



wwPDB EM Validation Summary Report ⓘ

Feb 20, 2025 – 09:48 AM EST

PDB ID : 3J7B
EMDB ID : EMD-6314
Title : Catalase solved at 3.2 Angstrom resolution by MicroED
Authors : Nannenga, B.L.; Shi, D.; Hattne, J.; Reyes, F.E.; Gonen, T.
Deposited on : 2014-06-09
Resolution : 3.20 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.dev117
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) : 2.41.4

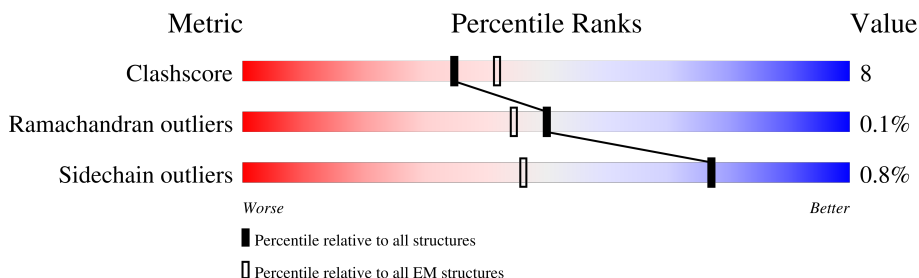
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON CRYSTALLOGRAPHY

The reported resolution of this entry is 3.20 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 ≥ 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	527	<div> <div>19%</div> <div>77%</div> <div>17%</div> <div>• 5%</div> </div>
1	B	527	<div> <div>23%</div> <div>76%</div> <div>19%</div> <div>5%</div> </div>
1	C	527	<div> <div>77%</div> <div>17%</div> <div>5%</div> </div>
1	D	527	<div> <div>61%</div> <div>76%</div> <div>18%</div> <div>• 5%</div> </div>

2 Entry composition [i](#)

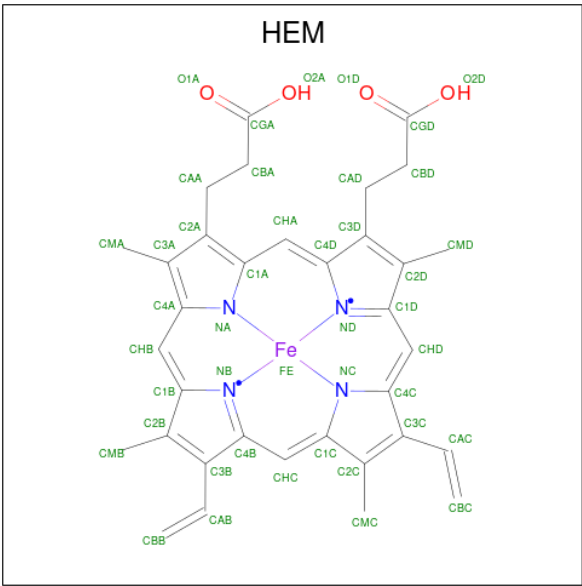
There are 3 unique types of molecules in this entry. The entry contains 16432 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Catalase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	499	Total	C	N	O	S	0	0
			4017	2548	717	738	14		
1	B	499	Total	C	N	O	S	0	0
			4017	2548	717	738	14		
1	C	499	Total	C	N	O	S	0	0
			4017	2548	717	738	14		
1	D	499	Total	C	N	O	S	0	0
			4017	2548	717	738	14		

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



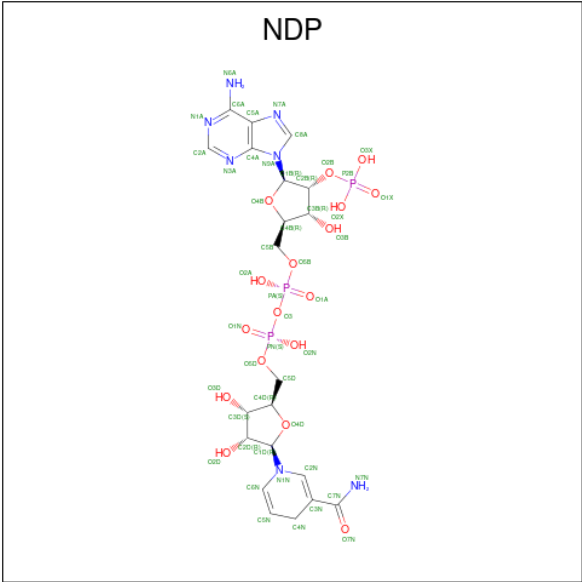
Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
2	B	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
2	C	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
2	D	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).

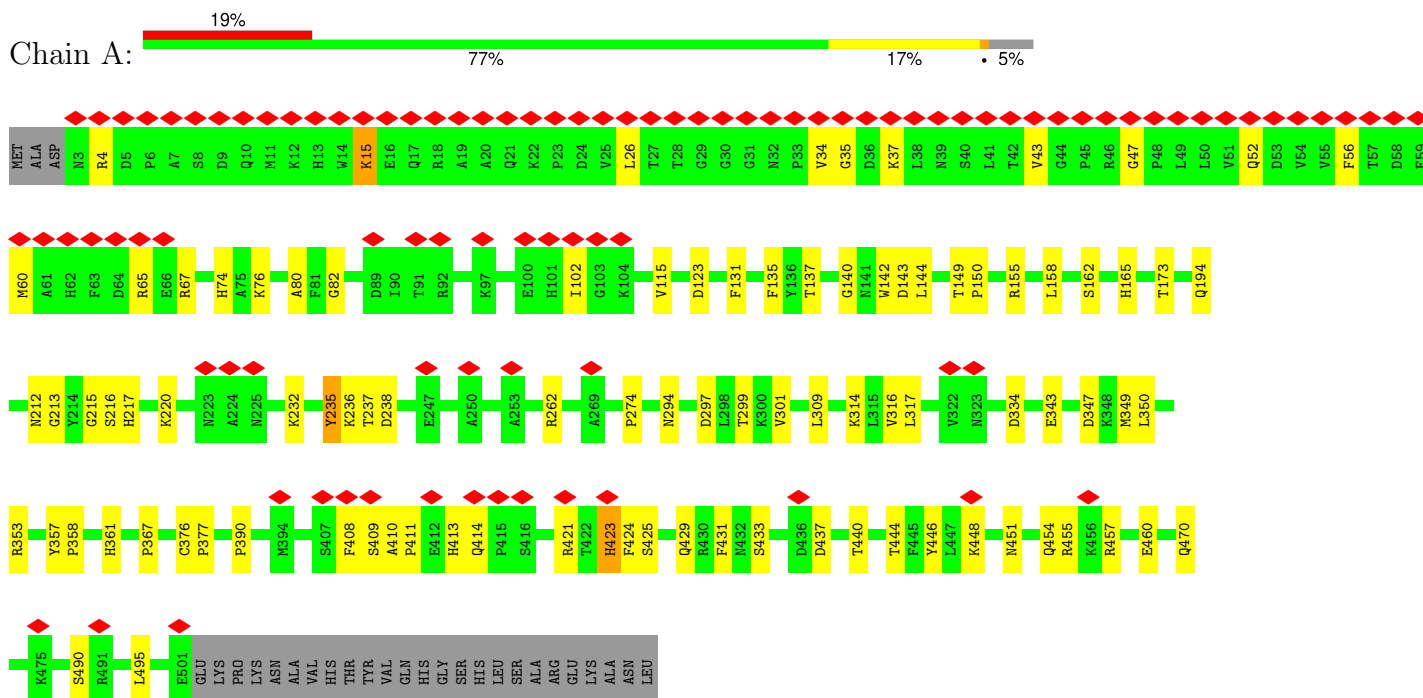


Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			48	21	7	17	3	
3	B	1	Total	C	N	O	P	0
			48	21	7	17	3	
3	C	1	Total	C	N	O	P	0
			48	21	7	17	3	
3	D	1	Total	C	N	O	P	0
			48	21	7	17	3	

