0.41
2:B:205:PHE:O	2:B:209:HIS:HB2	2.20	0.41
2:B:68:LEU:HA	2:B:68:LEU:HD23	1.85	0.41
2:B:412:GLY:O	2:B:415:PRO:HD2	2.20	0.41
2:B:479:TYR:CD1	2:B:514:PRO:HG3	2.56	0.40
5:N:94:TYR:O	5:N:119:GLY:HA2	2.21	0.40
2:B:413:VAL:CG2	2:B:443:TRP:CD1	3.04	0.40
2:B:22:ASN:ND2	2:B:107:MET:SD	2.95	0.40
1:A:105:LEU:O	1:A:108:ILE:HG22	2.22	0.40
2:B:156:ALA:HB2	2:B:169:LEU:HD11	2.04	0.40

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	Percentiles	
1	A	132/195 (68%)	131 (99%)	1 (1%)	0	100	100
2	B	521/570 (91%)	510 (98%)	11 (2%)	0	100	100
5	N	124/414 (30%)	122 (98%)	2 (2%)	0	100	100
All	All	777/1179 (66%)	763 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	100/150 (67%)	99 (99%)	1 (1%)	73	84
2	B	440/498 (88%)	435 (99%)	5 (1%)	70	82
5	N	93/350 (27%)	93 (100%)	0	100	100
All	All	633/998 (63%)	627 (99%)	6 (1%)	74	85

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	ASN
2	B	307	THR
2	B	414	THR
2	B	474	LEU
2	B	509	THR
2	B	530	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	22	ASN
2	B	527	HIS
5	N	103	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

3 monosaccharides 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	NAG	C	1	6,2	14,14,15	0.38	0	17,19,21	0.56	0
6	NAG	C	2	6	14,14,15	0.22	0	17,19,21	0.33	0
6	BMA	C	3	6	11,11,12	0.71	0	15,15,17	0.69	0

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	NAG	C	1	6,2	-	2/6/23/26	0/1/1/1
6	NAG	C	2	6	-	0/6/23/26	0/1/1/1
6	BMA	C	3	6	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

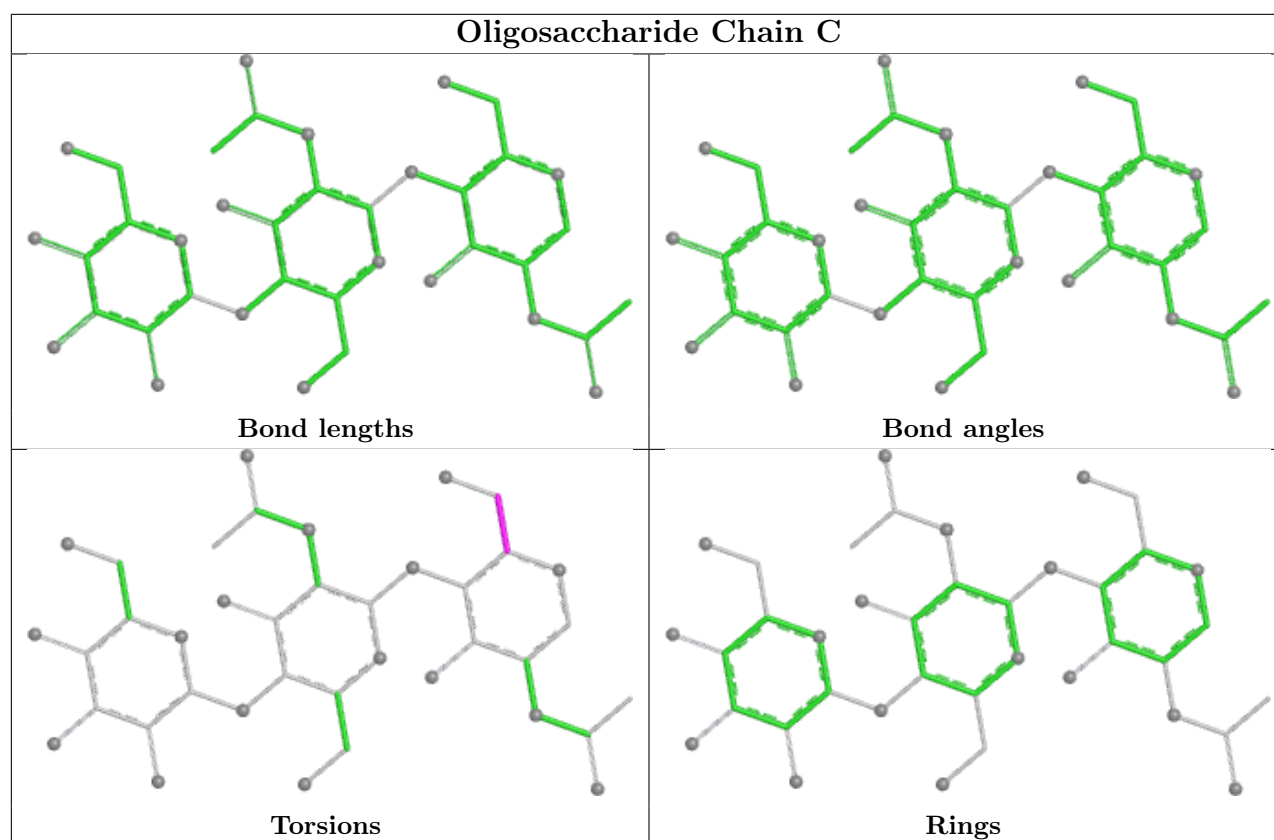
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	1	NAG	O5-C5-C6-O6
6	C	1	NAG	C4-C5-C6-O6

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 oligosaccharide.



## 5.6 Ligand geometry [i](#)

6 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	HEM	B	602	2	42,50,50	1.44	6 (14%)	46,82,82	2.08	14 (30%)
8	HEM	B	603	2	42,50,50	1.34	6 (14%)	46,82,82	1.88	14 (30%)
10	LBN	B	606	-	47,47,51	0.38	0	53,55,59	0.46	0
9	NAG	B	605	2	14,14,15	0.39	0	17,19,21	0.48	0
7	FAD	B	601	-	54,58,58	1.25	6 (11%)	71,89,89	1.30	8 (11%)
9	NAG	B	604	2	14,14,15	0.28	0	17,19,21	0.50	0

