



## Full wwPDB EM Validation Report ⓘ

Dec 16, 2023 – 02:28 PM EST

PDB ID : 8EC6  
EMDB ID : EMD-28013  
Title : Cryo-EM structure of the Glutaminase C core filament (fGAC)  
Authors : Ambrosio, A.L.; Dias, S.M.; Quesnay, J.E.; Portugal, R.V.; Cassago, A.; van Heel, M.G.; Islam, Z.; Rodrigues, C.T.  
Deposited on : 2022-09-01  
Resolution : 3.10 Å(reported)  
Based on initial model : 3SS3

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.dev70  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

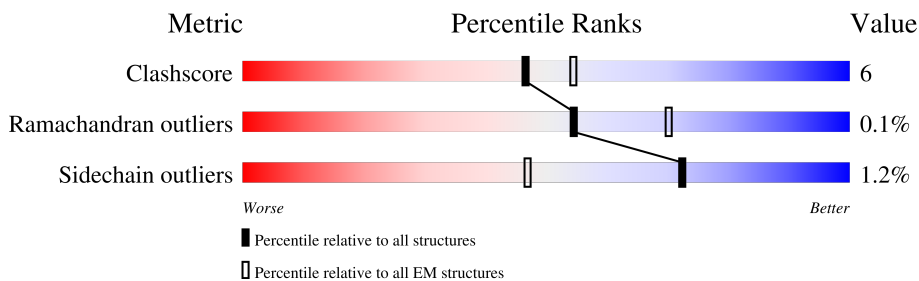
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	479	
1	B	479	
1	C	479	
1	D	479	
1	E	479	
1	F	479	
1	G	479	
1	H	479	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
2	PO4	B	701	-	-	X	-

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 19133 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 Isoform 2 of Glutaminase kidney isoform, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	310	2388	1527	395	443	23	0	0
1	B	310	2388	1527	395	443	23	0	0
1	C	310	2388	1527	395	443	23	0	0
1	D	310	2388	1527	395	443	23	0	0
1	E	309	2377	1518	394	442	23	0	0
1	F	310	2388	1527	395	443	23	0	0
1	G	310	2388	1527	395	443	23	0	0
1	H	310	2388	1527	395	443	23	0	0

There are 24 discrepancies between the modelled and reference sequences:

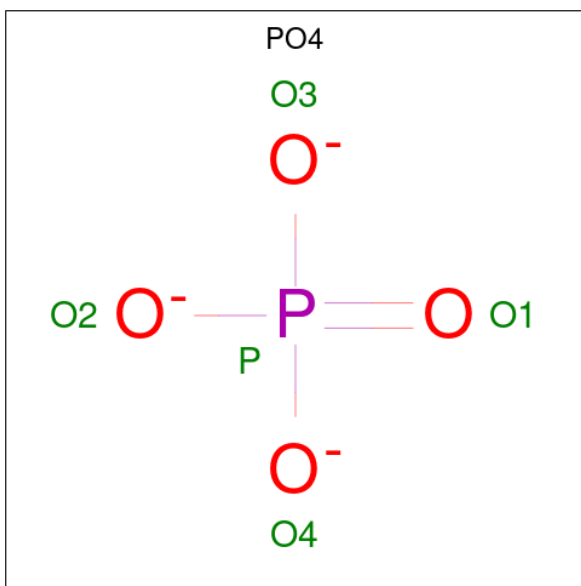
Chain	Residue	Modelled	Actual	Comment	Reference
A	125	GLY	-	expression tag	UNP D3Z7P3-2
A	126	SER	-	expression tag	UNP D3Z7P3-2
A	127	HIS	-	expression tag	UNP D3Z7P3-2
B	125	GLY	-	expression tag	UNP D3Z7P3-2
B	126	SER	-	expression tag	UNP D3Z7P3-2
B	127	HIS	-	expression tag	UNP D3Z7P3-2
C	125	GLY	-	expression tag	UNP D3Z7P3-2
C	126	SER	-	expression tag	UNP D3Z7P3-2
C	127	HIS	-	expression tag	UNP D3Z7P3-2
D	125	GLY	-	expression tag	UNP D3Z7P3-2
D	126	SER	-	expression tag	UNP D3Z7P3-2
D	127	HIS	-	expression tag	UNP D3Z7P3-2
E	125	GLY	-	expression tag	UNP D3Z7P3-2
E	126	SER	-	expression tag	UNP D3Z7P3-2

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Chain	Residue	Modelled	Actual	Comment	Reference
E	127	HIS	-	expression tag	UNP D3Z7P3-2
F	125	GLY	-	expression tag	UNP D3Z7P3-2
F	126	SER	-	expression tag	UNP D3Z7P3-2
F	127	HIS	-	expression tag	UNP D3Z7P3-2
G	125	GLY	-	expression tag	UNP D3Z7P3-2
G	126	SER	-	expression tag	UNP D3Z7P3-2
G	127	HIS	-	expression tag	UNP D3Z7P3-2
H	125	GLY	-	expression tag	UNP D3Z7P3-2
H	126	SER	-	expression tag	UNP D3Z7P3-2
H	127	HIS	-	expression tag	UNP D3Z7P3-2

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
2	A	1	Total	O	P	0
			5	4	1	
2	B	1	Total	O	P	0
			5	4	1	
2	C	1	Total	O	P	0
			5	4	1	
2	D	1	Total	O	P	0
			5	4	1	
2	E	1	Total	O	P	0
			5	4	1	
2	F	1	Total	O	P	0
			5	4	1	

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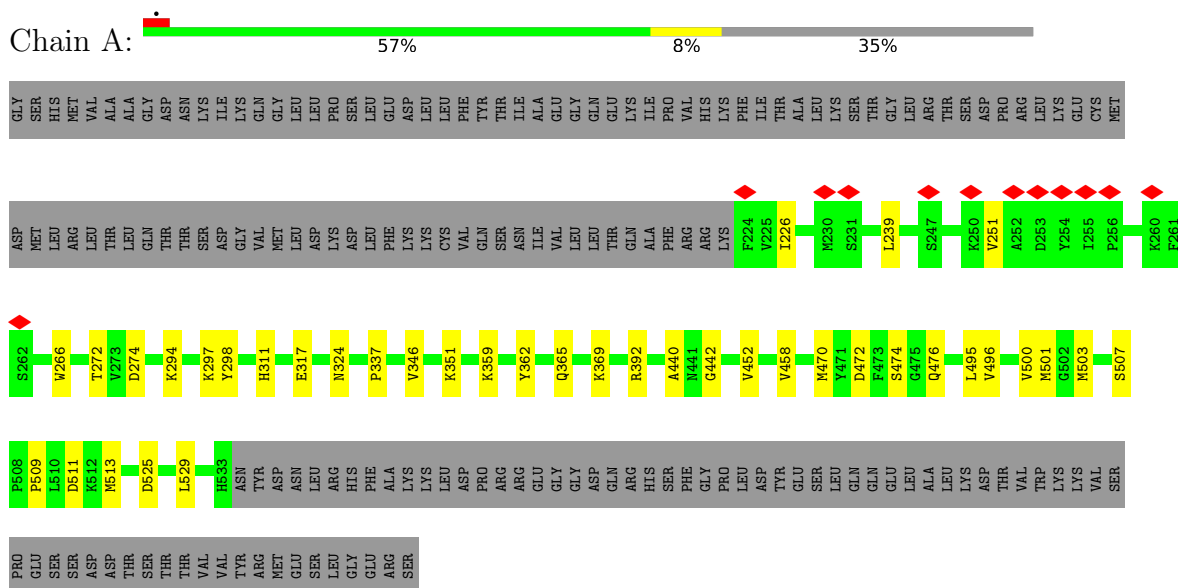
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>			<b>AltConf</b>
2	G	1	Total	O	P	0
			5	4	1	
2	H	1	Total	O	P	0
			5	4	1	

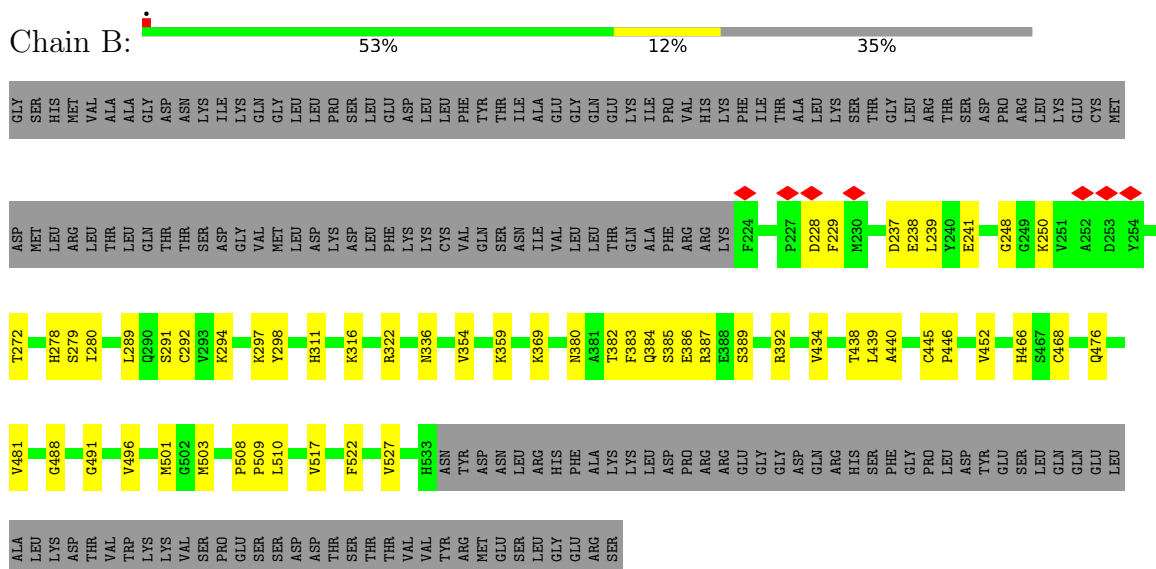
### 3 Residue-property plots [i](#)

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: Isoform 2 of Glutaminase kidney isoform, mitochondrial

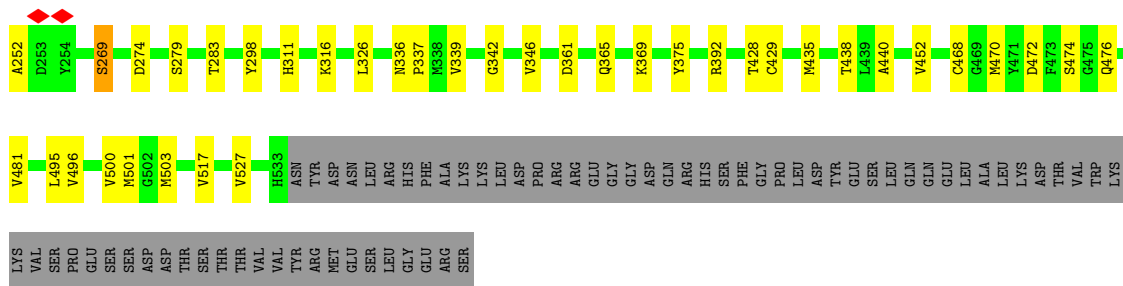


- Molecule 1: Isoform 2 of Glutaminase kidney isoform, mitochondrial

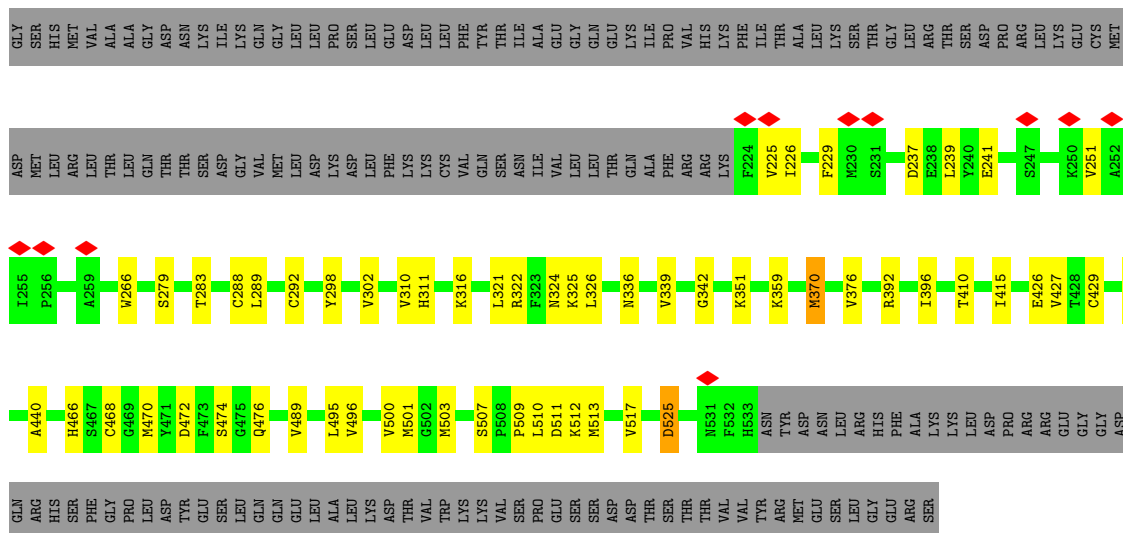




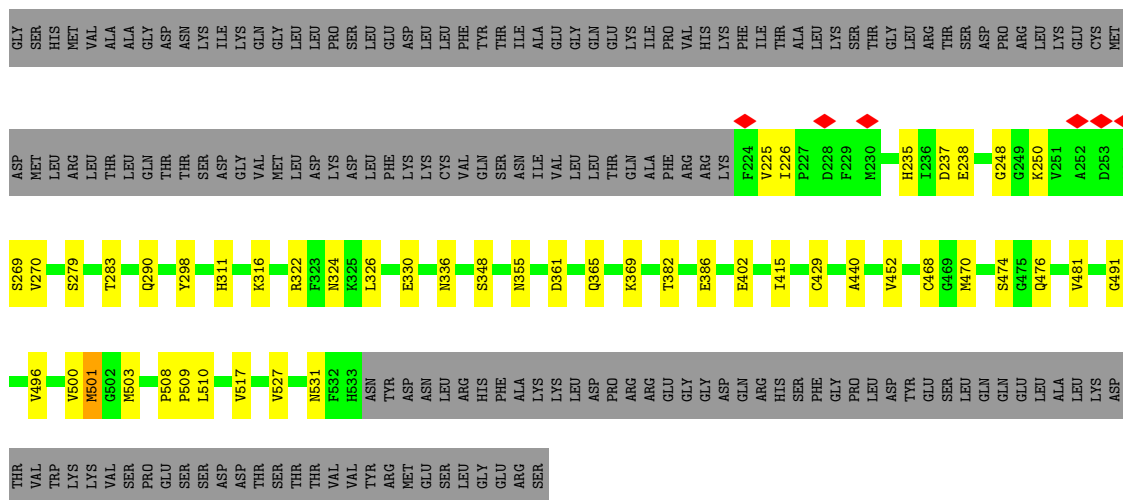




• Molecule 1: Isoform 2 of Glutaminase kidney isoform, mitochondrial



• Molecule 1: Isoform 2 of Glutaminase kidney isoform, mitochondrial



• Molecule 1: Isoform 2 of Glutaminase kidney isoform, mitochondrial



GLY SER HIS MET VAL ALA GLY ASP ASN LYS ILE LYS GLN GLY LEU LEU LEU PRO SER LEU ASP LEU PHE TYR THR THR ILE ALA GLU GLY GLN GLU ILE ILE PRO VAL HIS LYS PHE THR ALA THR LEU LYS SER THR GLY LEU ARG THR ASP PRO ARG LEU LYS GLU CYS MET