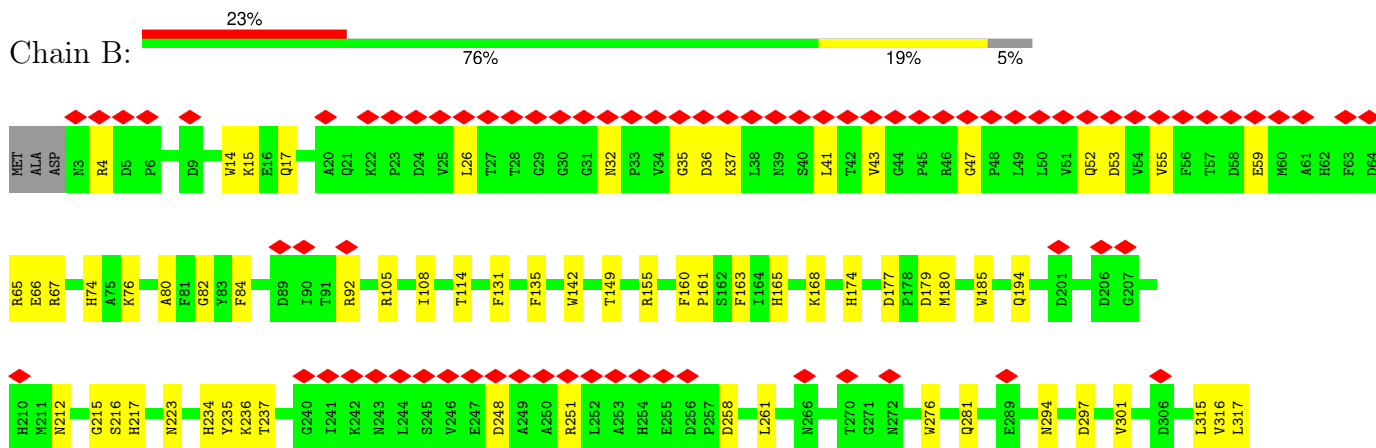
3 Residue-property plots

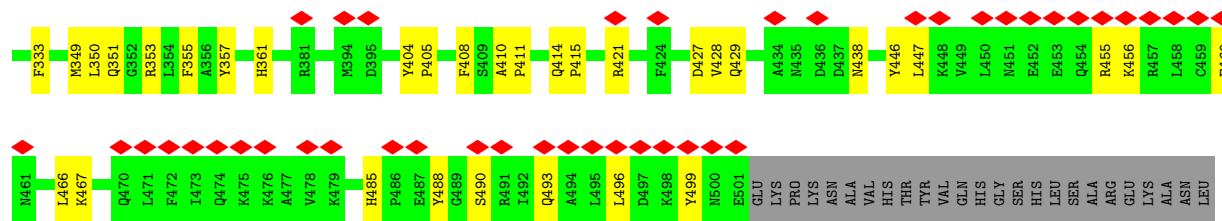
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



• Molecule 1: Catalase





ASN LEU	H465	P405	I310	T237	L175
	L466	M406	P311	D238	K176
	K467	S407	V312	Q239	D177
	D468	F408	G313	G240	P178
A469	S409	K314	I241	D179	
Q470	A410	L315	K242	M180	
L471	P411	V316	N243	V181	
F472	E412	L317	L244	W182	
I473	H413	E327	S245	D183	
Q474	Q414	F333	V246	F184	
K475	P415	D334	E247	W185	
K476	S416	P335	D248	S186	
A477	A417	S336	R251	L187	
V478	L418	N337	H254	R188	
K479	E419	M338	D258	P189	
M480	H420	P339	L261	E190	
F481	R421	P340	R262	S191	
S482	T422	G341	D263	L192	
D483	H423	I342	L264	H193	
V484	F424	E343	F265	Q194	
H485	S425	P344	S275	V195	
P486	G426	S345	W276	S196	
E487	D427	P346	T277	F197	
Y488	V428	D347	L278	L198	
G489	Q429	K348	Y279	F199	
S490	R430	M349	I280	S200	
R491	F431	L350	Q281	D201	
I492	N432	G351	V282	R202	
Q493	S433	G352	M283	G203	
A494	A434	R353	T284	I204	
L495	M435	L354	F285	P205	
L496	D436	F355	S286	G209	
D497	D437	A356	E287	H210	
K498	M438	Y357	A288	M211	
Y499	V439	P358	E289	N212	
N500	T440	D359	I290	G213	
E501	Q441	T360	F291	Y214	
GLU	V442	H361	P292	G215	
LYS	R443	R362	F293	S216	
PRO	T444	P367	N294	H217	
LYS	F445	N368	P295	T218	
LYS	Y446	V374	F296	F219	
ASN	L447	R381	D297	K220	
ALA	THR	V382	L298	L221	
ALA	VAL	A383	T299	V222	
VAL	GLN	N384	K300	N223	
VAL	HIS	Y385	V301	A224	
HIS	SER	Q386	W302	N225	
HIS	HIS	P390	H304	G226	
LEU	LEU	D395	G305	E227	
SER	SER	Y403	D306	A228	
ALA	ALA	Y404	Y307	V229	
ARG	ARG		P308	Y230	
GLU	GLU		L309	C231	
LYS	LYS			K232	
ALA	ALA			F233	
				H234	
				Y235	
				K236	

4 Experimental information

Property	Value	Source
EM reconstruction method	CRYSTALLOGRAPHY	Depositor
Imposed symmetry	3D CRYSTAL, a =Not provided Å, b =Not provided Å, c =Not provided Å, α =Not provided°, β =Not provided°, γ =Not provided°, space group=Not provided	Depositor
Number of images used	Not provided	
Resolution determination method	DIFFRACTION PATTERN/LAYERLINES	Depositor
CTF correction method	Not provided	
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	0.1	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	TVIPS TEMCAM-F416 (4k x 4k)	Depositor
Maximum map value	5.384	Depositor
Minimum map value	-3.715	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.5	Depositor
Map size (Å)	67.64004, 172.08072, 182.0712	wwPDB
Map dimensions	240, 216, 90	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.751556, 0.79667, 0.75863	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: HEM, NDP

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	0.32	0/4137	0.53	0/5619
1	B	0.34	0/4137	0.54	0/5619
1	C	0.32	0/4137	0.53	2/5619 (0.0%)
1	D	0.31	0/4137	0.51	0/5619
All	All	0.32	0/16548	0.53	2/22476 (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	D	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	427	ASP	CB-CG-OD2	-6.33	112.61	118.30
1	C	427	ASP	CB-CG-OD1	5.37	123.13	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	200	SER	Peptide

5.2 Too-close contacts ⓘ

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	4017	0	3844	66	0
1	B	4017	0	3844	84	0
1	C	4017	0	3844	71	0
1	D	4017	0	3844	71	0
2	A	43	0	30	2	0
2	B	43	0	30	3	0
2	C	43	0	30	1	0
2	D	43	0	30	2	0
3	A	48	0	26	2	0
3	B	48	0	26	3	0
3	C	48	0	26	3	0
3	D	48	0	26	1	0
All	All	16432	0	15600	250	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 250 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)
1:A:150:PRO:HG3	3:A:602:NDP:H41N	1.55	0.87
1:B:235:TYR:CZ	1:B:276:TRP:HB2	2.17	0.79
1:B:174:HIS:HB3	1:C:261:LEU:HD21	1.65	0.78
1:D:251:ARG:O	1:D:254:HIS:CD2	2.38	0.77
1:B:235:TYR:CE1	1:B:315:LEU:HD12	2.20	0.77

There are no symmetry-related clashes.

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	497/527 (94%)	481 (97%)	16 (3%)	0	100	100
1	B	497/527 (94%)	480 (97%)	17 (3%)	0	100	100
1	C	497/527 (94%)	481 (97%)	15 (3%)	1 (0%)	44	75
1	D	497/527 (94%)	479 (96%)	17 (3%)	1 (0%)	44	75
All	All	1988/2108 (94%)	1921 (97%)	65 (3%)	2 (0%)	50	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	427	ASP
1	D	216	SER

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	431/454 (95%)	424 (98%)	7 (2%)	58	79
1	B	431/454 (95%)	431 (100%)	0	100	100
1	C	431/454 (95%)	428 (99%)	3 (1%)	81	92
1	D	431/454 (95%)	427 (99%)	4 (1%)	75	89
All	All	1724/1816 (95%)	1710 (99%)	14 (1%)	77	90

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	89	ASP
1	C	131	PHE
1	D	499	TYR
1	D	254	HIS
1	D	498	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	52	GLN
1	D	39	ASN
1	D	167	GLN
1	D	413	HIS

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](#)

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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	C	601	1	42,50,50	1.88	7 (16%)	46,82,82	1.89	15 (32%)
3	NDP	A	602	-	47,52,52	2.62	7 (14%)	61,80,80	1.67	15 (24%)
3	NDP	B	602	-	47,52,52	2.52	7 (14%)	61,80,80	1.73	14 (22%)
2	HEM	A	601	1	42,50,50	1.88	6 (14%)	46,82,82	1.52	5 (10%)
3	NDP	D	602	-	47,52,52	2.83	6 (12%)	61,80,80	1.66	14 (22%)
3	NDP	C	602	-	47,52,52	2.82	6 (12%)	61,80,80	1.76	14 (22%)
2	HEM	B	601	1	42,50,50	2.02	7 (16%)	46,82,82	1.44	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	D	601	1	42,50,50	1.87	6 (14%)	46,82,82	1.52	10 (21%)

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
2	HEM	C	601	1	-	2/12/54/54	-
3	NDP	A	602	-	-	10/30/77/77	0/5/5/5
3	NDP	B	602	-	-	11/30/77/77	0/5/5/5
2	HEM	A	601	1	-	5/12/54/54	-
3	NDP	D	602	-	-	10/30/77/77	0/5/5/5
3	NDP	C	602	-	-	12/30/77/77	0/5/5/5
2	HEM	B	601	1	-	5/12/54/54	-
2	HEM	D	601	1	-	2/12/54/54	-

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	NDP	P2B-O2B	15.91	1.87	1.59
3	D	602	NDP	P2B-O2B	15.81	1.87	1.59
3	A	602	NDP	P2B-O2B	14.37	1.84	1.59
3	B	602	NDP	P2B-O2B	13.82	1.83	1.59
2	B	601	HEM	C3D-C2D	8.55	1.55	1.36

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	NDP	C4B-O4B-C1B	-6.37	104.09	109.92
3	C	602	NDP	C4B-O4B-C1B	-5.79	104.63	109.92
2	C	601	HEM	C4D-ND-C1D	5.76	112.03	105.21
2	A	601	HEM	C4D-ND-C1D	5.37	111.57	105.21
3	D	602	NDP	C4B-O4B-C1B	-5.25	105.11	109.92

There are no chirality outliers.