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
8	HEM	B	602	2	-	3/12/54/54	-
8	HEM	B	603	2	-	3/12/54/54	-
10	LBN	B	606	-	-	9/51/51/55	-
9	NAG	B	605	2	-	0/6/23/26	0/1/1/1
7	FAD	B	601	-	-	12/30/50/50	0/6/6/6
9	NAG	B	604	2	-	2/6/23/26	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	601	FAD	C9A-C5X	4.79	1.48	1.41
8	B	602	HEM	C1B-NB	-3.67	1.33	1.40
8	B	603	HEM	C1B-NB	-3.47	1.34	1.40
8	B	602	HEM	C4D-ND	-3.43	1.34	1.40
8	B	603	HEM	C4D-ND	-3.40	1.34	1.40
7	B	601	FAD	C8-C7	3.20	1.48	1.40
7	B	601	FAD	C4-N3	-2.73	1.33	1.38
8	B	603	HEM	FE-NB	2.61	2.12	1.98
8	B	602	HEM	FE-NB	2.51	2.12	1.98
8	B	603	HEM	C3B-C4B	2.30	1.49	1.44
8	B	602	HEM	C1D-ND	-2.29	1.34	1.38
8	B	602	HEM	C3B-C4B	2.29	1.49	1.44
8	B	603	HEM	CHB-C1B	2.20	1.40	1.34
7	B	601	FAD	C5X-N5	-2.20	1.35	1.39
8	B	602	HEM	O2A-CGA	-2.18	1.23	1.30
8	B	603	HEM	C1D-ND	-2.18	1.34	1.38
7	B	601	FAD	C2-N3	-2.14	1.34	1.39
7	B	601	FAD	C4X-N5	2.01	1.35	1.30

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	602	HEM	CBA-CAA-C2A	-5.77	102.84	112.54
8	B	602	HEM	CHD-C1D-ND	4.58	129.37	124.44
8	B	603	HEM	CHD-C1D-ND	4.41	129.18	124.44
8	B	602	HEM	CHB-C1B-NB	4.08	129.43	124.37
8	B	602	HEM	C3B-C4B-NB	-3.99	106.61	109.47
8	B	603	HEM	CHB-C1B-NB	3.94	129.26	124.37
8	B	603	HEM	CHA-C4D-ND	3.85	129.14	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	601	FAD	N3A-C2A-N1A	-3.68	123.68	128.67
8	B	602	HEM	CHC-C4B-NB	3.67	128.39	124.44
8	B	603	HEM	CHC-C4B-NB	3.66	128.37	124.44
8	B	603	HEM	C1B-NB-C4B	3.63	109.51	105.21
8	B	603	HEM	C3B-C4B-NB	-3.35	107.06	109.47
8	B	602	HEM	C1B-NB-C4B	3.23	109.03	105.21
8	B	602	HEM	CHA-C4D-ND	3.11	128.23	124.37
7	B	601	FAD	C4-C4X-N5	2.93	122.25	118.21
8	B	602	HEM	CHD-C1D-C2D	-2.85	120.52	125.03
7	B	601	FAD	C4A-C5A-N7A	-2.75	106.44	109.34
7	B	601	FAD	C4X-C10-N1	-2.60	118.23	124.59
8	B	603	HEM	CHA-C4D-C3D	-2.47	120.67	125.23
8	B	602	HEM	CHB-C1B-C2B	-2.46	119.97	126.94
8	B	602	HEM	CMA-C3A-C4A	-2.42	124.91	128.46
8	B	602	HEM	CAB-C3B-C2B	-2.36	120.76	128.43
8	B	603	HEM	C3B-C2B-C1B	2.35	108.18	106.41
7	B	601	FAD	C10-N1-C2	2.22	121.66	116.85
8	B	602	HEM	O2D-CGD-CBD	2.21	120.97	114.00
8	B	602	HEM	C4D-ND-C1D	2.19	107.81	105.21
7	B	601	FAD	C4X-C4-N3	2.19	118.83	113.25
7	B	601	FAD	O4-C4-C4X	-2.19	120.75	126.53
8	B	603	HEM	C4D-ND-C1D	2.14	107.74	105.21
8	B	603	HEM	CHD-C1D-C2D	-2.14	121.66	125.03
8	B	603	HEM	CHB-C1B-C2B	-2.12	120.95	126.94
7	B	601	FAD	C4-N3-C2	-2.11	121.89	125.64
8	B	603	HEM	CMC-C2C-C3C	2.07	128.82	124.68
8	B	603	HEM	O2D-CGD-CBD	2.05	120.48	114.00
8	B	603	HEM	CAB-C3B-C2B	-2.02	121.86	128.43
8	B	602	HEM	CMA-C3A-C2A	2.02	128.75	124.94

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	601	FAD	C5B-O5B-PA-O1A
7	B	601	FAD	C5B-O5B-PA-O2A
7	B	601	FAD	C5B-O5B-PA-O3P
7	B	601	FAD	C2'-C1'-N10-C10
7	B	601	FAD	O4'-C4'-C5'-O5'
9	B	604	NAG	C4-C5-C6-O6
9	B	604	NAG	O5-C5-C6-O6
8	B	602	HEM	C4B-C3B-CAB-CBB

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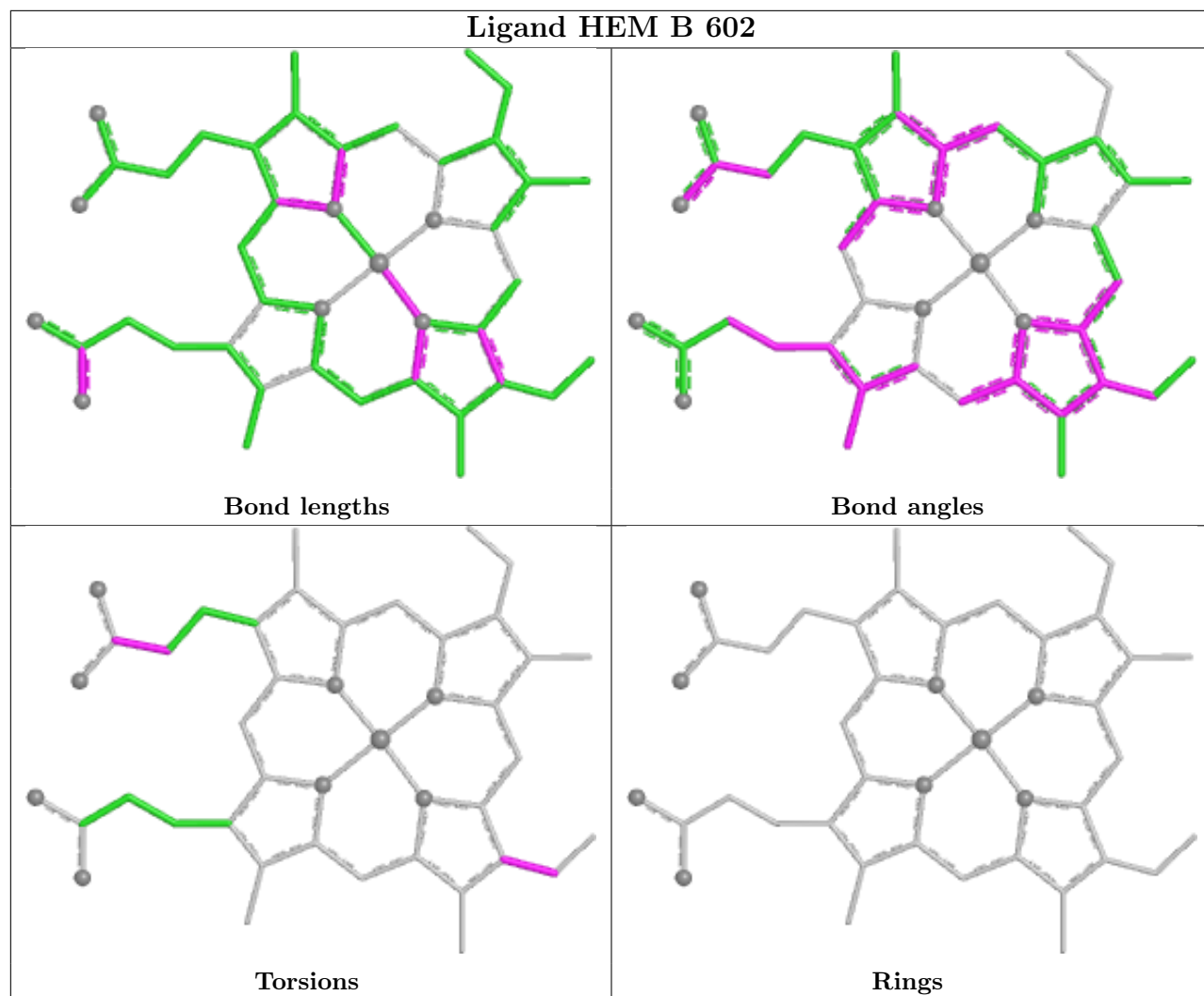
Mol	Chain	Res	Type	Atoms
10	B	606	LBN	C13-C10-C7-C4
7	B	601	FAD	C1'-C2'-C3'-O3'
10	B	606	LBN	C35-C36-C37-C38
8	B	603	HEM	C4B-C3B-CAB-CBB
10	B	606	LBN	N1-C6-C9-O2
10	B	606	LBN	C30-C31-C32-C33
10	B	606	LBN	C26-C27-C28-C29
8	B	603	HEM	C2A-CAA-CBA-CGA
10	B	606	LBN	C7-C10-C13-C16
7	B	601	FAD	P-O3P-PA-O2A
7	B	601	FAD	C3'-C4'-C5'-O5'
10	B	606	LBN	C3-C2-O7-C34
7	B	601	FAD	PA-O3P-P-O1P
10	B	606	LBN	C40-C41-C42-C5
7	B	601	FAD	P-O3P-PA-O1A
7	B	601	FAD	O2'-C2'-C3'-O3'
8	B	602	HEM	CAD-CBD-CGD-O2D
7	B	601	FAD	O2'-C2'-C3'-C4'
8	B	602	HEM	CAD-CBD-CGD-O1D
10	B	606	LBN	O5-C25-C26-C27
8	B	603	HEM	CAD-CBD-CGD-O2D