ASP MET LEU ARG THR LEU GLN THR SER ASP VAL MET LEU ASP LYS ASP LEU PHE LYS CYS VAL GLN SER ASN ILE VAL LEU LEU THR GLN ALA PHE ARG LYS F224 V225 I226 P227 D228 F229 M230 D237 E238 L239 Y240 E241 K245 Q246 S247 K250 V251 A252

D253 Y254 I255 P256 Q257 L258 A259 F260 F261 S262 W266 V270 D274 E277 L289 Q290 S291 C292 Y298 H311 K316 E317 R322 F323 N324 M336 V339 G342 K369 M370 A371 V376 T382 S385 E386 R392 V427 E430 M435

A440 V452 H466 C468 G469 M470 Y471 D472 F473 S474 G475 Q476 G488 G491 V496 V500 M501 G502 M503 S507 P508 P509 L510 D511 R512 M513 V517 K518 D525 H533 ASN TYR ASP ASN LEU ARG HIS PHE ALA LYS LEU ASP PRO ARG ARG GLY GLY ARG SER

ASP GLN ARG HIS SER PHE GLY PRO LEU ASP TYR GLU SER LEU LEU GLN GLU LEU ALA LEU LYS ASP THR VAL TRP LYS LYS VAL SER PRO GLU SER SER ASP THR THR VAL VAL TYR ARG MET GLU SER LEU GLY ARG ARG SER

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D2	Depositor
Number of particles used	229037	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 ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	8.759	Depositor
Minimum map value	-5.183	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.157	Depositor
Recommended contour level	1.0	Depositor
Map size ( $\text{\AA}$ )	440.0, 440.0, 440.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.1, 1.1, 1.1	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: PO4

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	0.25	0/2447	0.43	0/3309
1	B	0.26	0/2447	0.43	0/3309
1	C	0.26	0/2447	0.44	0/3309
1	D	0.26	0/2447	0.43	0/3309
1	E	0.26	0/2435	0.44	0/3293
1	F	0.25	0/2447	0.43	0/3309
1	G	0.25	0/2447	0.43	0/3309
1	H	0.25	0/2447	0.44	0/3309
All	All	0.26	0/19564	0.43	0/26456