5 of 57 torsion outliers are listed below:

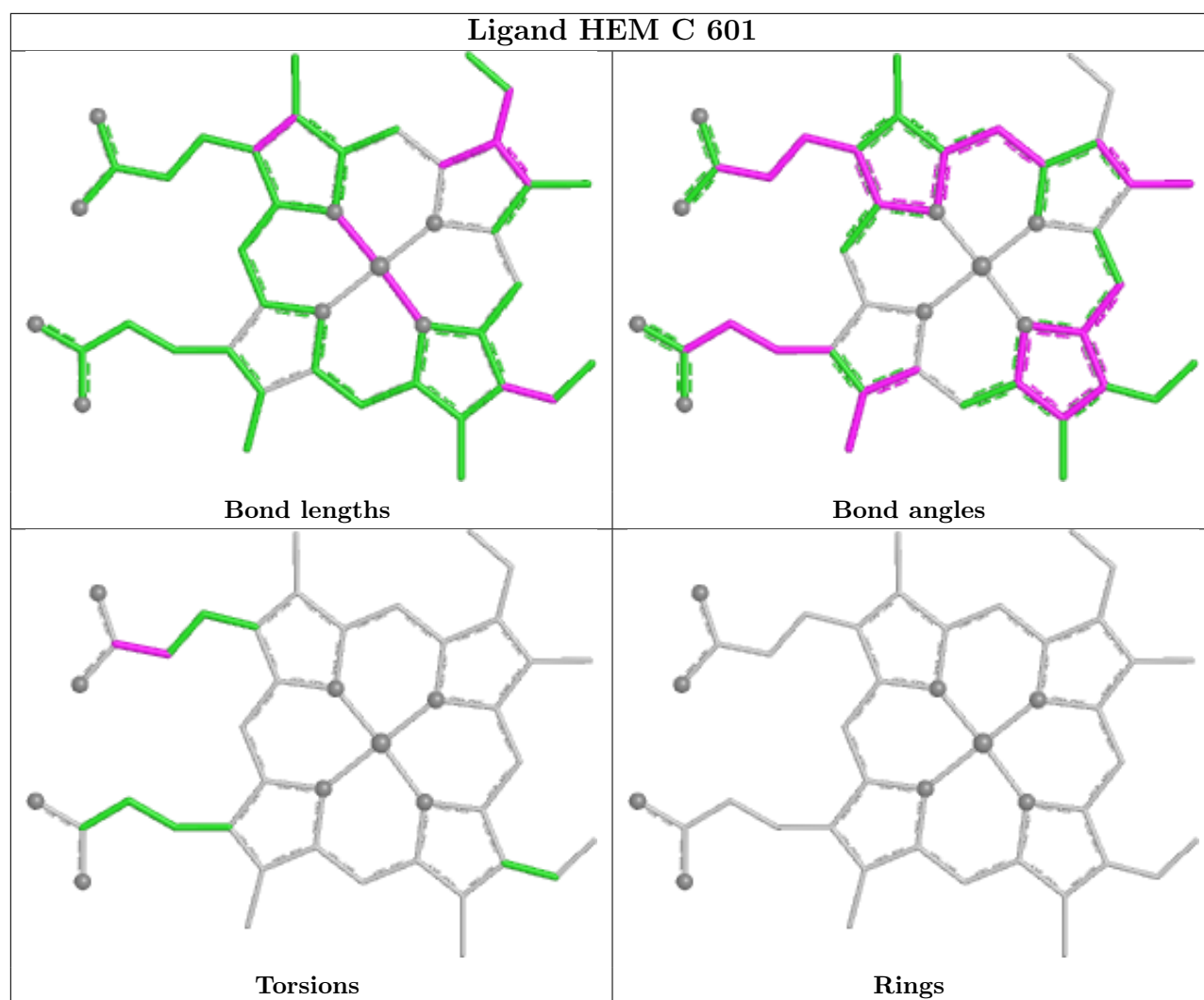
Mol	Chain	Res	Type	Atoms
2	B	601	HEM	C1A-C2A-CAA-CBA
2	B	601	HEM	C3A-C2A-CAA-CBA
2	B	601	HEM	C4D-C3D-CAD-CBD
3	A	602	NDP	C5B-O5B-PA-O3
3	B	602	NDP	C2N-C3N-C7N-N7N

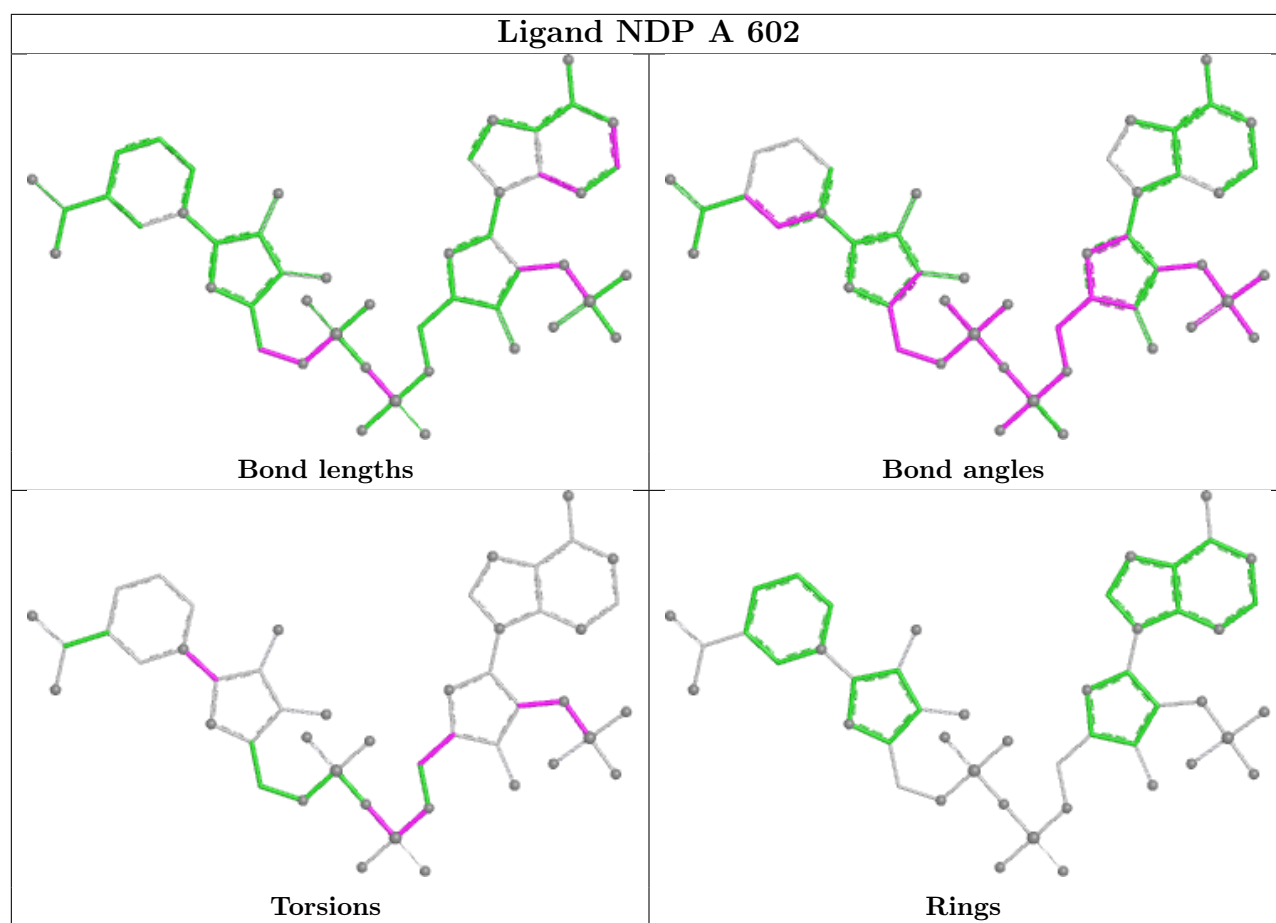
There are no ring outliers.