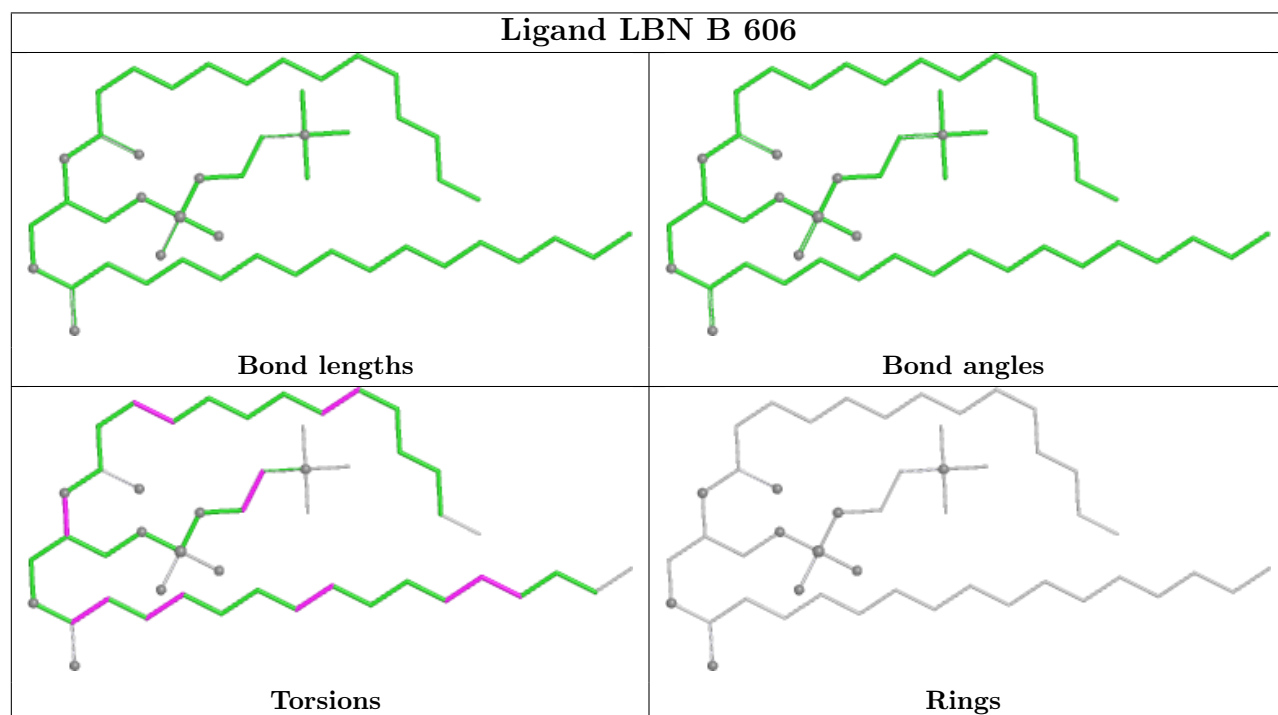
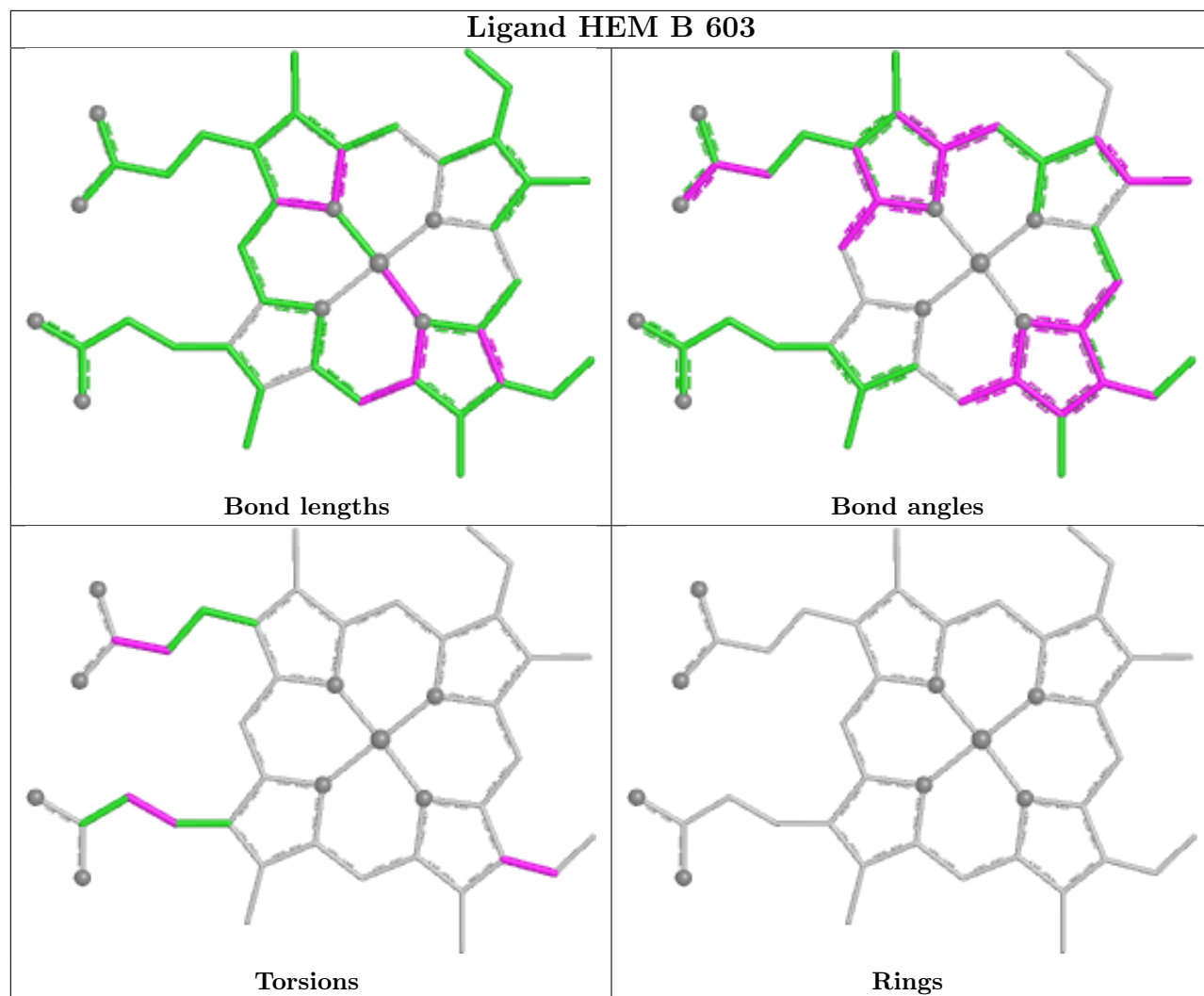
There are no ring outliers.