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	2388	0	2333	24	0
1	B	2388	0	2333	33	0
1	C	2388	0	2333	41	0
1	D	2388	0	2333	30	0
1	E	2377	0	2324	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2388	0	2333	33	0
1	G	2388	0	2333	32	0
1	H	2388	0	2333	34	0
2	A	5	0	0	1	0
2	B	5	0	0	2	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	1	0
2	G	5	0	0	1	0
2	H	5	0	0	1	0
All	All	19133	0	18655	244	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 (244) 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:298:TYR:HH	1:A:311:HIS:HE2	1.31	0.79
1:F:500:VAL:HG12	1:F:501:MET:HG2	1.64	0.78
1:C:298:TYR:HH	1:C:311:HIS:HE2	1.30	0.78
1:A:274:ASP:O	1:A:274:ASP:OD1	2.05	0.74
1:F:302:VAL:HG22	1:F:310:VAL:HG11	1.70	0.72
1:H:270:VAL:HG22	1:H:503:MET:HE3	1.73	0.70
1:H:298:TYR:HH	1:H:311:HIS:HE2	1.38	0.69
1:B:248:GLY:HA2	1:B:517:VAL:HG21	1.76	0.68
1:G:500:VAL:HG12	1:G:501:MET:HG2	1.76	0.67
1:F:298:TYR:HH	1:F:311:HIS:HE2	1.41	0.66
1:H:500:VAL:HG12	1:H:501:MET:HG2	1.79	0.65
1:B:336:ASN:ND2	1:B:468:CYS:SG	2.67	0.65
1:C:228:ASP:O	1:C:230:MET:N	2.29	0.65
1:B:278:HIS:CE1	1:B:280:ILE:HD11	2.31	0.65
1:A:324:ASN:O	1:A:392:ARG:NH1	2.31	0.64
1:C:263:PRO:HA	1:C:509:PRO:HD3	1.79	0.64
1:H:228:ASP:OD1	1:H:229:PHE:N	2.30	0.64
1:B:383:PHE:O	1:B:387:ARG:HG3	1.99	0.63
1:G:248:GLY:HA2	1:G:517:VAL:HG21	1.81	0.63
1:F:511:ASP:HB3	1:F:517:VAL:HG12	1.82	0.62
1:H:277:ARG:NH2	1:H:430:GLU:OE2	2.33	0.62
1:H:336:ASN:ND2	1:H:468:CYS:SG	2.73	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:472:ASP:OD1	1:H:472:ASP:N	2.34	0.61
1:D:369:LYS:HD2	1:D:452:VAL:HG23	1.83	0.61
1:A:495:LEU:HD11	1:A:503:MET:HE3	1.81	0.61
1:F:239:LEU:HD22	1:F:525:ASP:HB3	1.83	0.60
1:B:434:VAL:O	1:B:438:THR:HG23	2.01	0.60
1:B:369:LYS:HD2	1:B:452:VAL:HG23	1.85	0.59
1:A:274:ASP:OD1	1:A:274:ASP:C	2.41	0.59
1:C:472:ASP:OD1	1:C:472:ASP:N	2.34	0.59
1:F:336:ASN:ND2	1:F:468:CYS:SG	2.73	0.59
1:G:470:MET:HB2	1:G:474:SER:HA	1.84	0.58
1:G:225:VAL:HG23	1:G:226:ILE:HG12	1.86	0.57
1:G:322:ARG:NH2	2:G:701:PO4:O4	2.37	0.57
1:G:476:GLN:HG3	1:H:316:LYS:HD2	1.86	0.57
1:H:322:ARG:NH2	2:H:701:PO4:O1	2.38	0.56
1:D:336:ASN:ND2	1:D:468:CYS:SG	2.78	0.56
1:B:228:ASP:OD1	1:B:229:PHE:N	2.39	0.56
1:G:361:ASP:O	1:G:365:GLN:HG3	2.06	0.56
1:E:470:MET:HB2	1:E:474:SER:HA	1.88	0.56
1:B:322:ARG:NH2	2:B:701:PO4:O3	2.38	0.55
1:A:470:MET:H	1:A:474:SER:HB3	1.71	0.55
1:G:369:LYS:HD2	1:G:452:VAL:HG23	1.89	0.55
1:C:226:ILE:HD11	1:C:500:VAL:HG13	1.87	0.55
1:G:476:GLN:N	1:H:317:GLU:OE2	2.30	0.55
1:C:317:GLU:OE2	1:D:476:GLN:N	2.35	0.54
1:A:317:GLU:OE2	1:B:476:GLN:N	2.34	0.54
1:C:440:ALA:HB2	1:C:496:VAL:HG13	1.90	0.54
1:C:511:ASP:OD1	1:C:513:MET:HG2	2.08	0.53
1:D:440:ALA:HB2	1:D:496:VAL:HG13	1.89	0.53
1:H:291:SER:HB2	1:H:488:GLY:HA2	1.91	0.53
1:H:369:LYS:HE3	1:H:452:VAL:HG23	1.89	0.53
1:B:385:SER:O	1:B:389:SER:HB3	2.09	0.53
1:A:472:ASP:OD1	1:A:472:ASP:N	2.40	0.53
1:D:248:GLY:HA2	1:D:517:VAL:HG21	1.91	0.52
1:G:330:GLU:N	1:G:330:GLU:OE1	2.38	0.52
1:E:476:GLN:HG3	1:F:316:LYS:HD2	1.90	0.52
1:E:392:ARG:NH1	1:G:402:GLU:OE2	2.43	0.52
1:E:298:TYR:OH	1:E:311:HIS:NE2	2.42	0.52
1:B:440:ALA:HB2	1:B:496:VAL:HG13	1.90	0.51
1:A:239:LEU:HD22	1:A:525:ASP:HB3	1.93	0.51
1:D:370:MET:HG3	1:D:438:THR:HG21	1.92	0.51
1:E:316:LYS:HD2	1:F:476:GLN:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:283:THR:HB	1:G:429:CYS:HB2	1.91	0.51
1:G:440:ALA:HB2	1:G:496:VAL:HG13	1.91	0.51
1:C:229:PHE:O	1:C:233:THR:HG23	2.10	0.51
1:E:225:VAL:HG13	1:E:226:ILE:H	1.76	0.51
1:E:369:LYS:HD2	1:E:452:VAL:HG23	1.92	0.51
1:B:294:LYS:HA	1:B:297:LYS:HD2	1.94	0.50
1:E:225:VAL:N	1:E:274:ASP:OD2	2.45	0.50
1:D:239:LEU:HD22	1:D:525:ASP:HB3	1.93	0.50
1:D:508:PRO:HB2	1:D:509:PRO:HD3	1.93	0.50
1:G:316:LYS:HD2	1:H:476:GLN:HG3	1.92	0.50
1:G:336:ASN:ND2	1:G:468:CYS:SG	2.85	0.50
1:A:369:LYS:HE2	1:A:452:VAL:HG23	1.94	0.49
1:D:481:VAL:HA	1:D:527:VAL:HG21	1.94	0.49
1:A:440:ALA:HB2	1:A:496:VAL:HG13	1.94	0.49
1:E:375:TYR:HD2	1:E:428:THR:HG23	1.77	0.49
1:E:440:ALA:HB2	1:E:496:VAL:HG13	1.94	0.49
1:A:362:TYR:O	1:A:365:GLN:HG3	2.13	0.49
1:B:491:GLY:HA2	1:B:510:LEU:HD21	1.93	0.49
1:F:336:ASN:OD1	1:F:336:ASN:N	2.45	0.49
1:G:322:ARG:NE	1:G:324:ASN:OD1	2.46	0.49
1:B:237:ASP:O	1:B:241:GLU:HG2	2.13	0.48
1:E:241:GLU:OE1	1:E:244:LYS:NZ	2.33	0.48
1:A:476:GLN:HG3	1:B:316:LYS:HD2	1.93	0.48
1:C:246:GLN:OE1	1:C:521:HIS:ND1	2.46	0.48
1:C:442:GLY:HA2	1:C:458:VAL:HG21	1.94	0.48
1:F:289:LEU:HD22	1:F:292:CYS:HB2	1.95	0.48
1:H:336:ASN:OD1	1:H:336:ASN:N	2.46	0.48
1:G:500:VAL:HG12	1:G:501:MET:CG	2.43	0.48
1:H:225:VAL:HG13	1:H:226:ILE:HG12	1.96	0.48
1:G:279:SER:OG	1:G:283:THR:OG1	2.31	0.48
1:A:337:PRO:HB3	1:A:346:VAL:HG21	1.96	0.48
1:C:240:TYR:CE2	1:C:266:TRP:CD1	3.01	0.48
1:E:336:ASN:ND2	1:E:468:CYS:SG	2.87	0.48
1:G:270:VAL:HG22	1:G:503:MET:HE3	1.94	0.48
1:G:481:VAL:HA	1:G:527:VAL:HG21	1.96	0.48
1:D:278:HIS:CE1	1:D:280:ILE:HD11	2.49	0.48
1:E:481:VAL:HA	1:E:527:VAL:HG21	1.95	0.48
1:D:298:TYR:OH	1:D:311:HIS:NE2	2.47	0.47
1:F:472:ASP:OD1	1:F:472:ASP:N	2.47	0.47
1:C:279:SER:HB3	1:C:283:THR:HG21	1.96	0.47
1:C:337:PRO:HB3	1:C:346:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:470:MET:HB2	1:D:474:SER:HA	1.95	0.47
1:E:228:ASP:C	1:E:230:MET:H	2.18	0.47
1:A:392:ARG:NH2	2:A:701:PO4:O4	2.43	0.47
1:A:511:ASP:OD1	1:A:513:MET:HG2	2.14	0.47
1:F:266:TRP:CE3	1:F:507:SER:HB2	2.49	0.47
1:C:362:TYR:O	1:C:365:GLN:HG3	2.14	0.47
1:D:250:LYS:H	1:D:250:LYS:HD2	1.80	0.47
1:G:290:GLN:NE2	1:G:386:GLU:OE2	2.46	0.47
1:H:440:ALA:HB2	1:H:496:VAL:HG13	1.96	0.47
1:F:440:ALA:HB2	1:F:496:VAL:HG13	1.96	0.47
1:E:495:LEU:HD11	1:E:503:MET:SD	2.55	0.47
1:H:289:LEU:HD22	1:H:292:CYS:HB2	1.97	0.47
1:F:470:MET:HB2	1:F:474:SER:HA	1.97	0.46
1:C:470:MET:HB2	1:C:474:SER:HA	1.96	0.46
1:B:354:VAL:O	1:B:359:LYS:HE3	2.16	0.46
1:H:266:TRP:CE3	1:H:507:SER:HB2	2.51	0.46
1:H:376:VAL:HG22	1:H:427:VAL:HG12	1.98	0.46
1:G:298:TYR:OH	1:G:311:HIS:NE2	2.41	0.46
1:E:326:LEU:HD13	1:G:326:LEU:HD23	1.99	0.45
1:B:298:TYR:OH	1:B:311:HIS:NE2	2.49	0.45
1:B:392:ARG:NH2	2:B:701:PO4:O1	2.49	0.45
1:D:495:LEU:HD11	1:D:503:MET:SD	2.56	0.45
1:G:330:GLU:H	1:G:330:GLU:CD	2.16	0.45
1:B:508:PRO:HB2	1:B:509:PRO:HD3	1.99	0.45
1:D:235:HIS:O	1:D:238:GLU:HG2	2.17	0.45
1:F:321:LEU:HD13	1:F:325:LYS:HD2	1.99	0.45
1:G:508:PRO:HB2	1:G:509:PRO:HD3	1.99	0.45
1:H:324:ASN:O	1:H:392:ARG:NH2	2.50	0.45
1:C:257:GLN:HG3	1:C:385:SER:OG	2.18	0.44
1:H:339:VAL:HG23	1:H:342:GLY:H	1.82	0.44
1:D:330:GLU:CD	1:D:330:GLU:H	2.20	0.44
1:A:503:MET:HE2	1:A:503:MET:HB2	1.79	0.44
1:B:438:THR:HG22	1:B:445:CYS:HA	1.99	0.44
1:D:351:LYS:HB3	1:D:359:LYS:HG2	1.99	0.44
1:F:279:SER:HB3	1:F:283:THR:HG21	1.99	0.44
1:C:470:MET:H	1:C:474:SER:HB3	1.83	0.44
1:F:288:CYS:HA	1:F:426:GLU:HA	1.99	0.44
1:F:410:THR:HB	1:F:415:ILE:HD11	1.99	0.44
1:A:294:LYS:HA	1:A:297:LYS:HG2	2.00	0.44
1:B:503:MET:HE1	1:B:522:PHE:HE1	1.82	0.44
1:E:435:MET:O	1:E:438:THR:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:376:VAL:HG22	1:F:427:VAL:HG12	1.99	0.44
1:H:237:ASP:O	1:H:241:GLU:HG2	2.18	0.44
1:H:511:ASP:HB3	1:H:517:VAL:HG12	2.00	0.44
1:C:392:ARG:NH2	2:C:701:PO4:O2	2.40	0.44
1:F:503:MET:HE2	1:F:503:MET:HB2	1.79	0.44
1:G:348:SER:HA	1:G:415:ILE:HD12	2.00	0.44
1:A:251:VAL:HG22	1:A:509:PRO:HA	2.00	0.43
1:C:258:LEU:HA	1:C:261:PHE:CE1	2.53	0.43
1:G:531:ASN:OD1	1:G:531:ASN:N	2.47	0.43
1:B:291:SER:HB2	1:B:488:GLY:HA2	2.00	0.43
1:C:495:LEU:HG	1:C:503:MET:HB2	1.99	0.43
1:H:508:PRO:HB2	1:H:509:PRO:HD3	2.00	0.43
1:F:326:LEU:HD21	1:F:396:ILE:HA	1.99	0.43
1:F:339:VAL:HG23	1:F:342:GLY:H	1.83	0.43
1:H:382:THR:O	1:H:386:GLU:HG3	2.17	0.43
1:C:225:VAL:HG13	1:C:226:ILE:CD1	2.49	0.43
1:H:470:MET:HB2	1:H:474:SER:HA	2.01	0.43
1:G:382:THR:O	1:G:386:GLU:HG3	2.19	0.43
1:C:266:TRP:CE3	1:C:507:SER:HB2	2.53	0.43
1:E:279:SER:HB2	1:E:283:THR:HG21	2.00	0.43
1:F:495:LEU:HD11	1:F:503:MET:HE3	2.00	0.43
1:C:294:LYS:HA	1:C:297:LYS:HG2	2.00	0.43
1:D:354:VAL:O	1:D:359:LYS:HE3	2.19	0.43
1:F:351:LYS:O	1:F:359:LYS:HE2	2.19	0.43
1:G:491:GLY:HA2	1:G:510:LEU:HD21	2.01	0.43
1:H:371:ALA:HB2	1:H:435:MET:HE2	2.00	0.43
1:D:290:GLN:NE2	1:D:386:GLU:OE2	2.47	0.43
1:C:269:SER:HB2	1:C:429:CYS:HB3	2.01	0.43
1:C:339:VAL:HG23	1:C:342:GLY:H	1.84	0.43
1:E:235:HIS:O	1:E:238:GLU:HG2	2.19	0.43
1:H:491:GLY:HA2	1:H:510:LEU:HD21	2.01	0.43
1:C:263:PRO:HA	1:C:509:PRO:CD	2.46	0.42
1:C:229:PHE:CE1	1:C:276:GLN:HB3	2.53	0.42
1:D:233:THR:HG22	1:D:278:HIS:ND1	2.34	0.42
1:F:251:VAL:HG22	1:F:509:PRO:HA	2.01	0.42
1:C:489:VAL:O	1:C:510:LEU:HD11	2.19	0.42
1:F:322:ARG:NH2	2:F:701:PO4:O1	2.50	0.42
1:B:383:PHE:CZ	1:B:387:ARG:HD2	2.54	0.42
1:C:376:VAL:HG22	1:C:427:VAL:HG12	2.01	0.42
1:F:266:TRP:HE3	1:F:507:SER:HB2	1.85	0.42
1:A:266:TRP:CE3	1:A:507:SER:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:THR:HG22	1:B:446:PRO:HD2	2.02	0.42
1:C:382:THR:O	1:C:386:GLU:HG3	2.19	0.42
1:D:503:MET:HE1	1:D:522:PHE:HE2	1.85	0.42
1:E:361:ASP:O	1:E:365:GLN:HG3	2.19	0.42
1:H:266:TRP:HE3	1:H:507:SER:HB2	1.83	0.42
1:A:226:ILE:HG21	1:A:272:THR:HG21	2.02	0.42
1:C:270:VAL:HG22	1:C:503:MET:CE	2.50	0.42
1:E:337:PRO:HB3	1:E:346:VAL:HG21	2.00	0.42
1:F:489:VAL:O	1:F:510:LEU:HD11	2.20	0.42
1:B:272:THR:HA	1:B:501:MET:HB2	2.02	0.42
1:F:237:ASP:O	1:F:241:GLU:HG2	2.19	0.42
1:C:258:LEU:HA	1:C:261:PHE:HE1	1.85	0.41
1:E:248:GLY:HA3	1:E:517:VAL:HG21	2.02	0.41
1:A:351:LYS:O	1:A:359:LYS:HE2	2.20	0.41
1:B:239:LEU:HB3	1:B:522:PHE:CE2	2.55	0.41
1:C:237:ASP:O	1:C:241:GLU:HG2	2.21	0.41
1:G:250:LYS:HB2	1:G:250:LYS:HE2	1.85	0.41
1:B:439:LEU:HD23	1:B:439:LEU:HA	1.88	0.41
1:D:370:MET:HG2	1:D:435:MET:HG2	2.01	0.41
1:E:500:VAL:HG12	1:E:501:MET:HG2	2.03	0.41
1:G:235:HIS:O	1:G:238:GLU:HG2	2.20	0.41
1:H:239:LEU:HD22	1:H:525:ASP:HB3	2.02	0.41
1:C:476:GLN:HG3	1:D:316:LYS:HD2	2.02	0.41
1:D:291:SER:HB2	1:D:488:GLY:HA2	2.03	0.41
1:B:481:VAL:HA	1:B:527:VAL:HG21	2.01	0.41
1:C:308:GLU:HG2	1:C:309:TYR:N	2.36	0.41
1:E:237:ASP:O	1:E:241:GLU:HG2	2.21	0.41
1:G:355:ASN:OD1	1:G:355:ASN:N	2.44	0.41
1:B:250:LYS:HE2	1:B:250:LYS:HB2	1.82	0.41
1:B:380:ASN:O	1:B:384:GLN:HG2	2.21	0.41
1:B:382:THR:O	1:B:386:GLU:HG3	2.20	0.41
1:D:272:THR:HA	1:D:501:MET:HB2	2.02	0.41
1:F:225:VAL:HG13	1:F:226:ILE:HG22	2.03	0.41
1:C:351:LYS:O	1:C:359:LYS:HE2	2.21	0.41
1:E:250:LYS:HE2	1:E:250:LYS:HB2	1.75	0.41
1:F:324:ASN:O	1:F:392:ARG:NH2	2.53	0.41
1:F:370:MET:HG2	1:F:435:MET:HG3	2.03	0.41
1:H:241:GLU:O	1:H:245:LYS:HE2	2.20	0.41
1:H:257:GLN:HG3	1:H:385:SER:OG	2.20	0.41
1:C:298:TYR:OH	1:C:311:HIS:NE2	2.34	0.41
1:C:324:ASN:O	1:C:392:ARG:NH2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:383:PHE:CZ	1:D:387:ARG:HD2	2.57	0.41
1:D:289:LEU:HD22	1:D:292:CYS:HB2	2.03	0.40
1:H:517:VAL:CG2	1:H:518:LYS:N	2.84	0.40
1:C:411:ASP:O	1:C:415:ILE:HG12	2.21	0.40
1:D:376:VAL:HG22	1:D:427:VAL:HG12	2.02	0.40
1:D:401:LYS:HD3	1:D:412:MET:HB2	2.03	0.40
1:B:279:SER:C	1:B:280:ILE:HD12	2.42	0.40
1:D:439:LEU:HD23	1:D:439:LEU:HA	1.92	0.40
1:A:442:GLY:HA2	1:A:458:VAL:HG21	2.03	0.40
1:E:269:SER:HB2	1:E:429:CYS:HB3	2.04	0.40
1:E:339:VAL:HG23	1:E:342:GLY:H	1.87	0.40
1:F:283:THR:HB	1:F:429:CYS:HB2	2.04	0.40
1:A:500:VAL:HG12	1:A:501:MET:HB2	2.03	0.40
1:B:289:LEU:HD22	1:B:292:CYS:HB2	2.03	0.40
1:C:283:THR:HB	1:C:429:CYS:HB2	2.03	0.40
1:E:472:ASP:N	1:E:472:ASP:OD1	2.54	0.40
1:H:517:VAL:HG23	1:H:518:LYS:N	2.36	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	308/479 (64%)	289 (94%)	19 (6%)	0	100	100
1	B	308/479 (64%)	291 (94%)	17 (6%)	0	100	100
1	C	308/479 (64%)	287 (93%)	20 (6%)	1 (0%)	41	73
1	D	308/479 (64%)	290 (94%)	17 (6%)	1 (0%)	41	73
1	E	307/479 (64%)	291 (95%)	15 (5%)	1 (0%)	41	73
1	F	308/479 (64%)	287 (93%)	21 (7%)	0	100	100
1	G	308/479 (64%)	291 (94%)	17 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	308/479 (64%)	293 (95%)	15 (5%)	0	100	100
All	All	2463/3832 (64%)	2319 (94%)	141 (6%)	3 (0%)	54	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	229	PHE
1	D	225	VAL
1	E	252	ALA

### 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	263/415 (63%)	262 (100%)	1 (0%)	91	96
1	B	263/415 (63%)	261 (99%)	2 (1%)	81	92
1	C	263/415 (63%)	258 (98%)	5 (2%)	57	81
1	D	263/415 (63%)	262 (100%)	1 (0%)	91	96
1	E	262/415 (63%)	259 (99%)	3 (1%)	73	89
1	F	263/415 (63%)	257 (98%)	6 (2%)	50	77
1	G	263/415 (63%)	260 (99%)	3 (1%)	73	89
1	H	263/415 (63%)	258 (98%)	5 (2%)	57	81
All	All	2103/3320 (63%)	2077 (99%)	26 (1%)	72	88

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	529	LEU
1	B	238	GLU
1	B	466	HIS
1	C	238	GLU
1	C	269	SER

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Mol	Chain	Res	Type
1	C	391	ASP
1	C	511	ASP
1	C	529	LEU
1	D	466	HIS
1	E	229	PHE
1	E	250	LYS
1	E	269	SER
1	F	229	PHE
1	F	370	MET
1	F	466	HIS
1	F	512	LYS
1	F	513	MET
1	F	525	ASP
1	G	237	ASP
1	G	269	SER
1	G	501	MET
1	H	274	ASP
1	H	466	HIS
1	H	472	ASP
1	H	501	MET
1	H	513	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	246	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

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	PO4	F	701	-	4,4,4	0.94	0	6,6,6	0.43	0
2	PO4	G	701	-	4,4,4	0.92	0	6,6,6	0.43	0
2	PO4	A	701	-	4,4,4	0.92	0	6,6,6	0.43	0
2	PO4	E	701	-	4,4,4	0.93	0	6,6,6	0.42	0
2	PO4	C	701	-	4,4,4	0.93	0	6,6,6	0.43	0
2	PO4	B	701	-	4,4,4	0.94	0	6,6,6	0.43	0
2	PO4	D	701	-	4,4,4	0.93	0	6,6,6	0.44	0
2	PO4	H	701	-	4,4,4	0.92	0	6,6,6	0.43	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