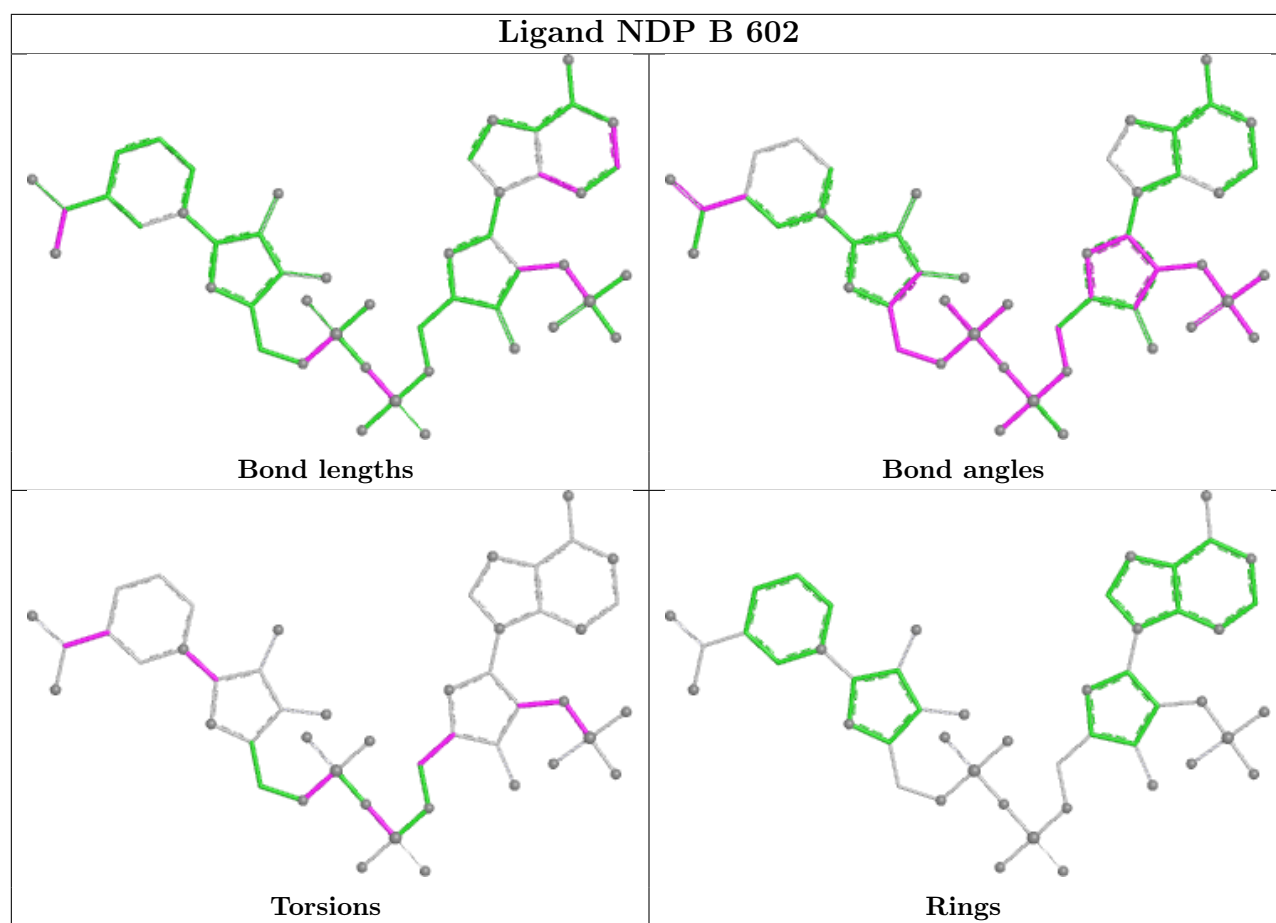
8 monomers are involved in 17 short contacts:

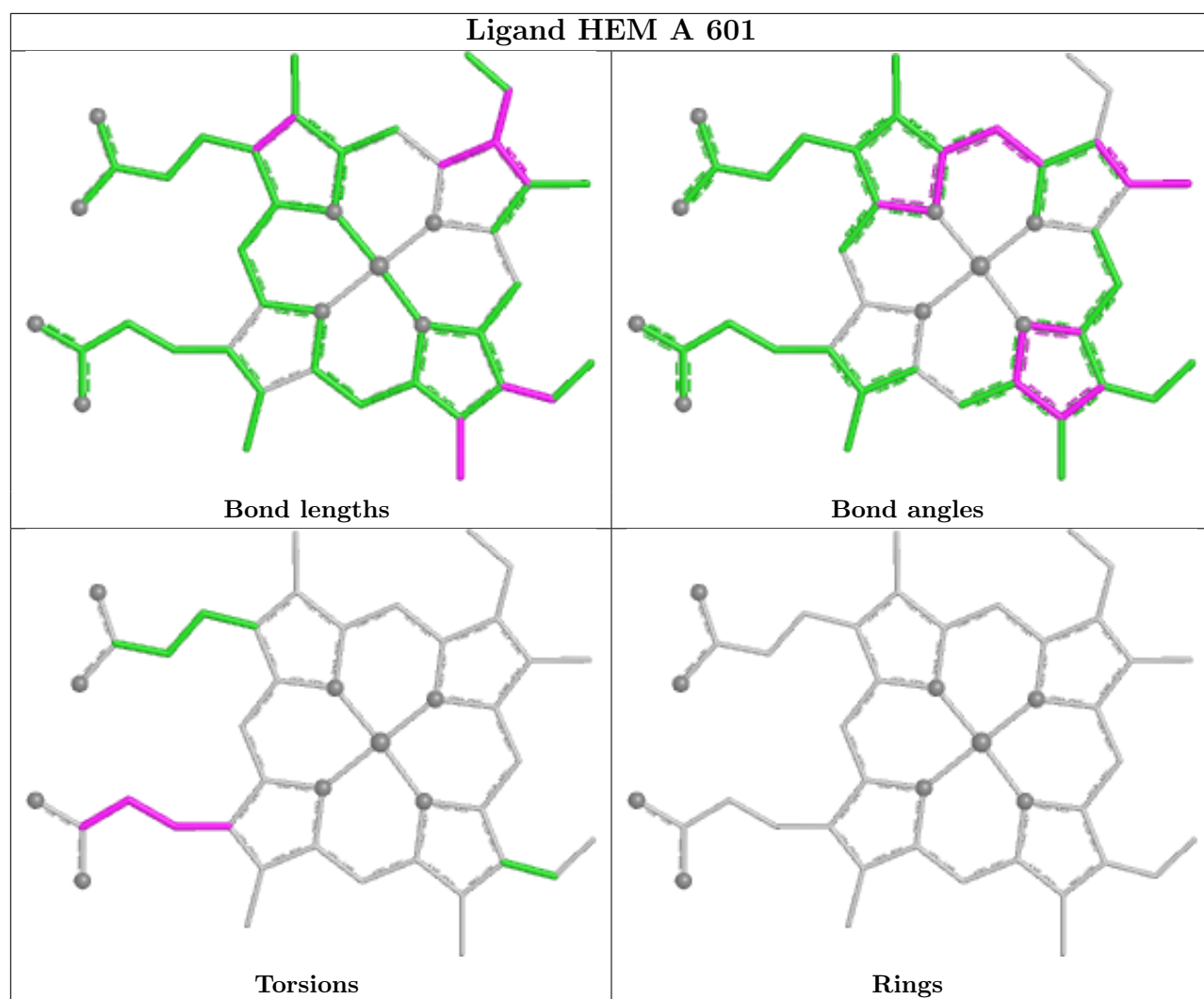
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	HEM	1	0
3	A	602	NDP	2	0
3	B	602	NDP	3	0
2	A	601	HEM	2	0
3	D	602	NDP	1	0
3	C	602	NDP	3	0
2	B	601	HEM	3	0
2	D	601	HEM	2	0

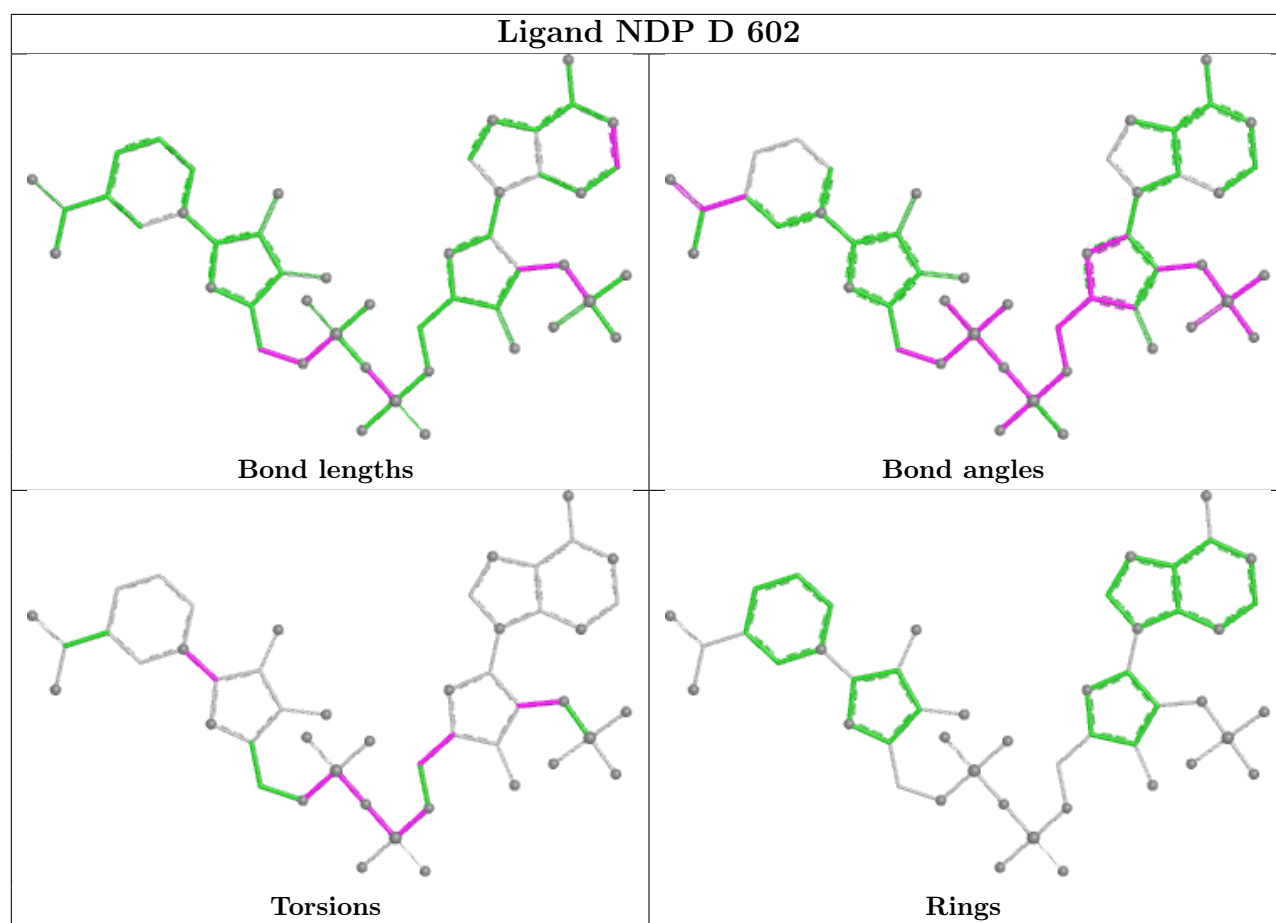
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