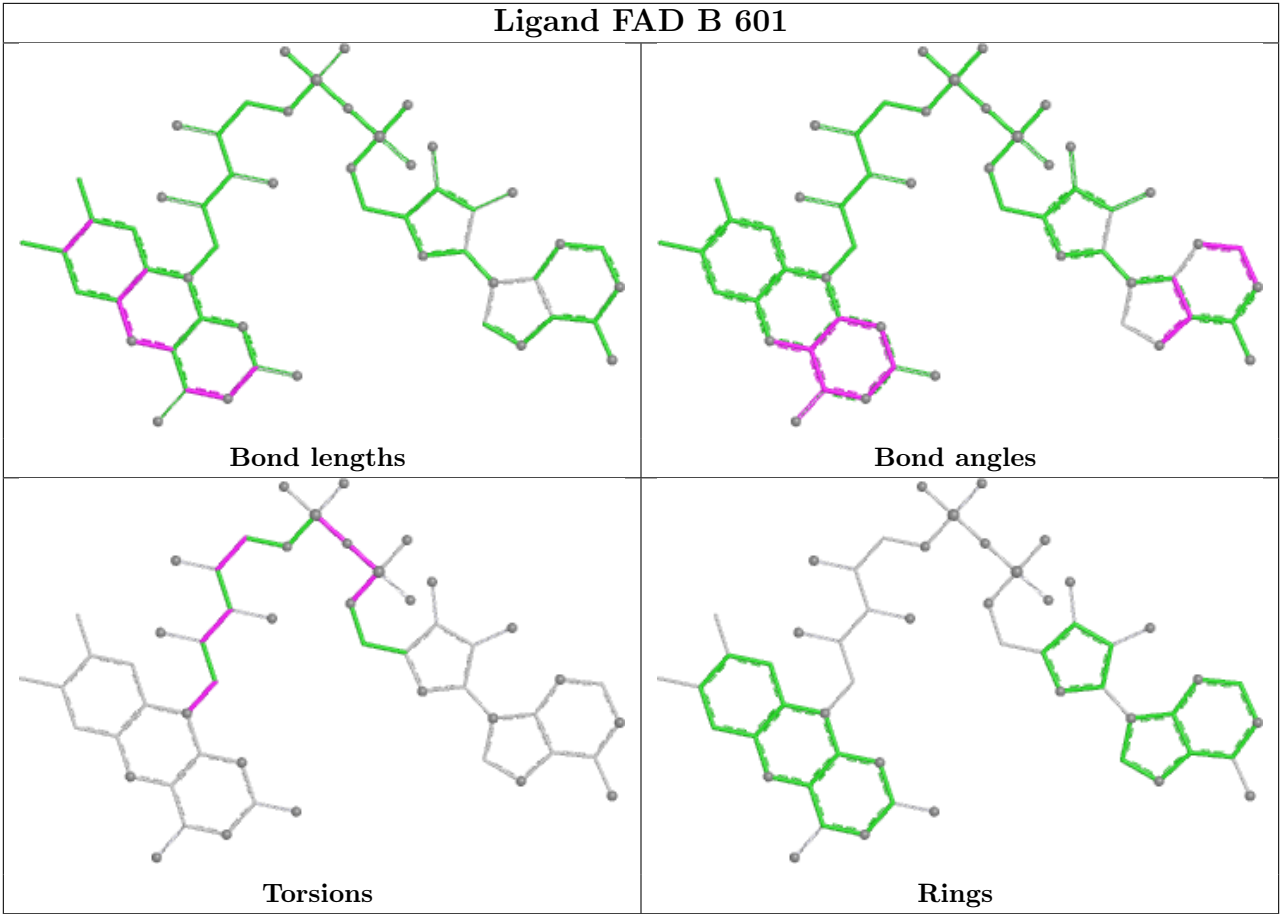
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	602	HEM	2	0
8	B	603	HEM	1	0
7	B	601	FAD	3	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 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	H	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	133:UNK	C	139:UNK	N	10.36

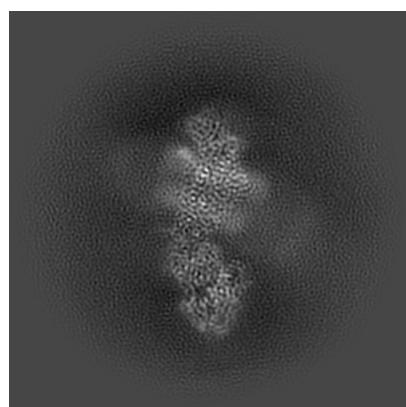
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34389. These allow visual inspection of the internal detail of the map and identification of artifacts.