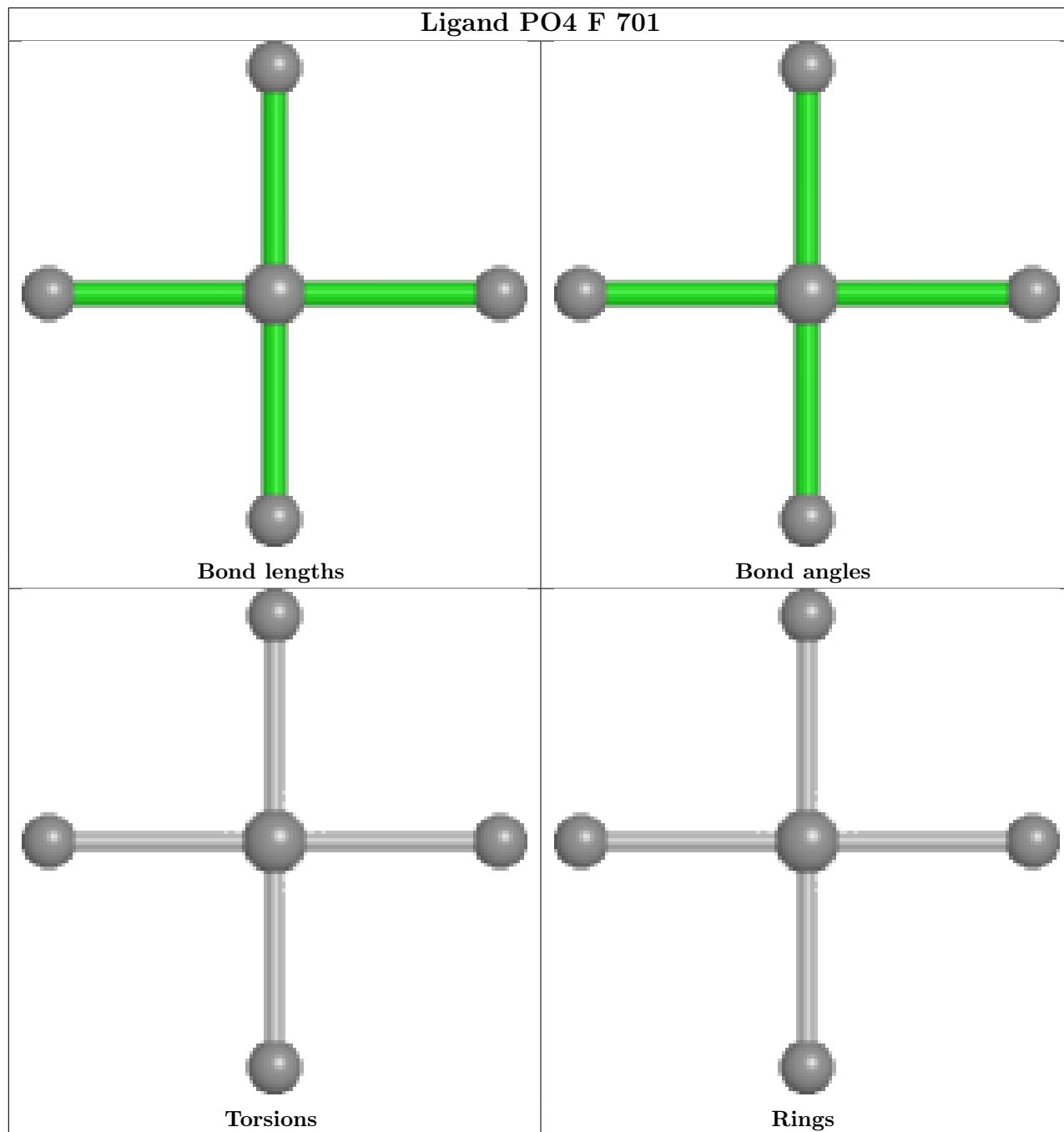
There are no ring outliers.

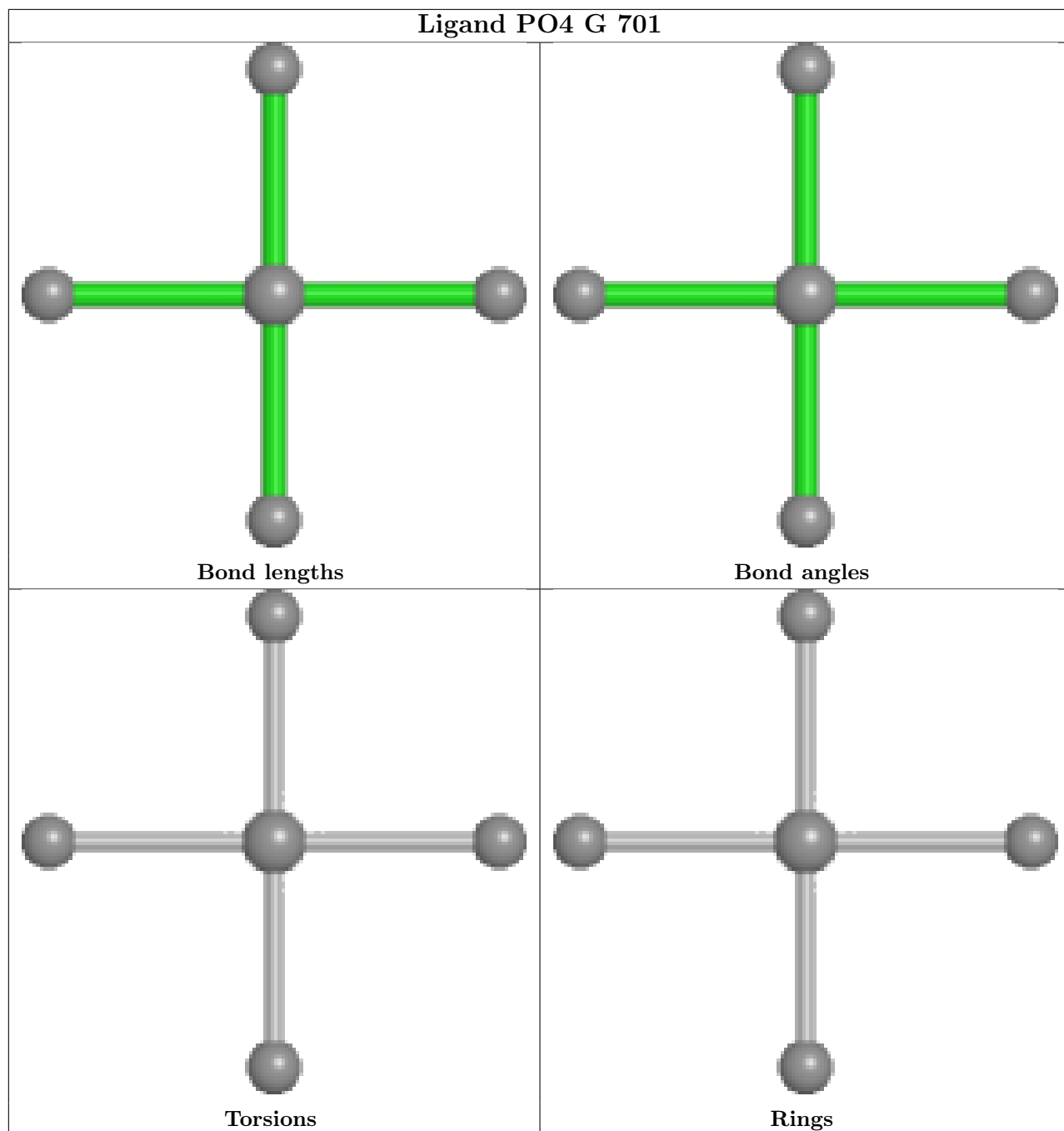
6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	701	PO4	1	0
2	G	701	PO4	1	0
2	A	701	PO4	1	0
2	C	701	PO4	1	0
2	B	701	PO4	2	0
2	H	701	PO4	1	0

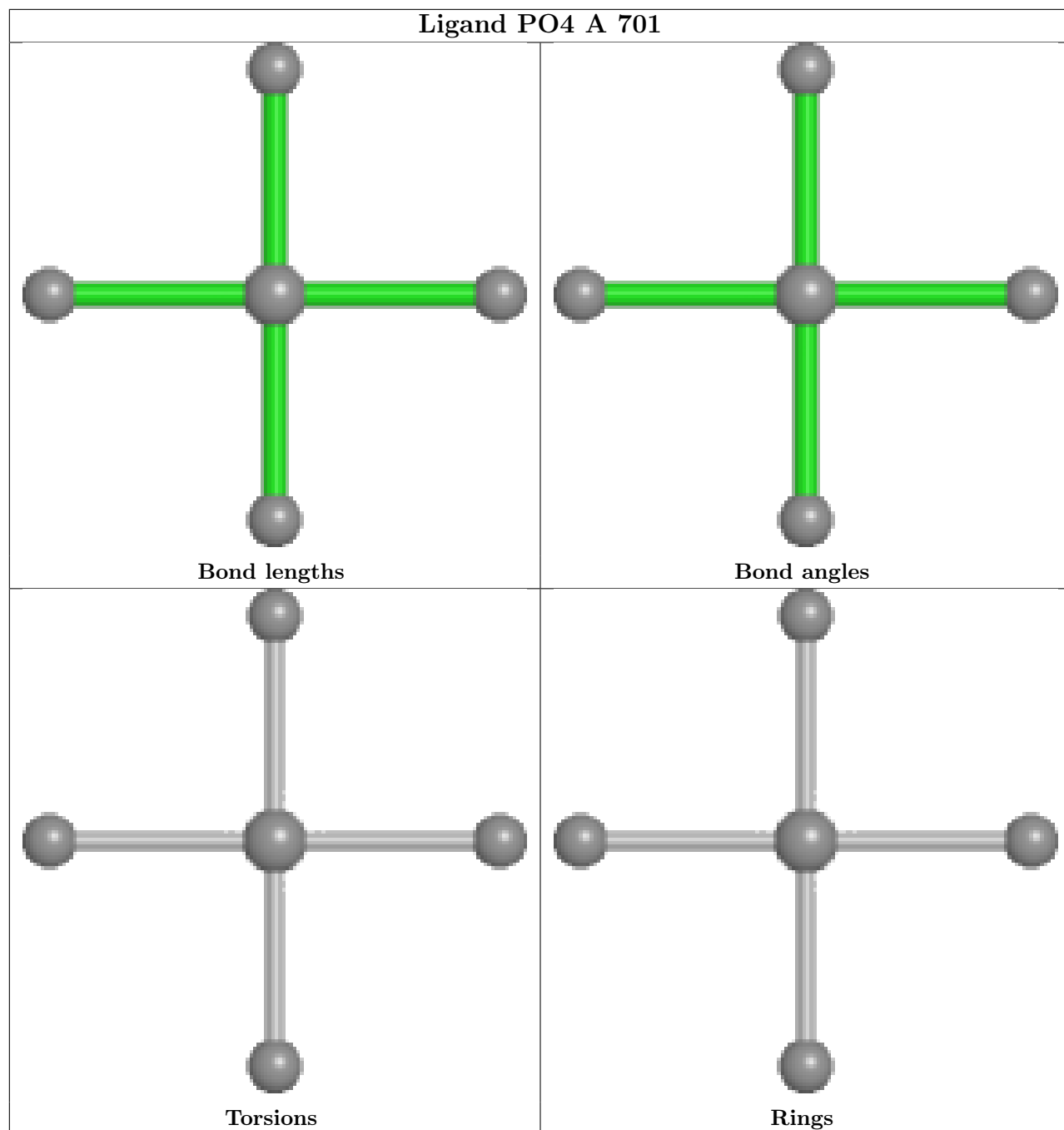
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight  $> 250$  and outliers as shown on the validation Tables will also be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

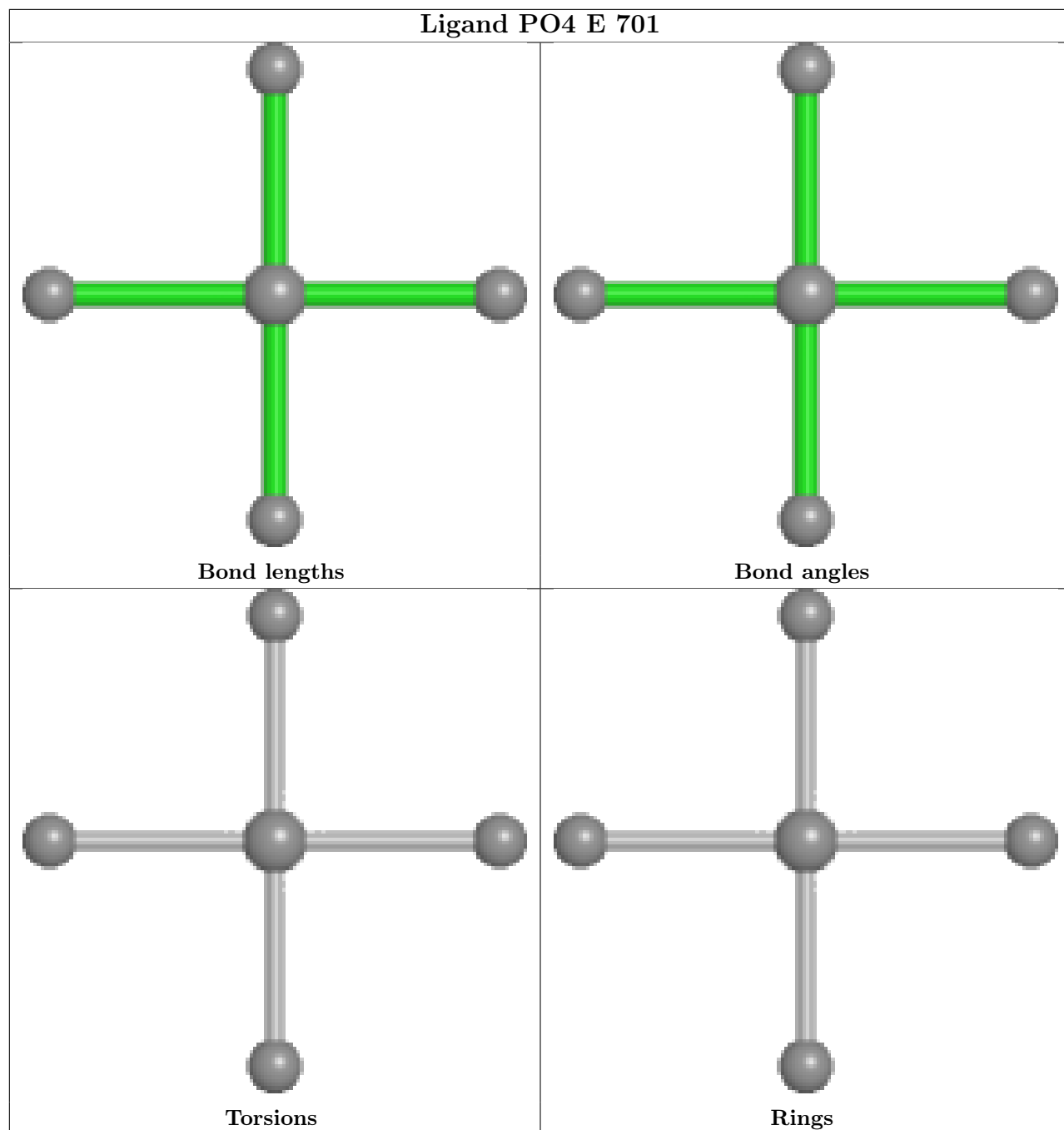
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