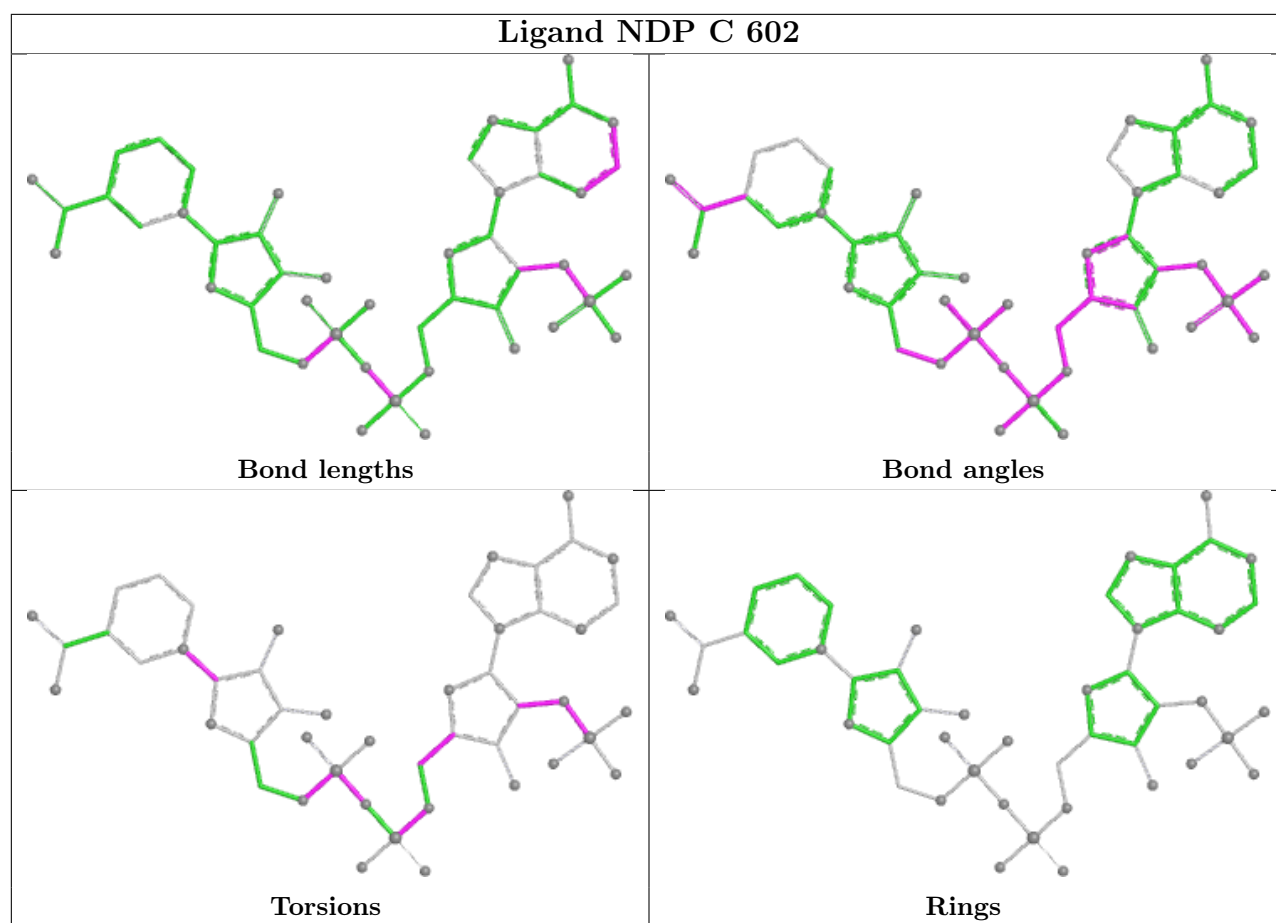


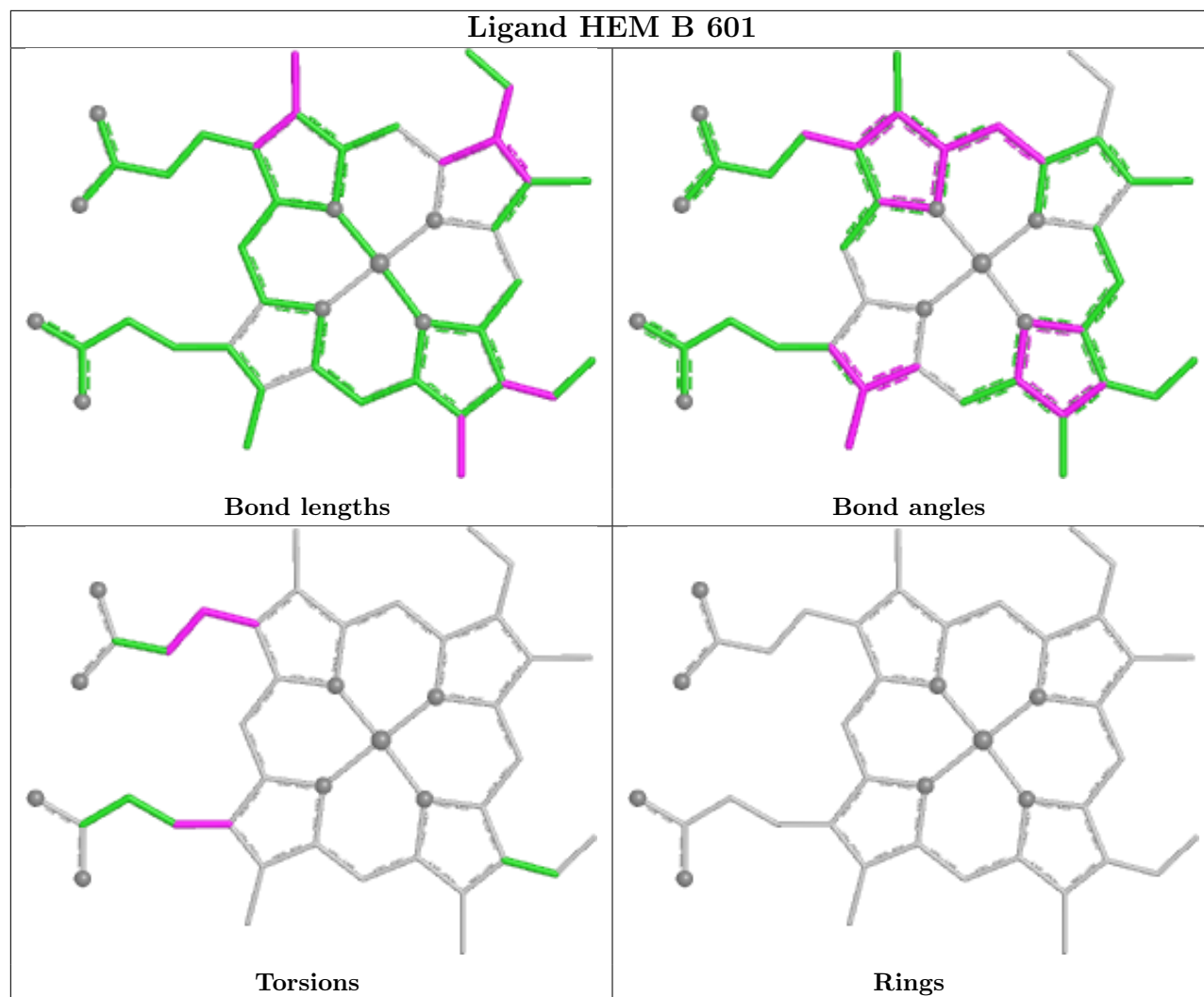


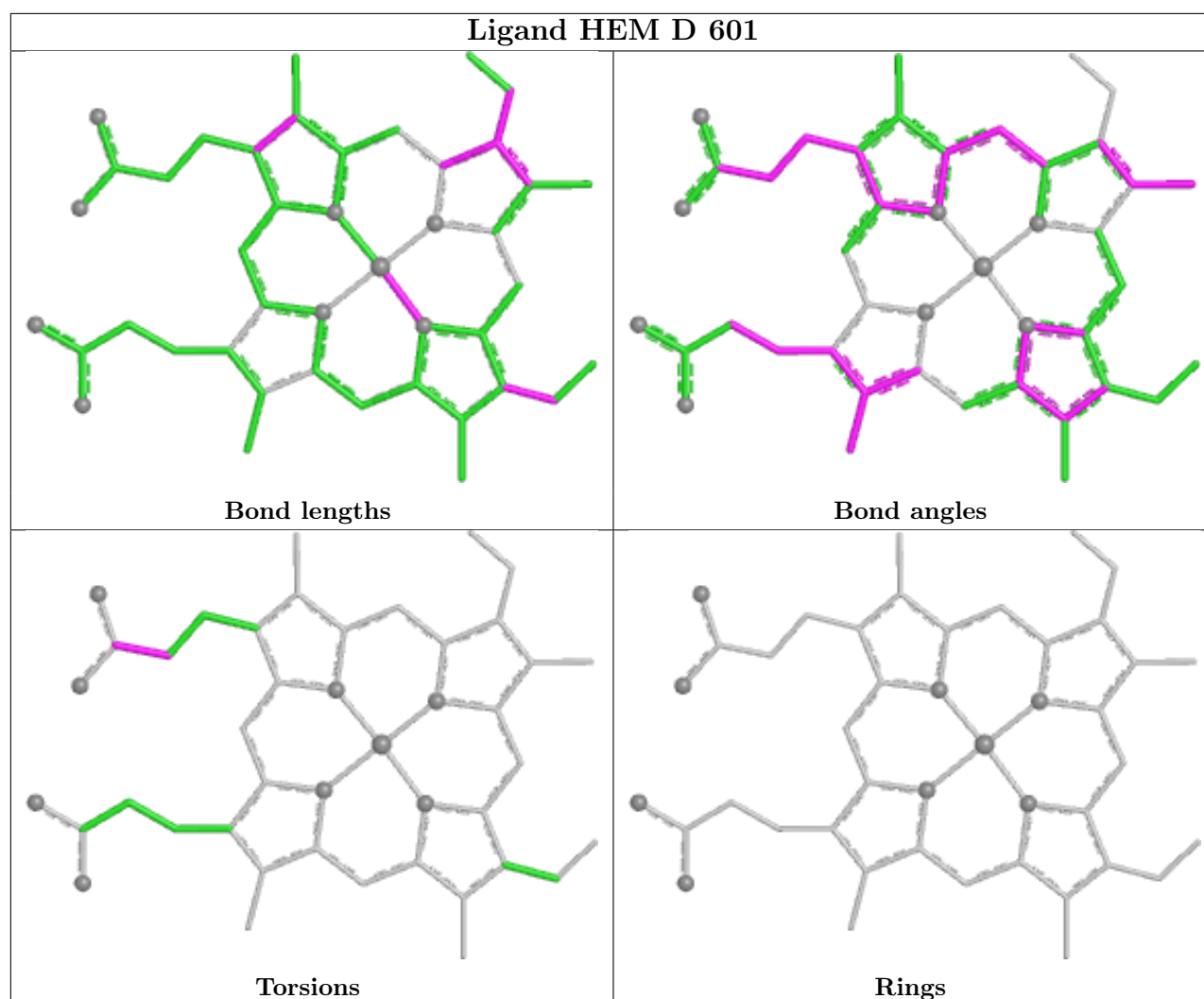












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

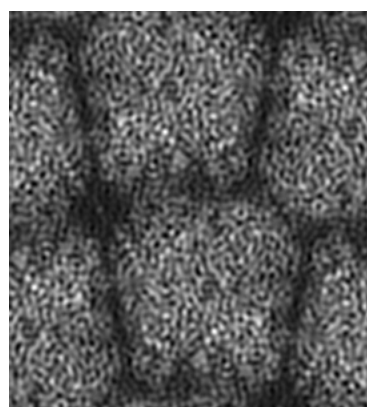
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6314. These allow visual inspection of the internal detail of the map and identification of artifacts.

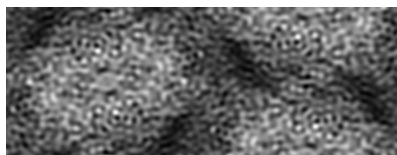
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

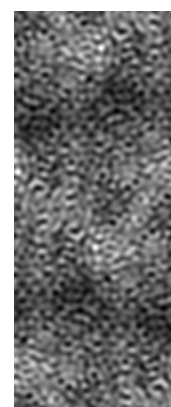
6.1.1 Primary map



X



Y

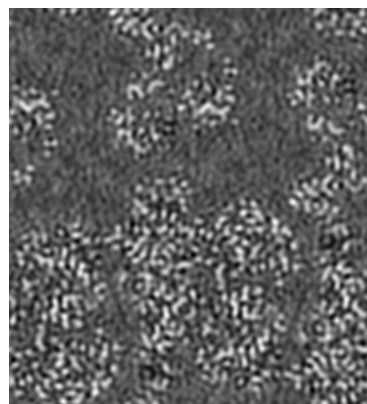


Z