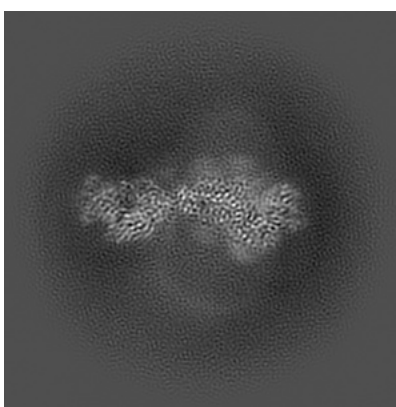
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

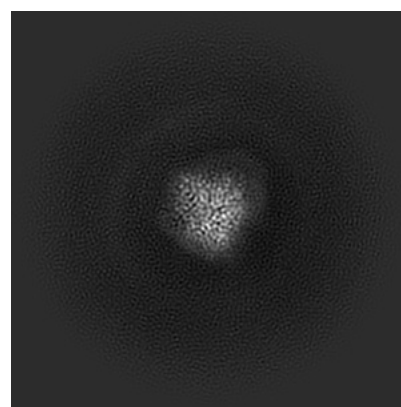
#### 6.1.1 Primary map



X



Y

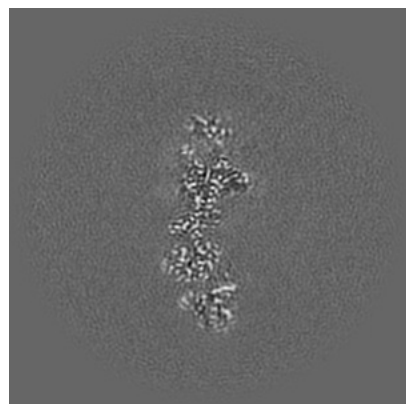


Z

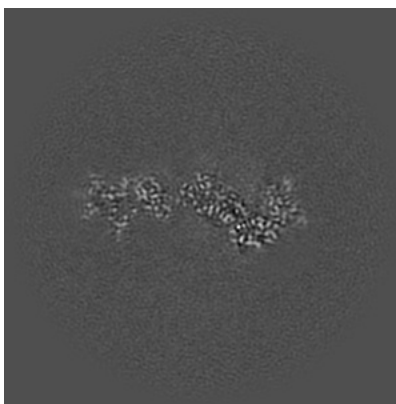
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

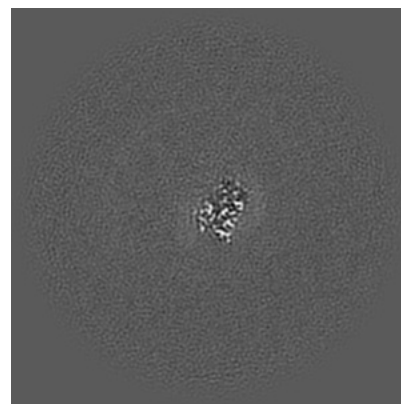
#### 6.2.1 Primary map



X Index: 140



Y Index: 140



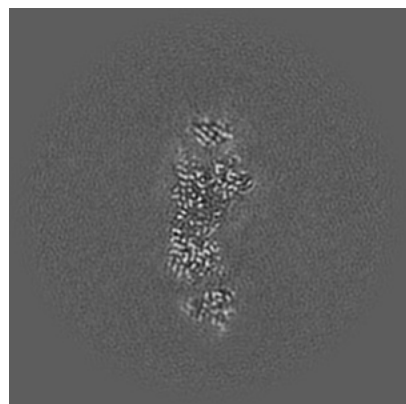
Z Index: 140



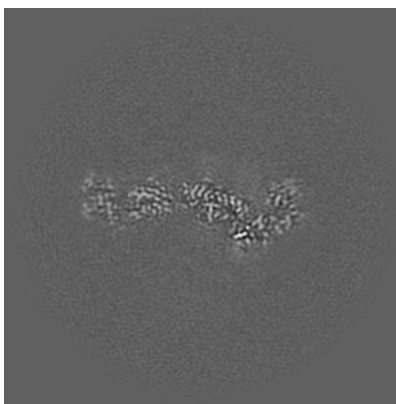
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

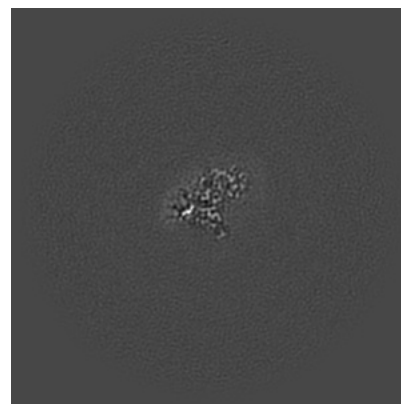
### 6.3.1 Primary map



X Index: 145



Y Index: 135

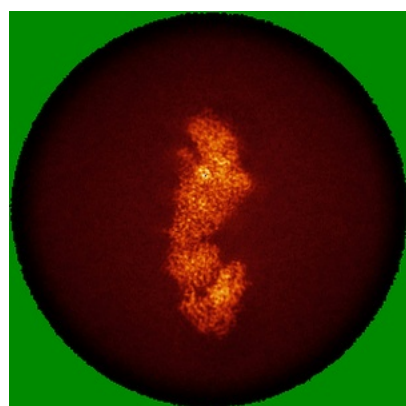


Z Index: 164

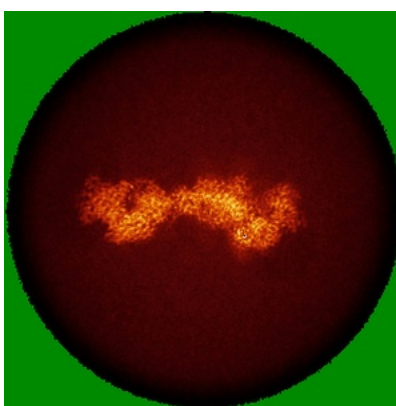
The images above show the largest variance slices of the map in three orthogonal directions.

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

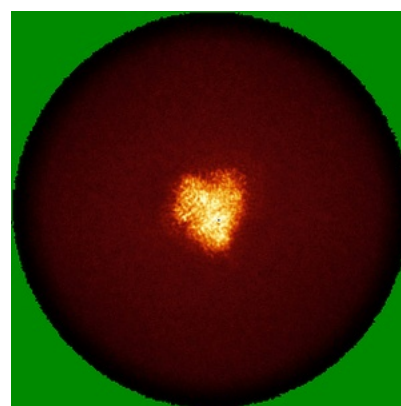
### 6.4.1 Primary map



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](#)

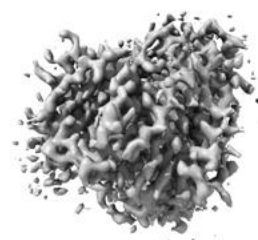
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 1.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