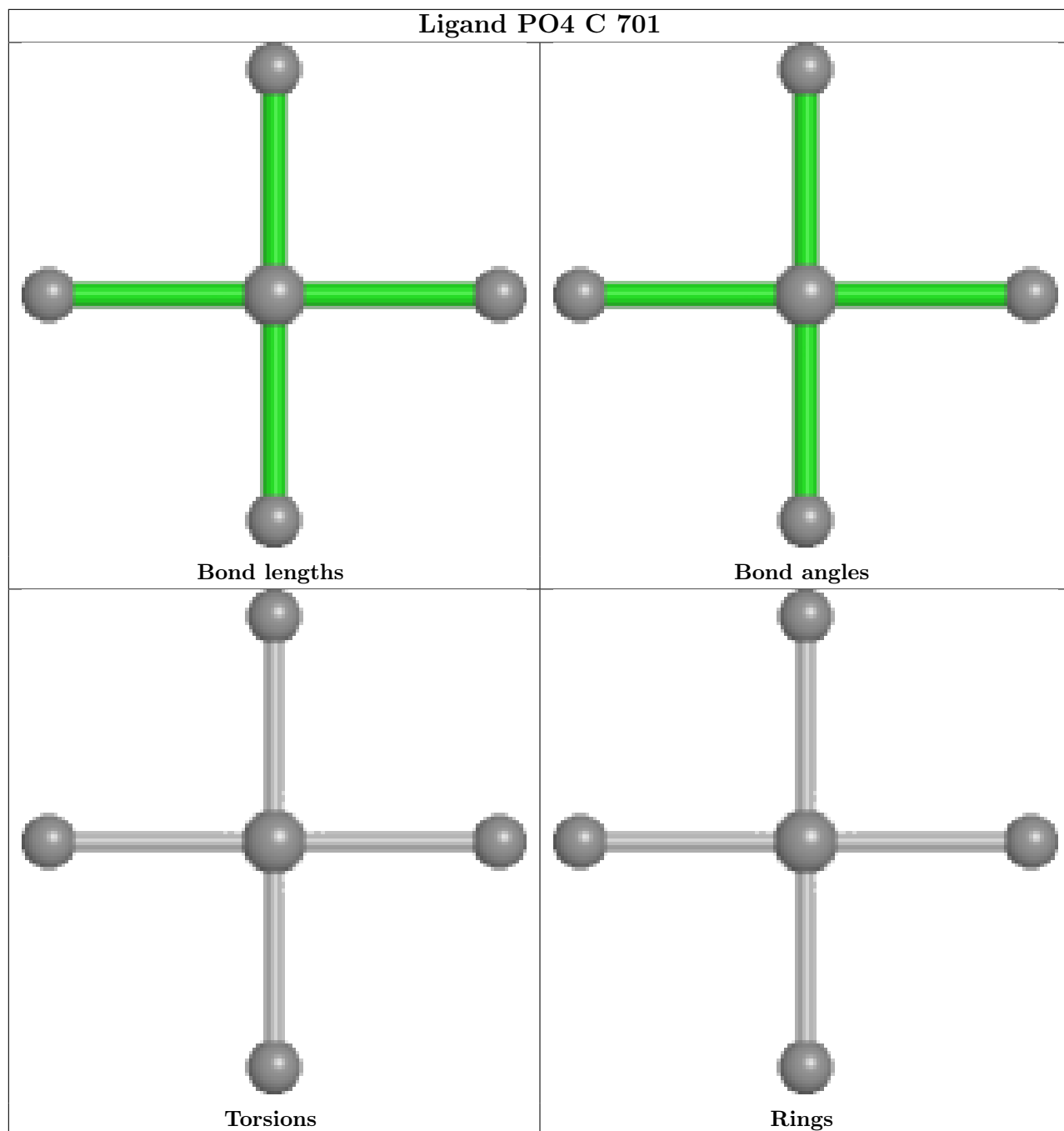


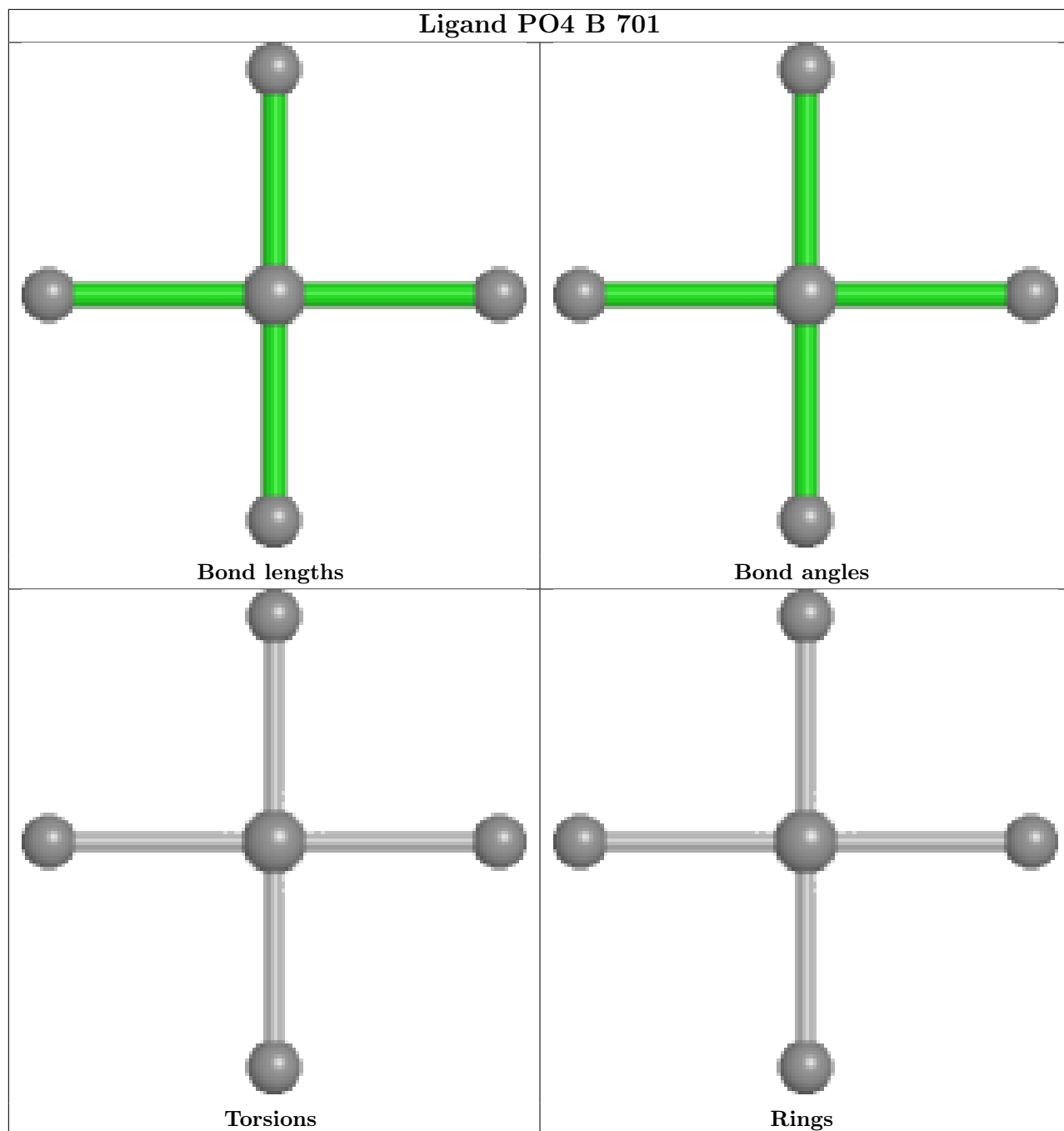


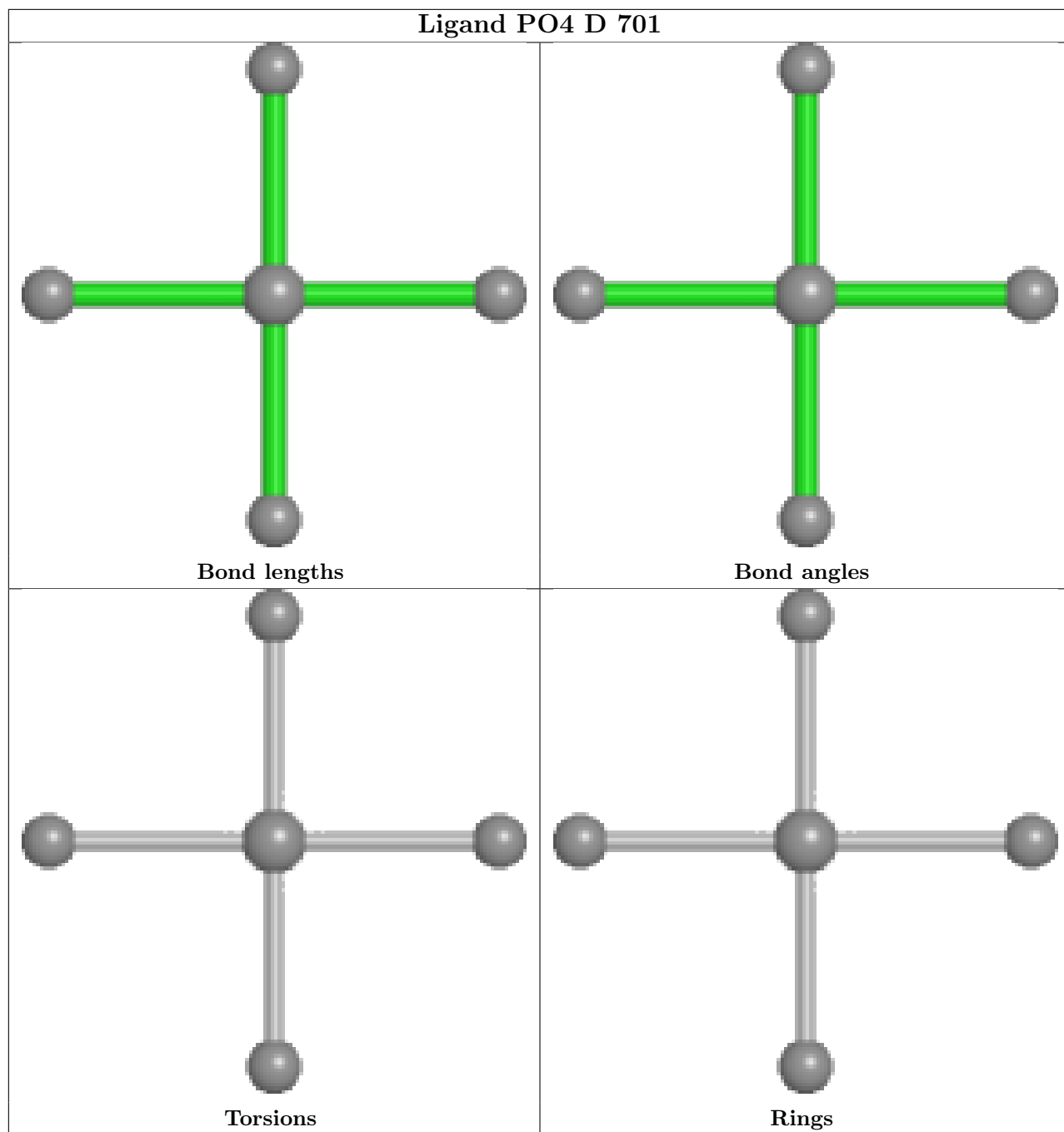


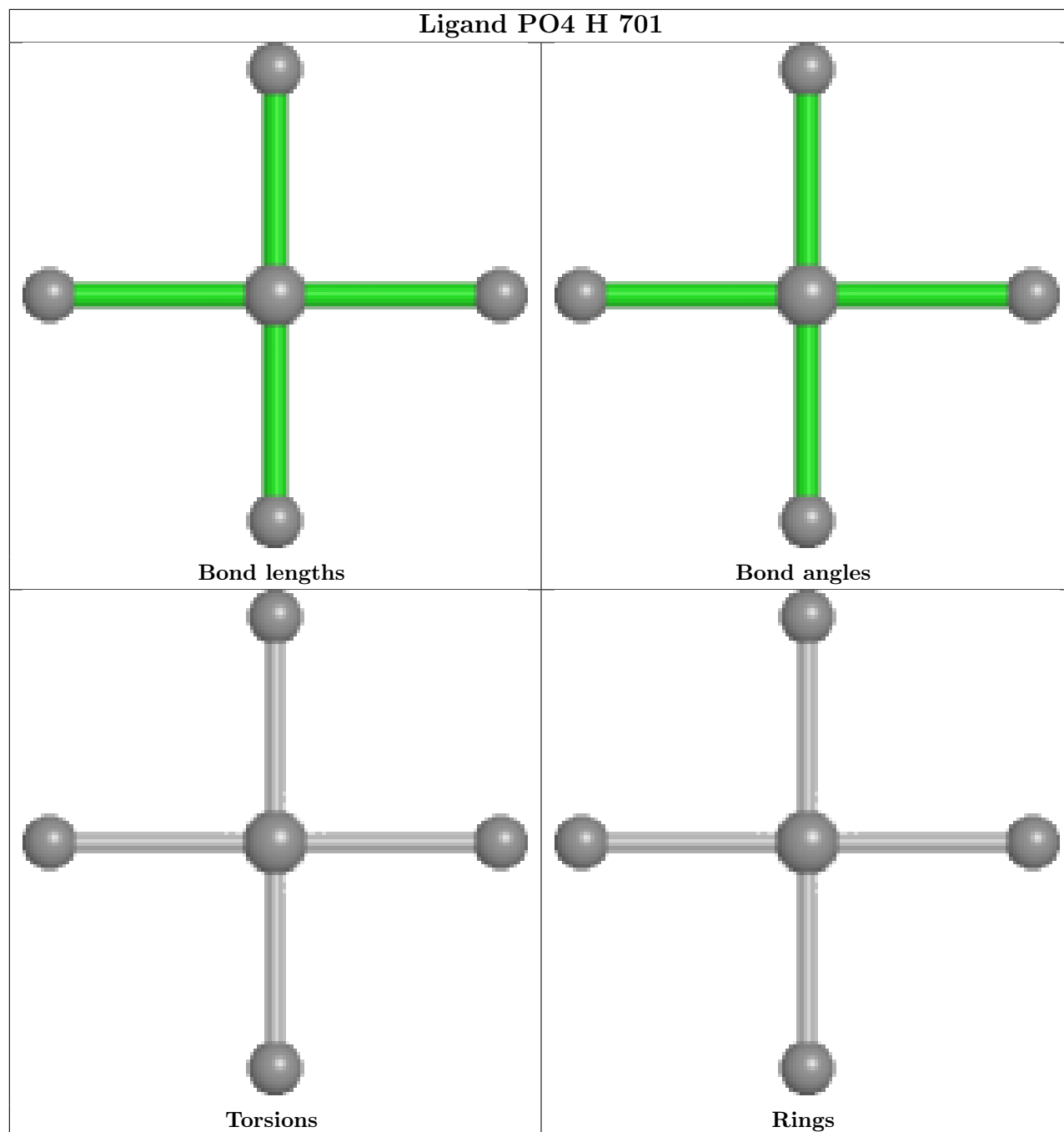












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

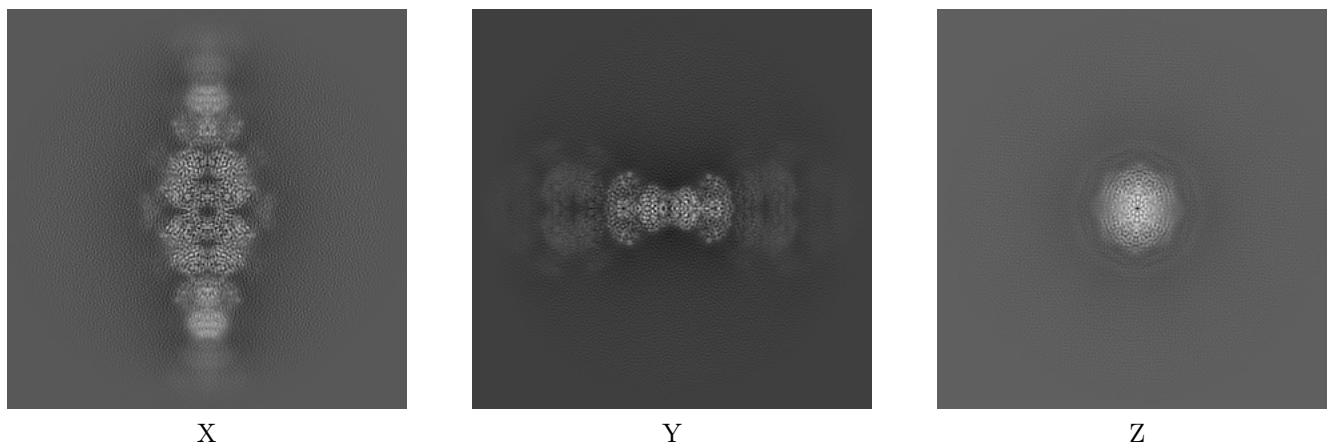
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28013. These allow visual inspection of the internal detail of the map and identification of artifacts.

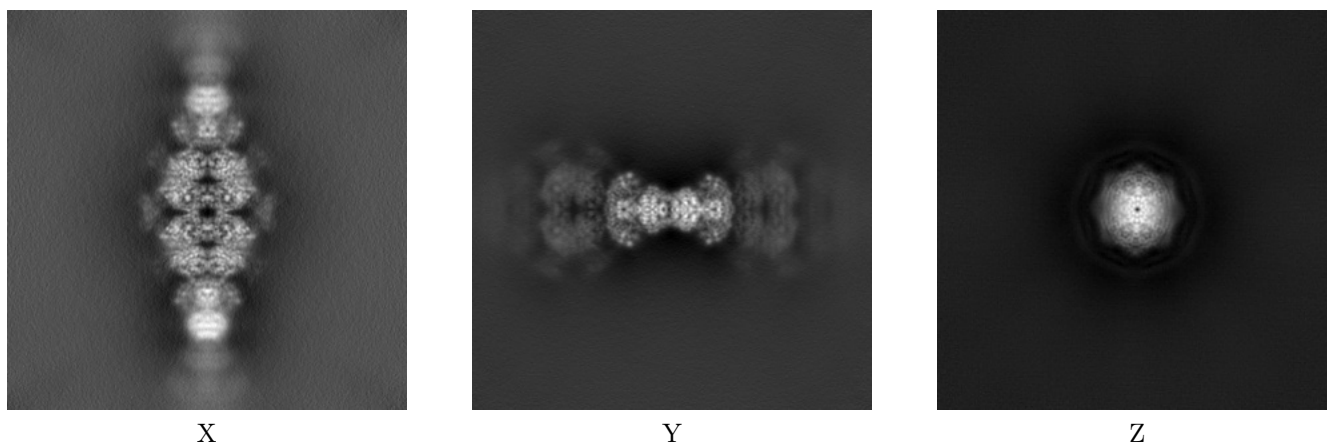
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

#### 6.1.1 Primary map



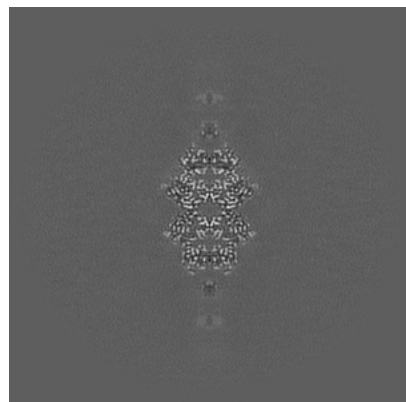
#### 6.1.2 Raw map



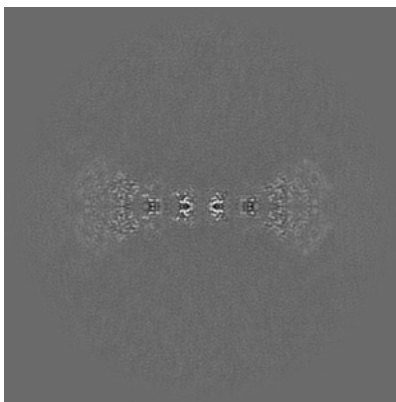
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

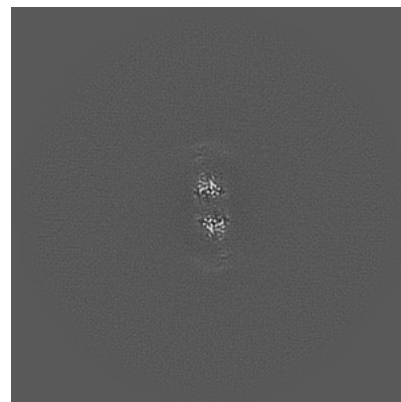
### 6.2.1 Primary map



X Index: 200

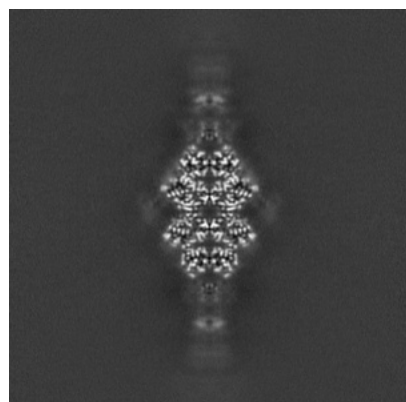