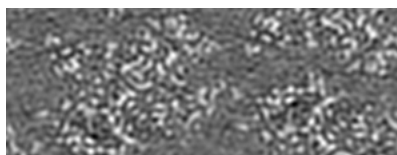
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

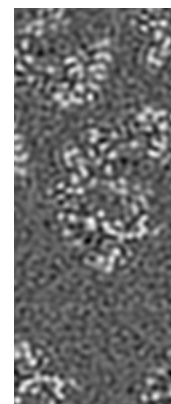
6.2.1 Primary map



X Index: 45



Y Index: 108

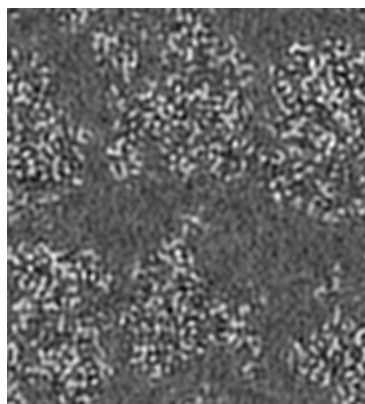


Z Index: 120

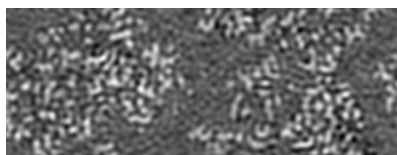
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

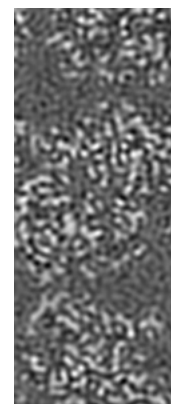
6.3.1 Primary map



X Index: 19



Y Index: 202

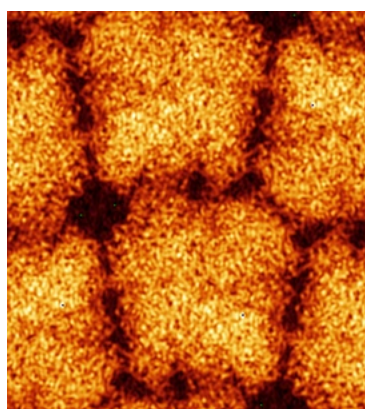


Z Index: 56

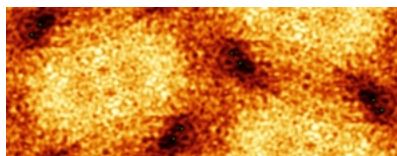
The images above show the largest variance slices of the map in three orthogonal directions.