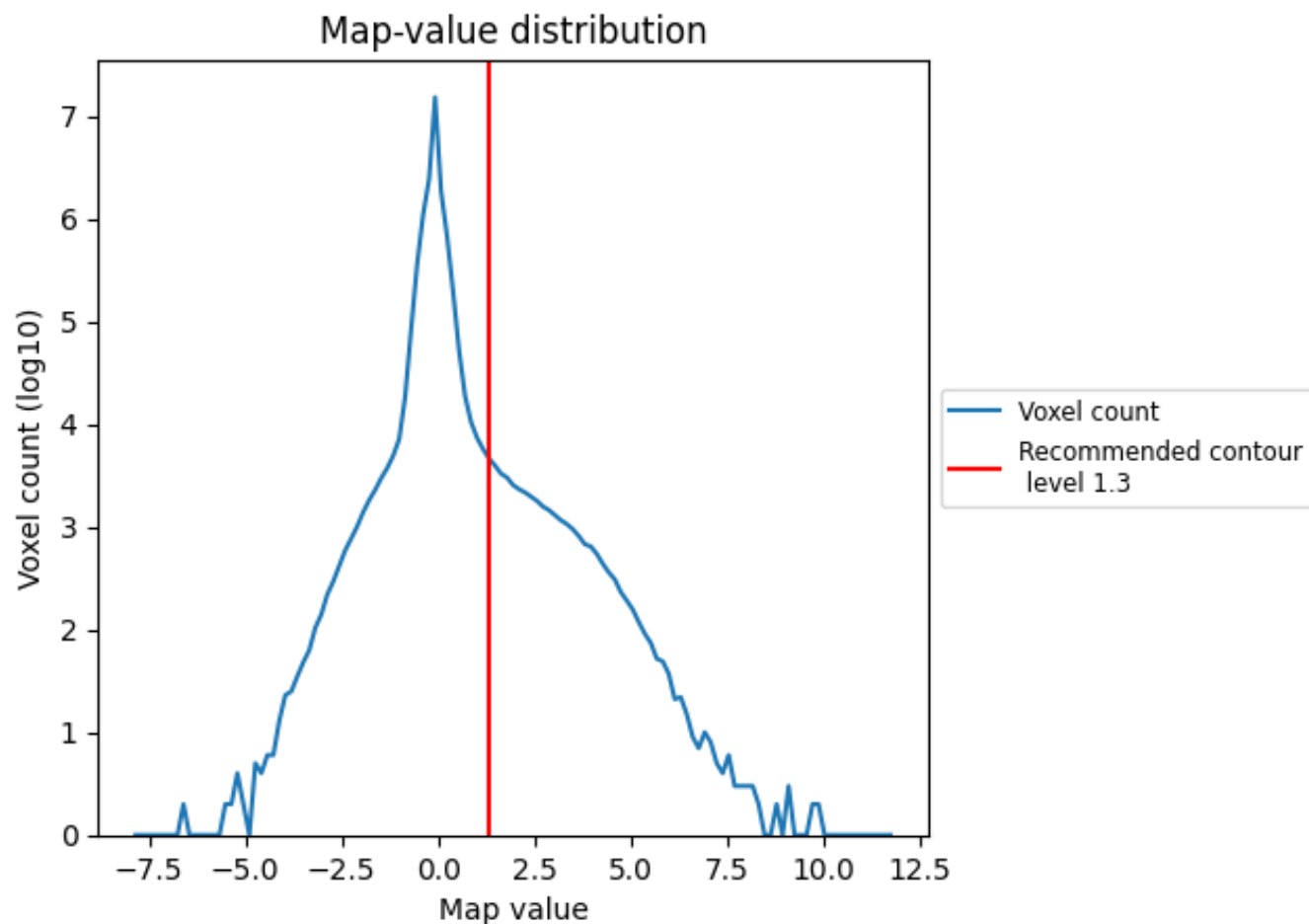
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

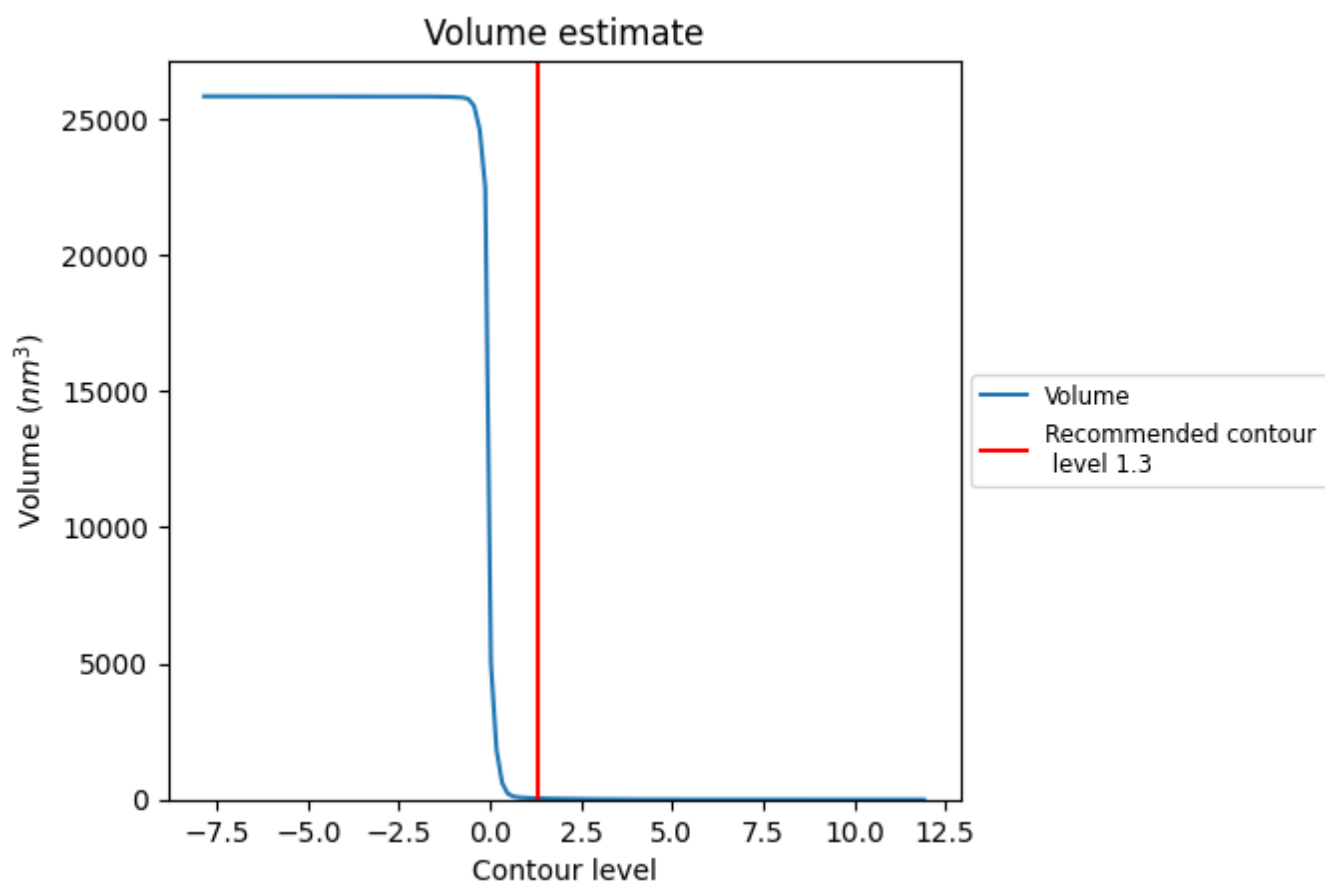
This section contains the results of statistical analysis of the map.