Y Index: 200

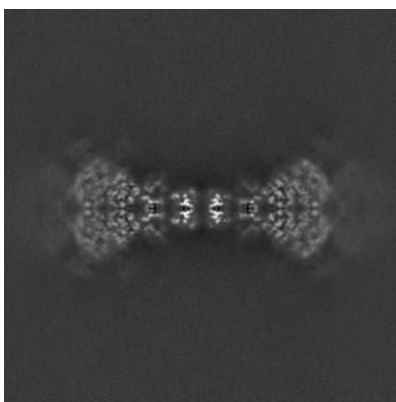


Z Index: 200

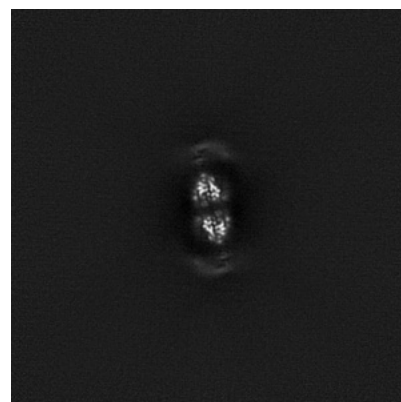
### 6.2.2 Raw map



X Index: 200



Y Index: 200



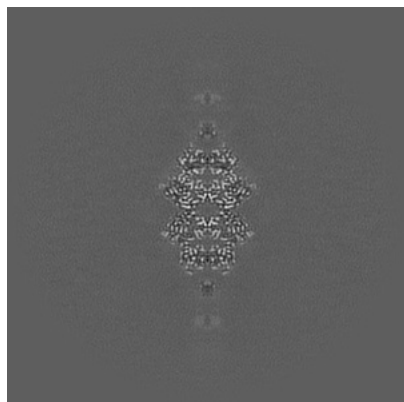
Z Index: 200

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

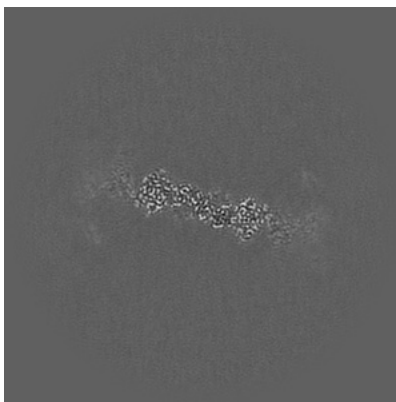


## 6.3 Largest variance slices [i](#)

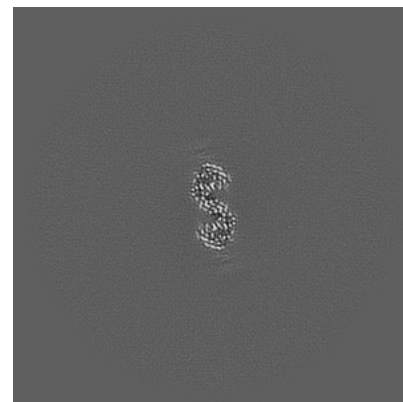
### 6.3.1 Primary map



X Index: 200

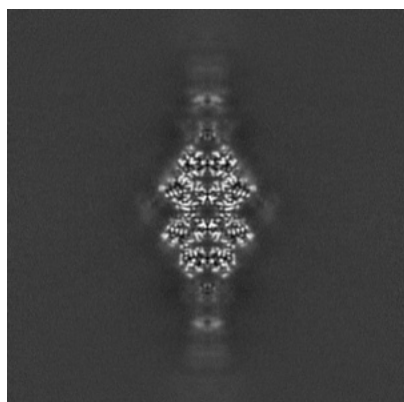


Y Index: 216

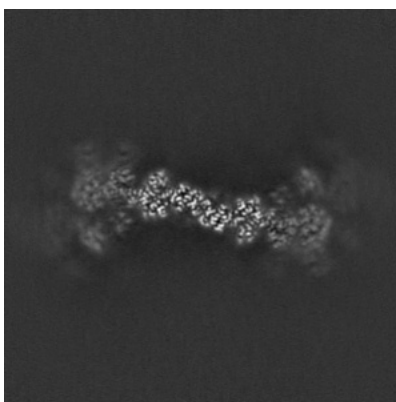


Z Index: 213

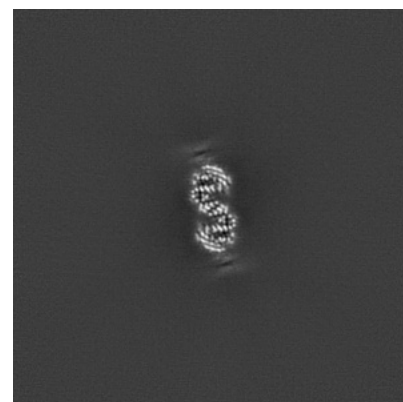
### 6.3.2 Raw map



X Index: 200



Y Index: 212

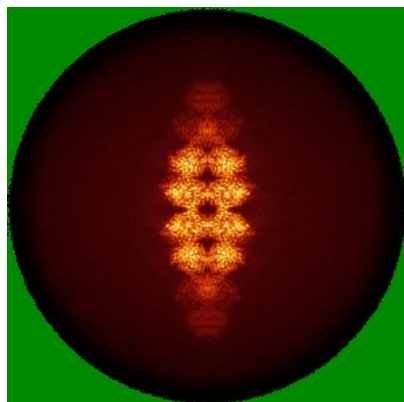


Z Index: 213

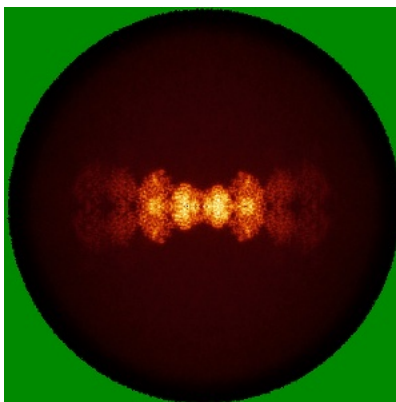
The images above show the largest variance slices of the map in three orthogonal directions.