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

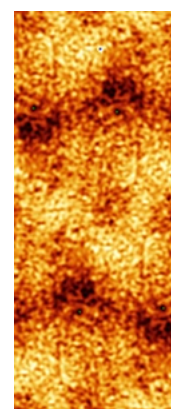
6.4.1 Primary map



X



Y

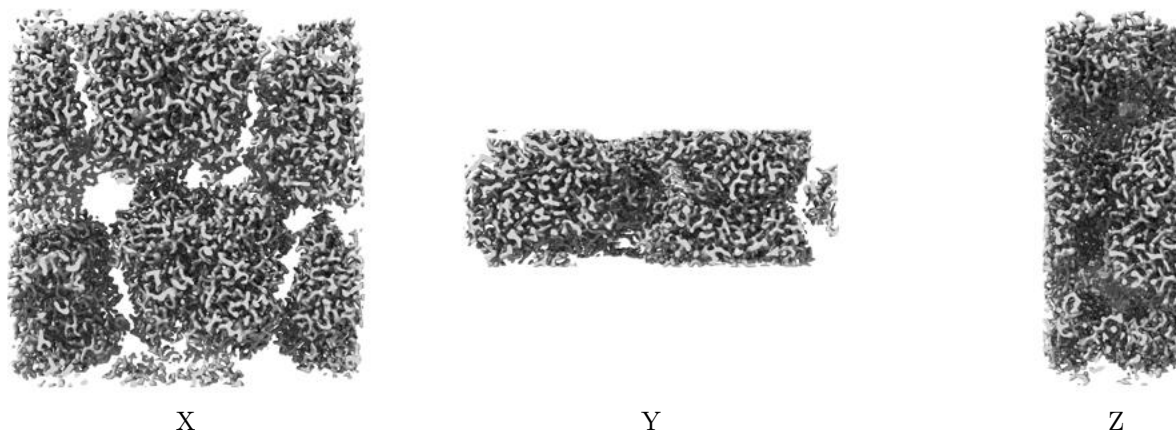


Z

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

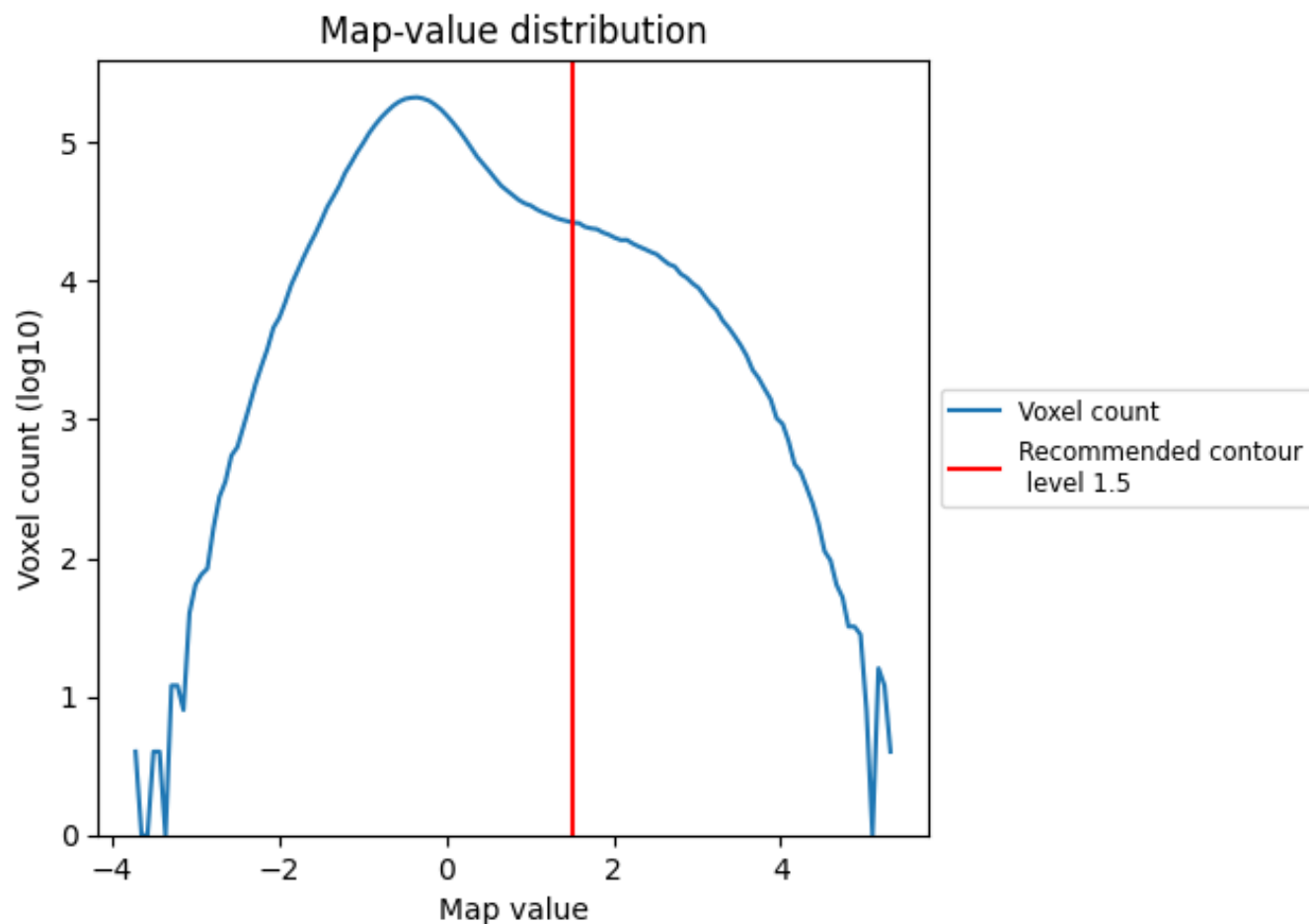
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

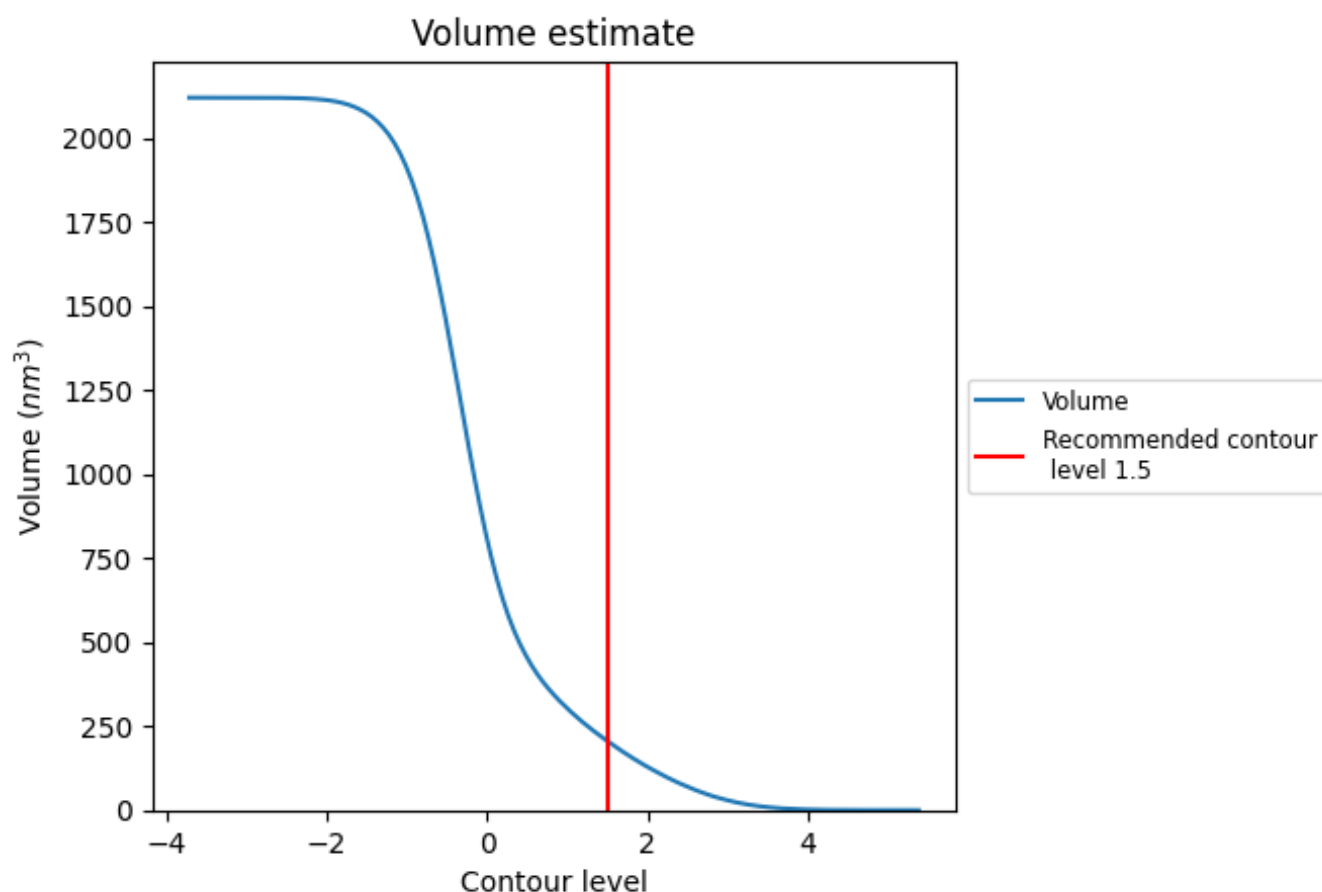
This section contains the results of statistical analysis of the map.