### 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.

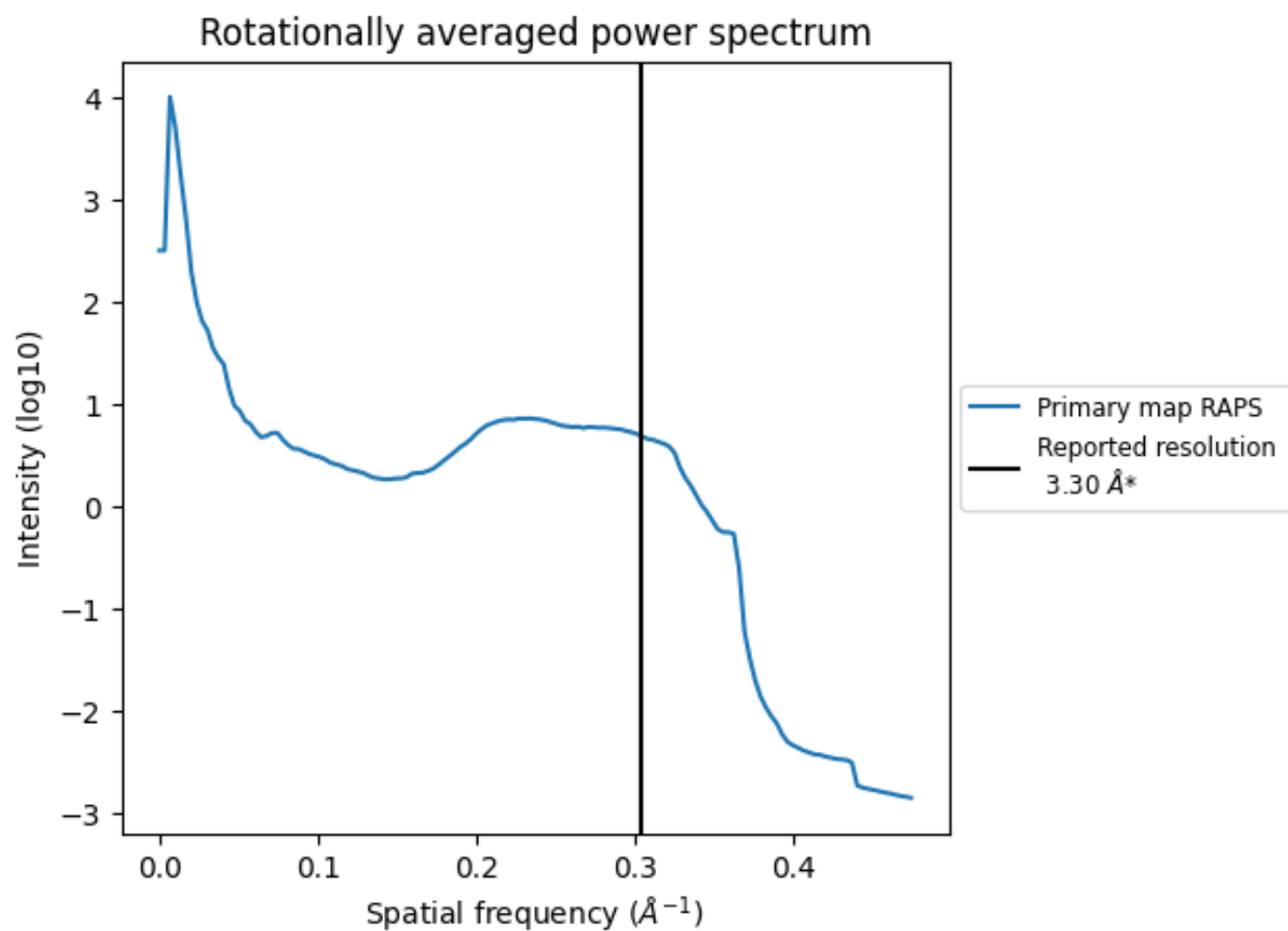
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 46 nm<sup>3</sup>; this corresponds to an approximate mass of 42 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 0.303 Å<sup>-1</sup>

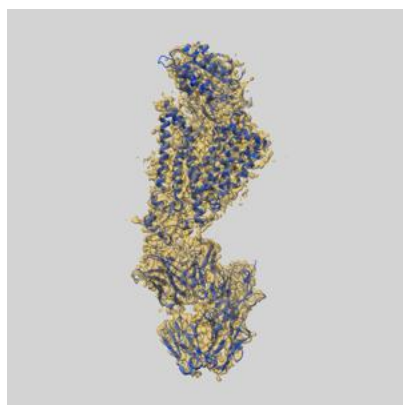
## 8 Fourier-Shell correlation ⓘ

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

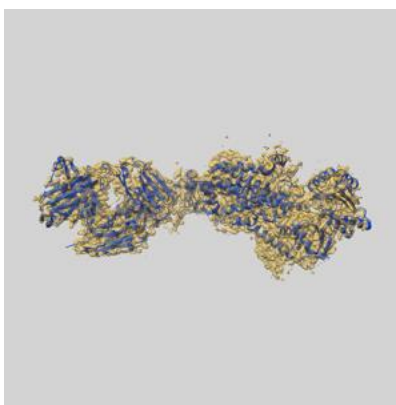
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34389 and PDB model 8GZ3. Per-residue inclusion information can be found in section [3](#) on page [7](#).

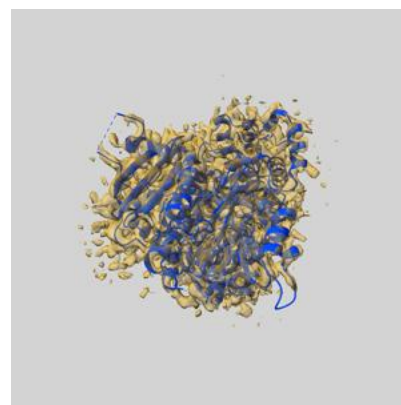
### 9.1 Map-model overlay [i](#)