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

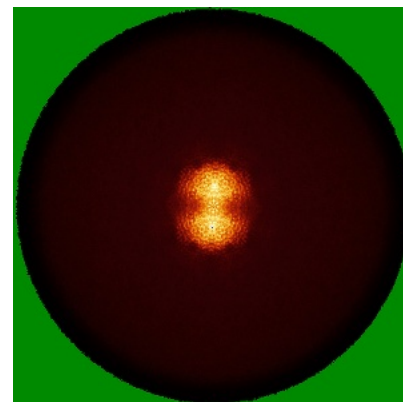
### 6.4.1 Primary map



X

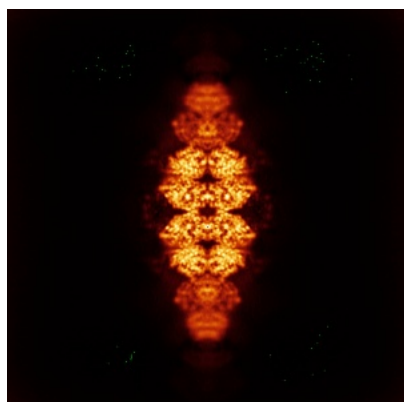


Y

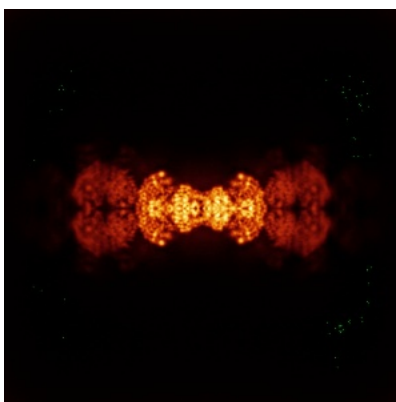


Z

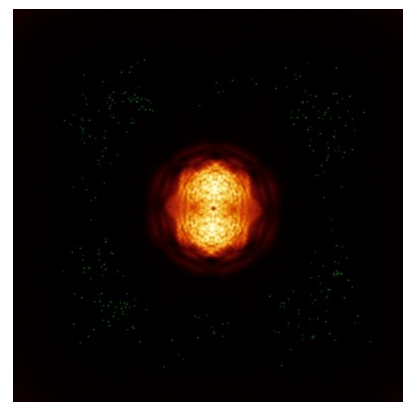
### 6.4.2 Raw map



X



Y

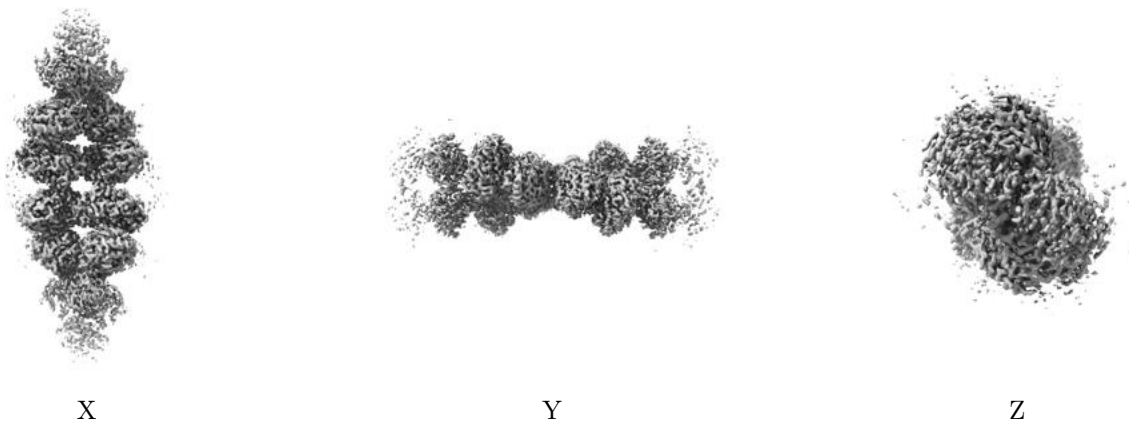


Z

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.

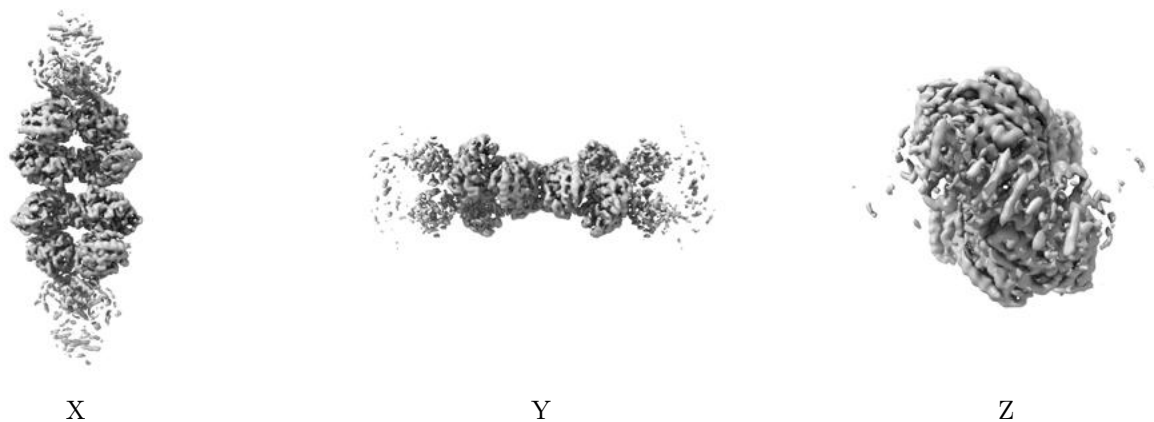
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

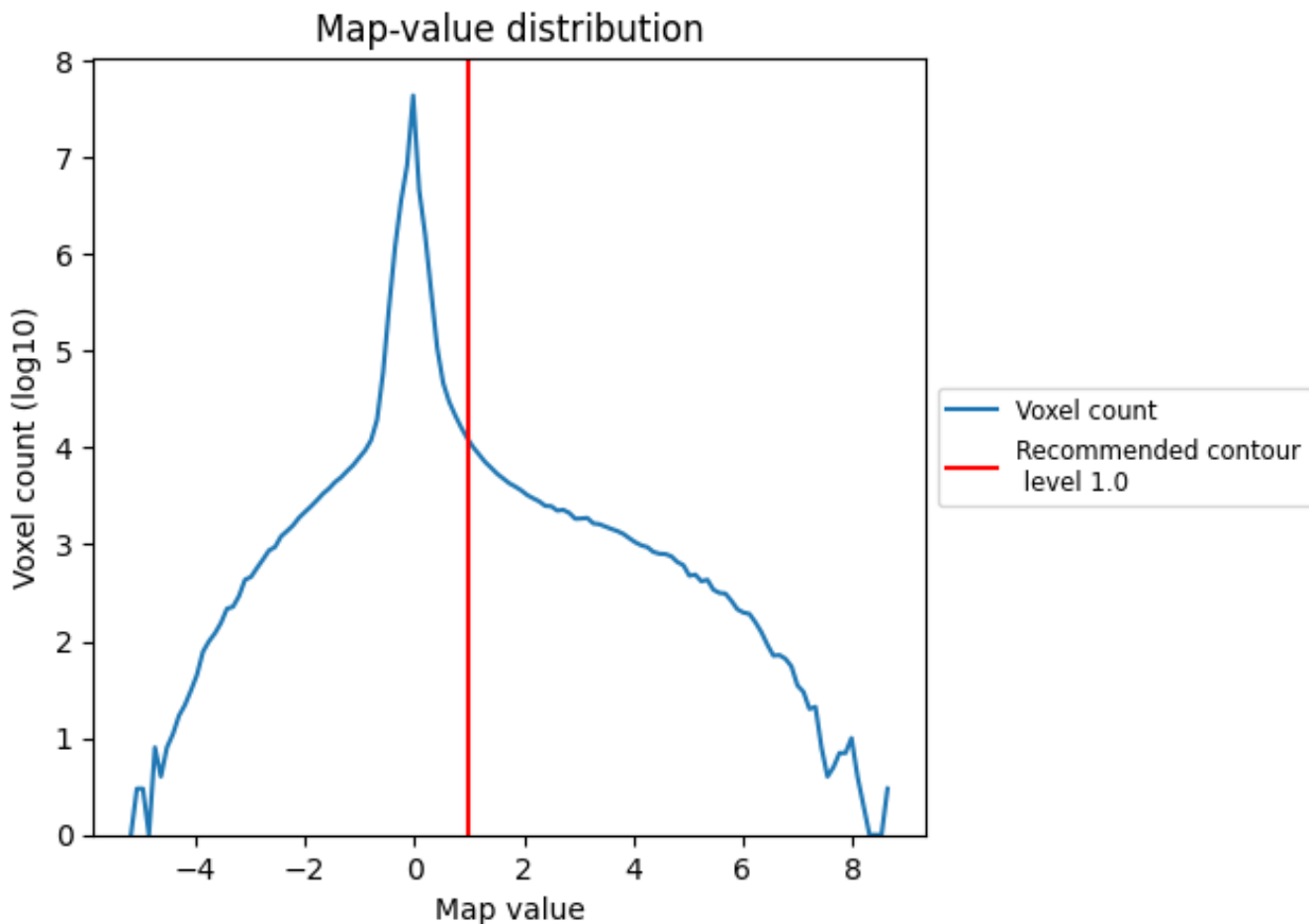
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

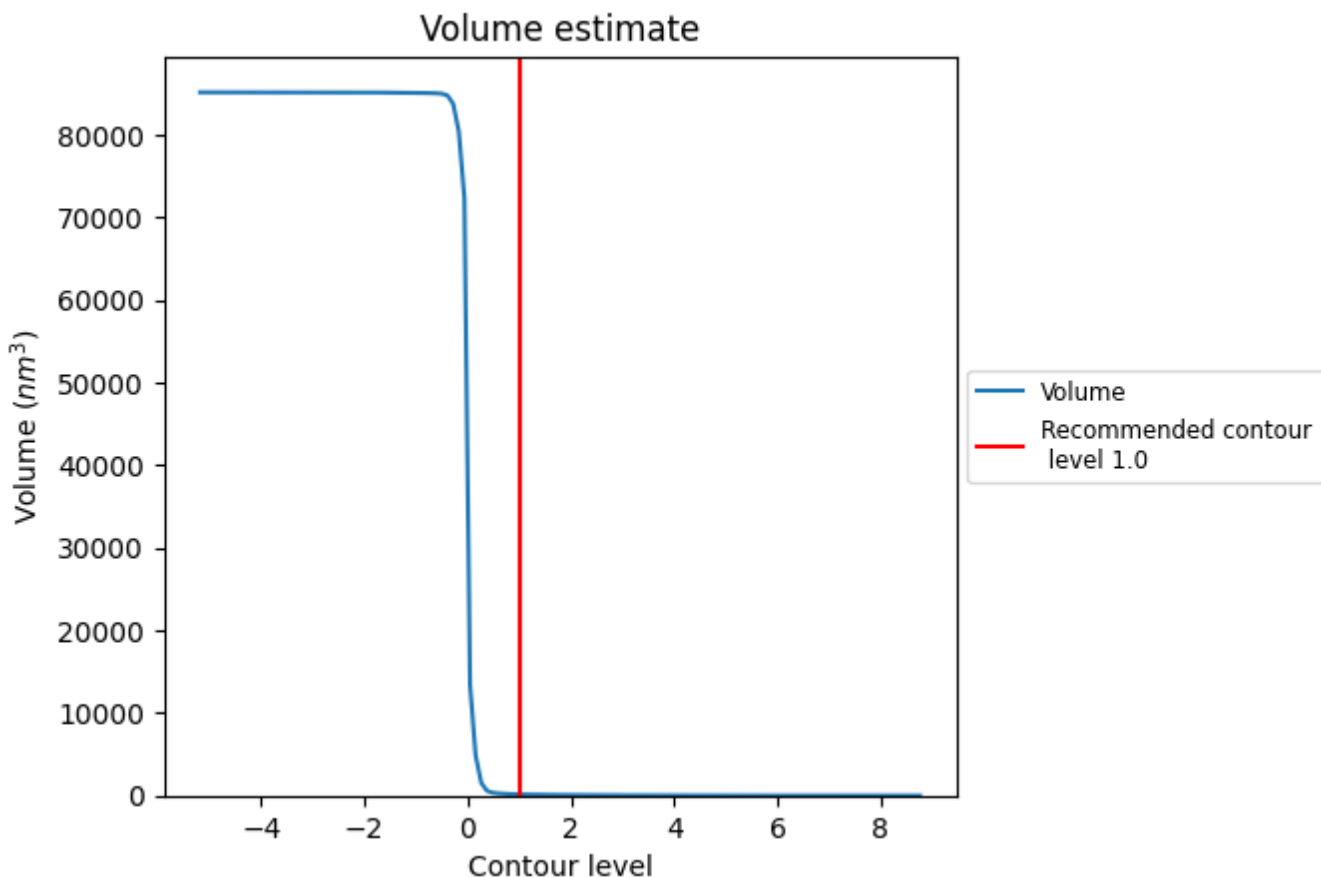
This section contains the results of statistical analysis of the map.