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 206 nm³; this corresponds to an approximate mass of 186 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](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

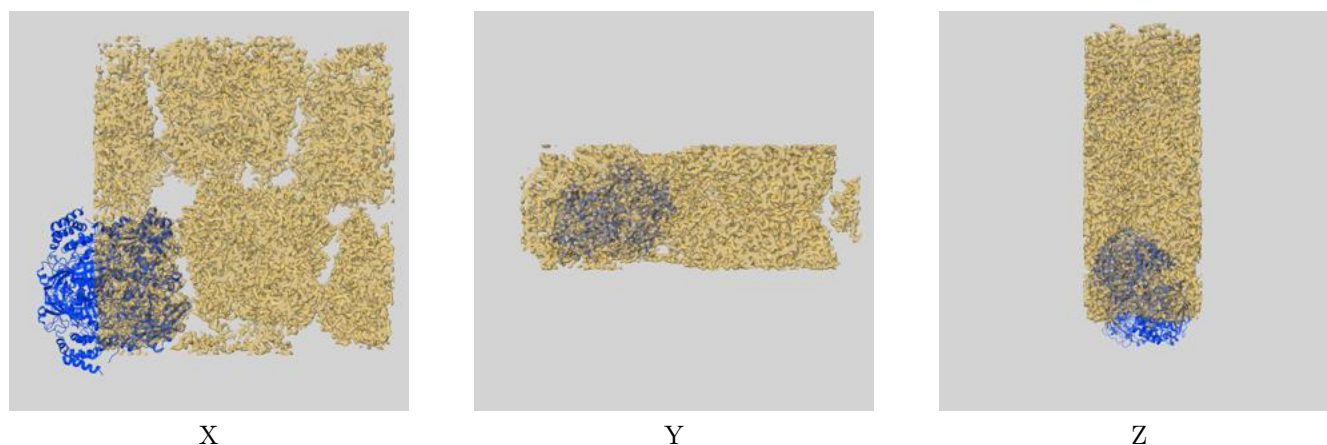
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

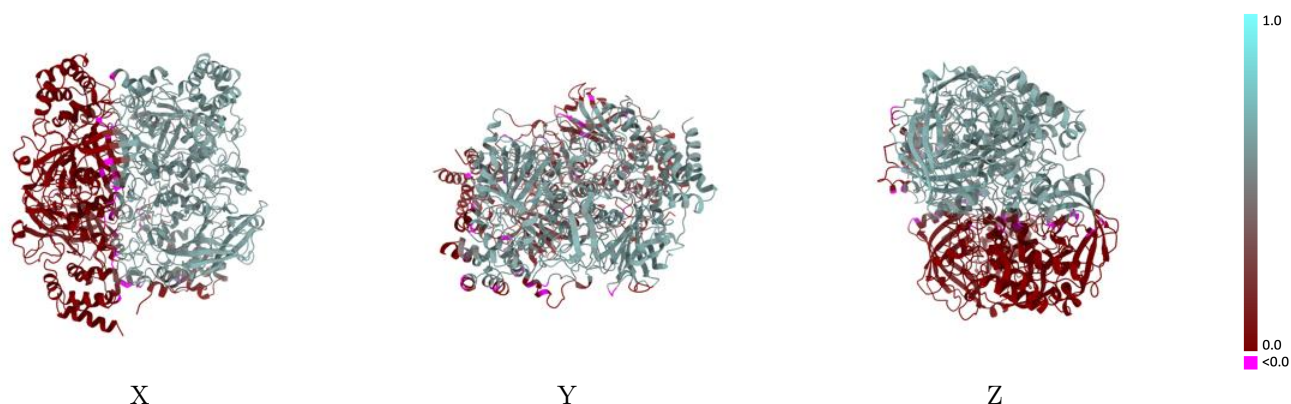
This section contains information regarding the fit between EMDB map EMD-6314 and PDB model 3J7B. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

9.1 Map-model overlay [i](#)



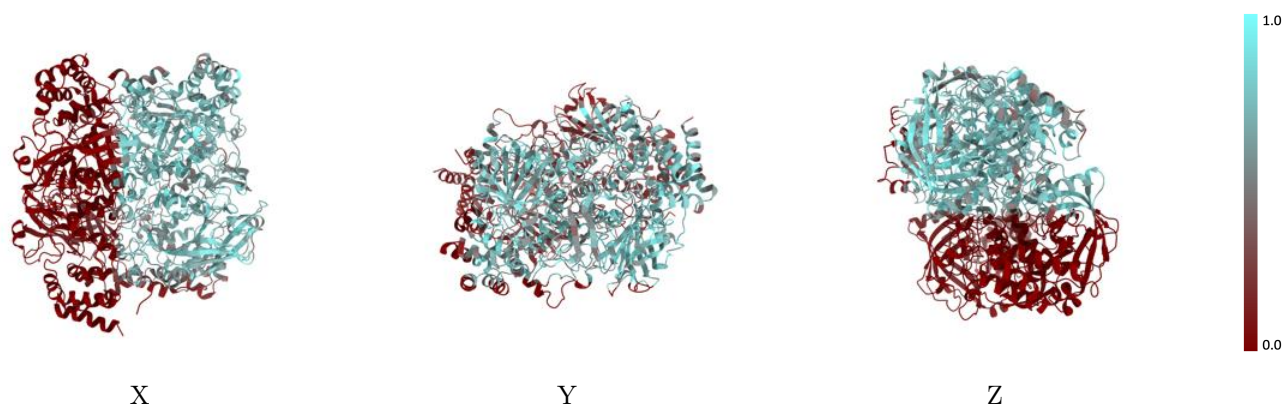
The images above show the 3D surface view of the map at the recommended contour level 1.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



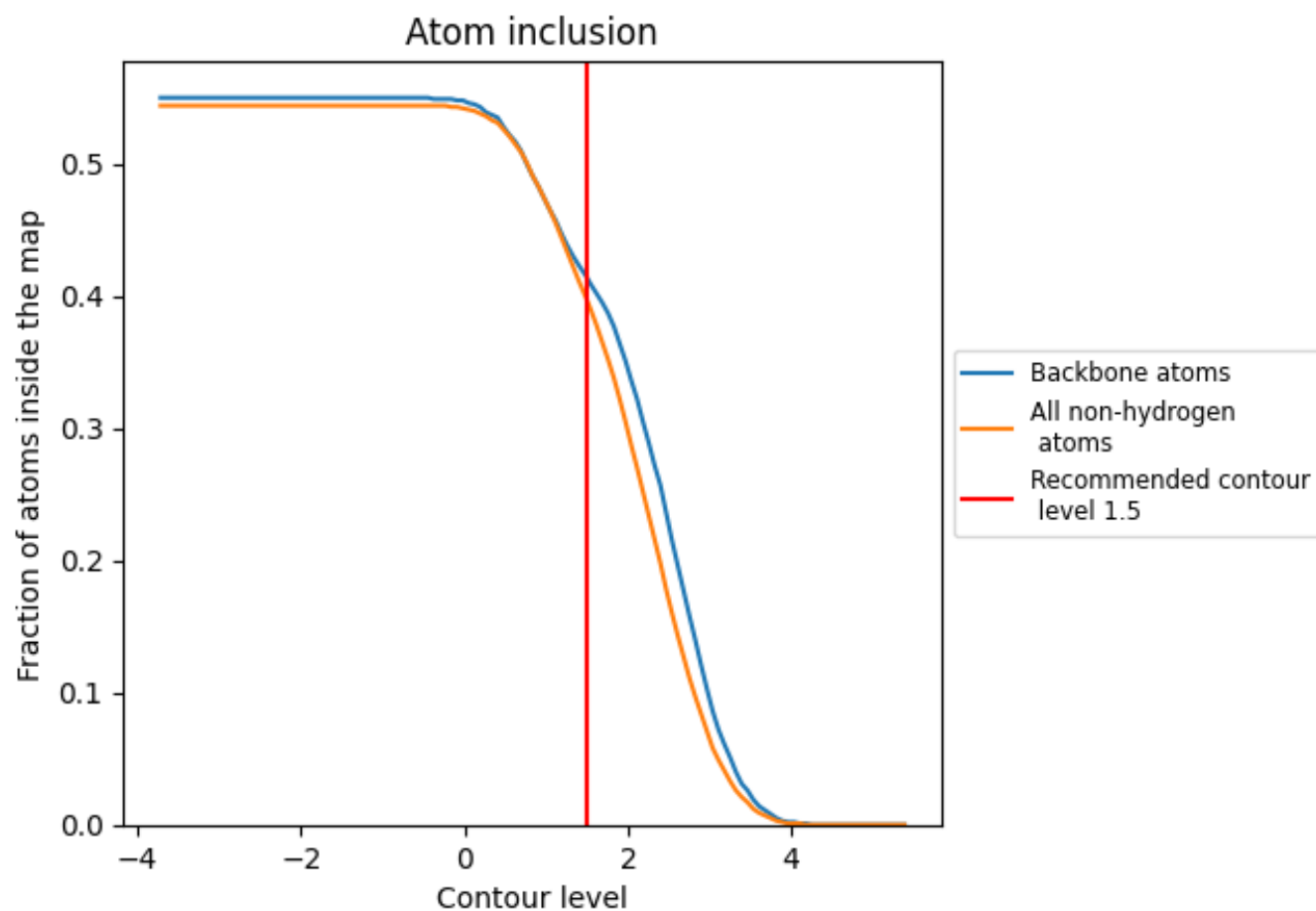
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 41% of all backbone atoms, 40% 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 (1.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.3970	<div></div> 0.3350
A	<div></div> 0.6260	<div></div> 0.5130
B	<div></div> 0.5800	<div></div> 0.4910
C	<div></div> 0.1300	<div></div> 0.1160
D	<div></div> 0.2540	<div></div> 0.2190