X



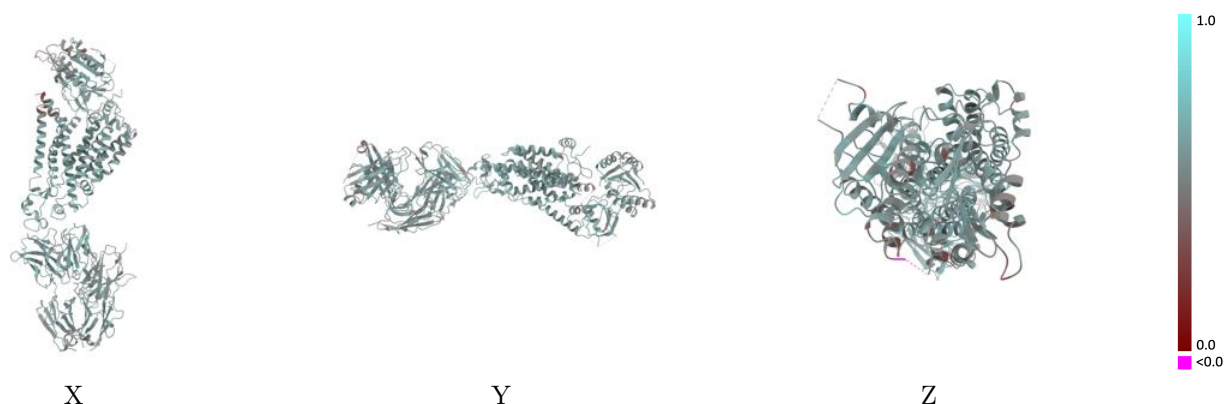
Y



Z

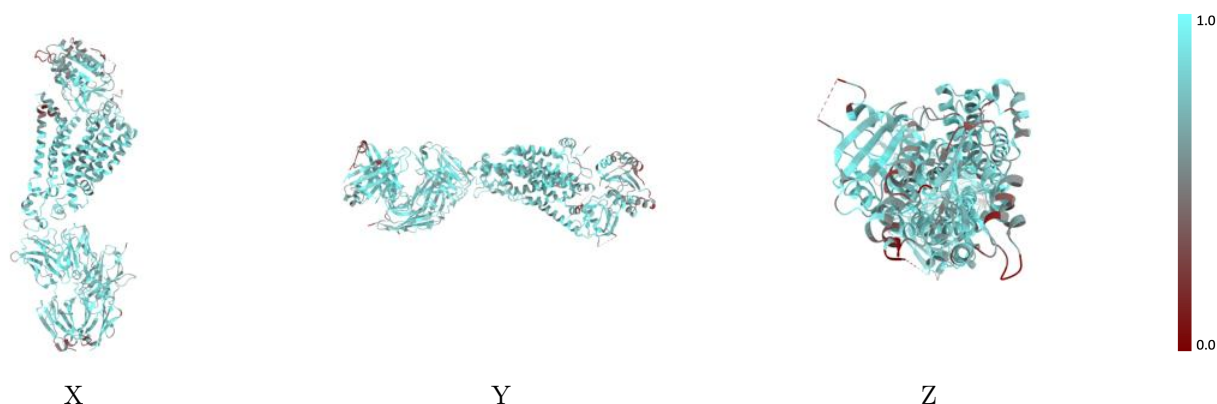
The images above show the 3D surface view of the map at the recommended contour level 1.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



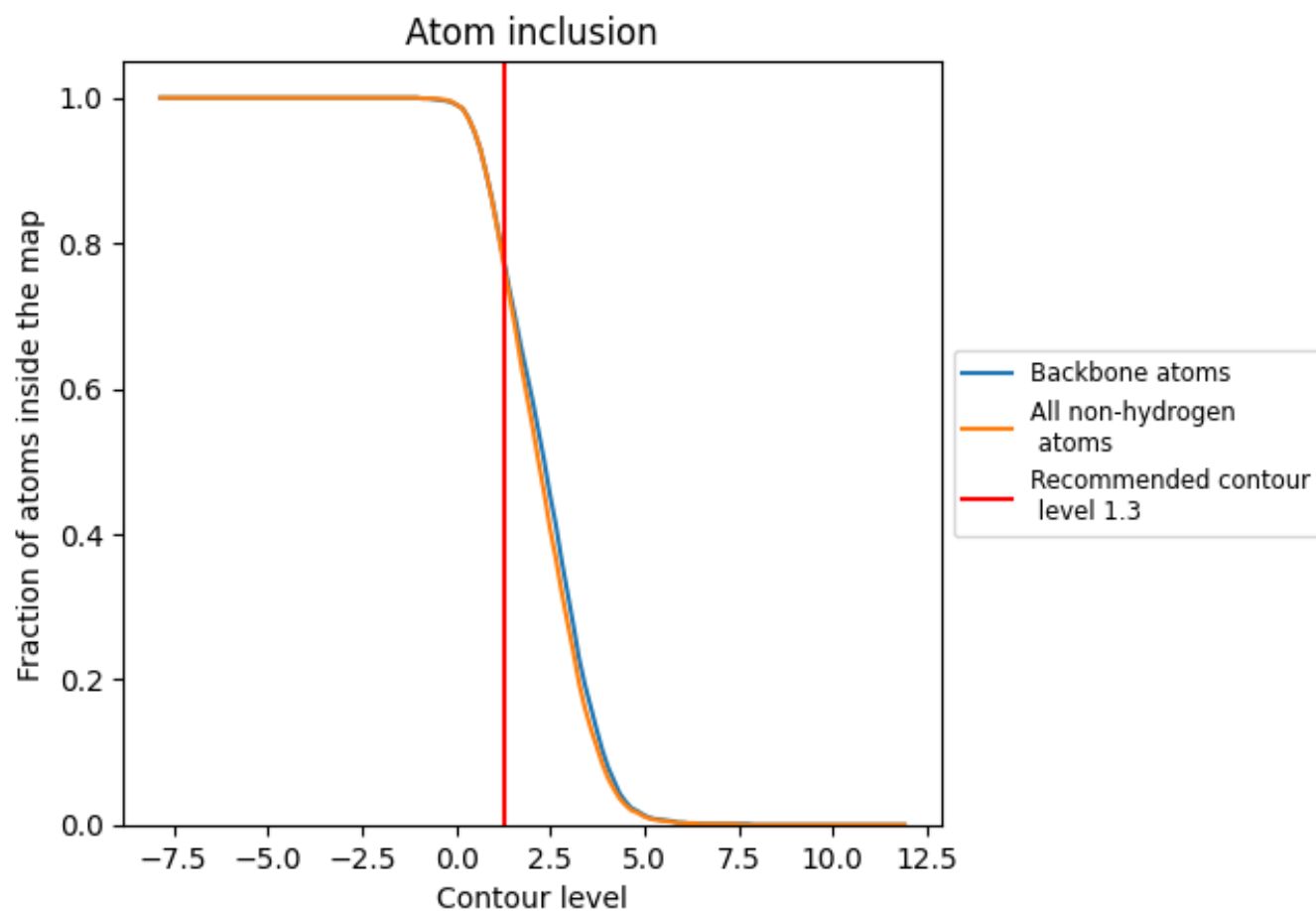
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.3).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 76% 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 (1.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7620	<div><div></div></div> 0.5590
A	<div><div></div></div> 0.7590	<div><div></div></div> 0.5660
B	<div><div></div></div> 0.7550	<div><div></div></div> 0.5670
C	<div><div></div></div> 0.3330	<div><div></div></div> 0.4990
H	<div><div></div></div> 0.7800	<div><div></div></div> 0.5480
L	<div><div></div></div> 0.7880	<div><div></div></div> 0.5560
N	<div><div></div></div> 0.7740	<div><div></div></div> 0.5360

1.0

0.0

<0.0