### 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.

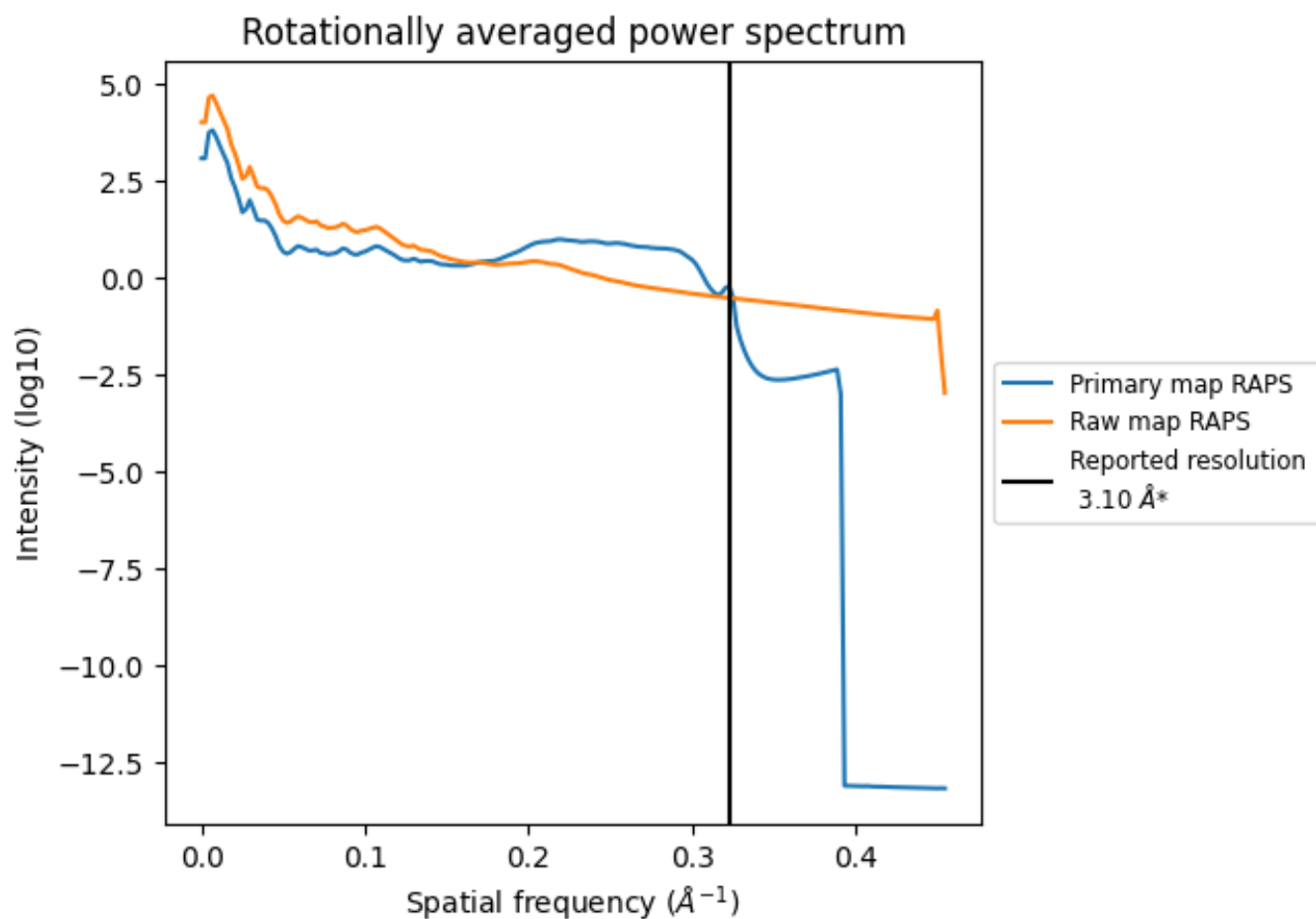
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 147  $\text{nm}^3$ ; this corresponds to an approximate mass of 133 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum i

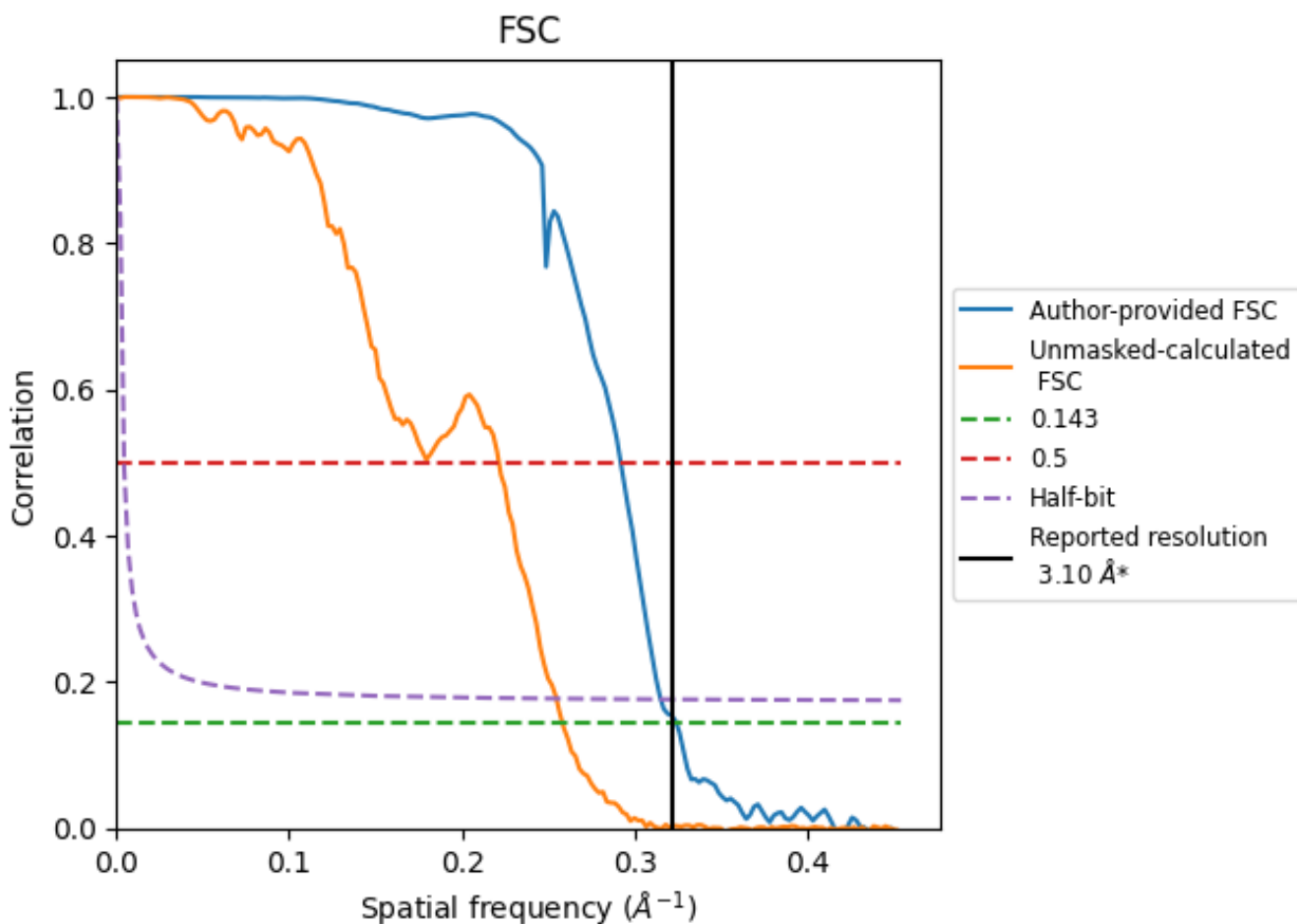


\*Reported resolution corresponds to spatial frequency of  $0.323 \text{ \AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.323 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.08	3.42	3.17
Unmasked-calculated*	3.87	4.51	3.92

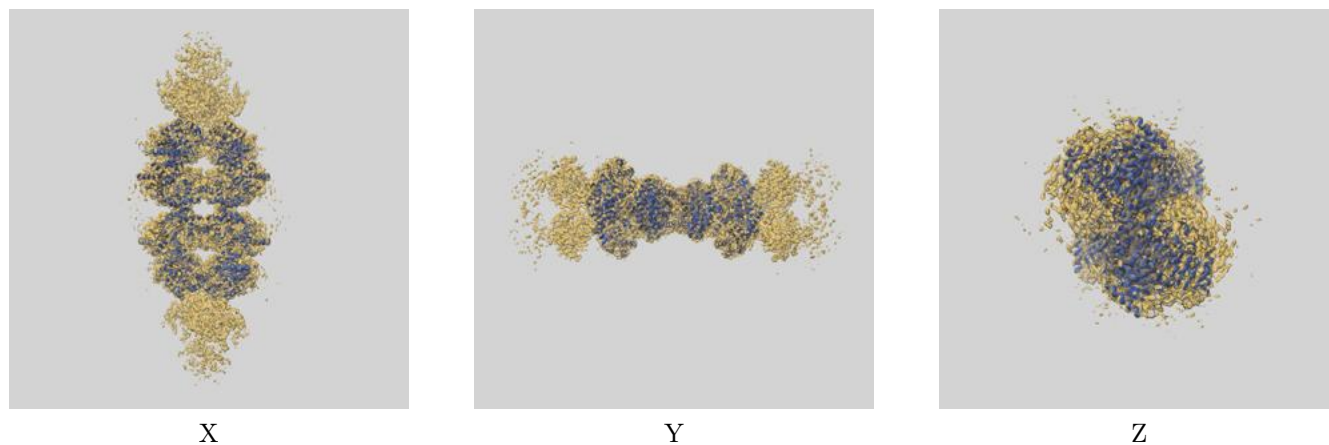
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.87 differs from the reported value 3.1 by more than 10 %



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

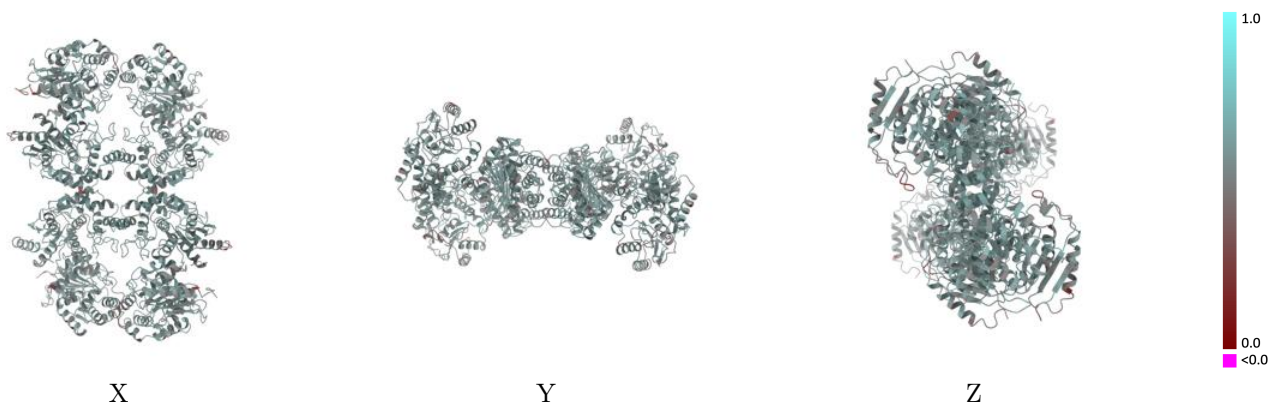
This section contains information regarding the fit between EMDB map EMD-28013 and PDB model 8EC6. Per-residue inclusion information can be found in section 3 on page 7.

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



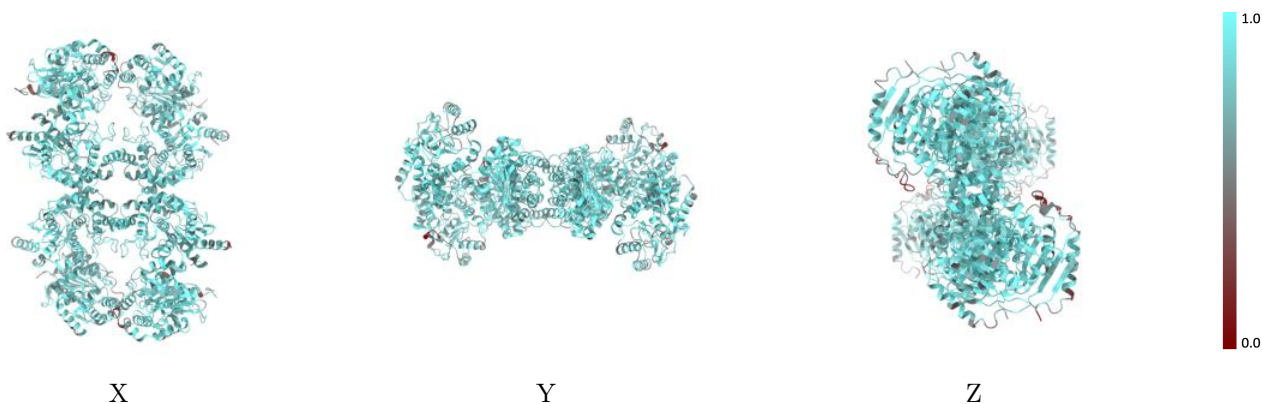
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



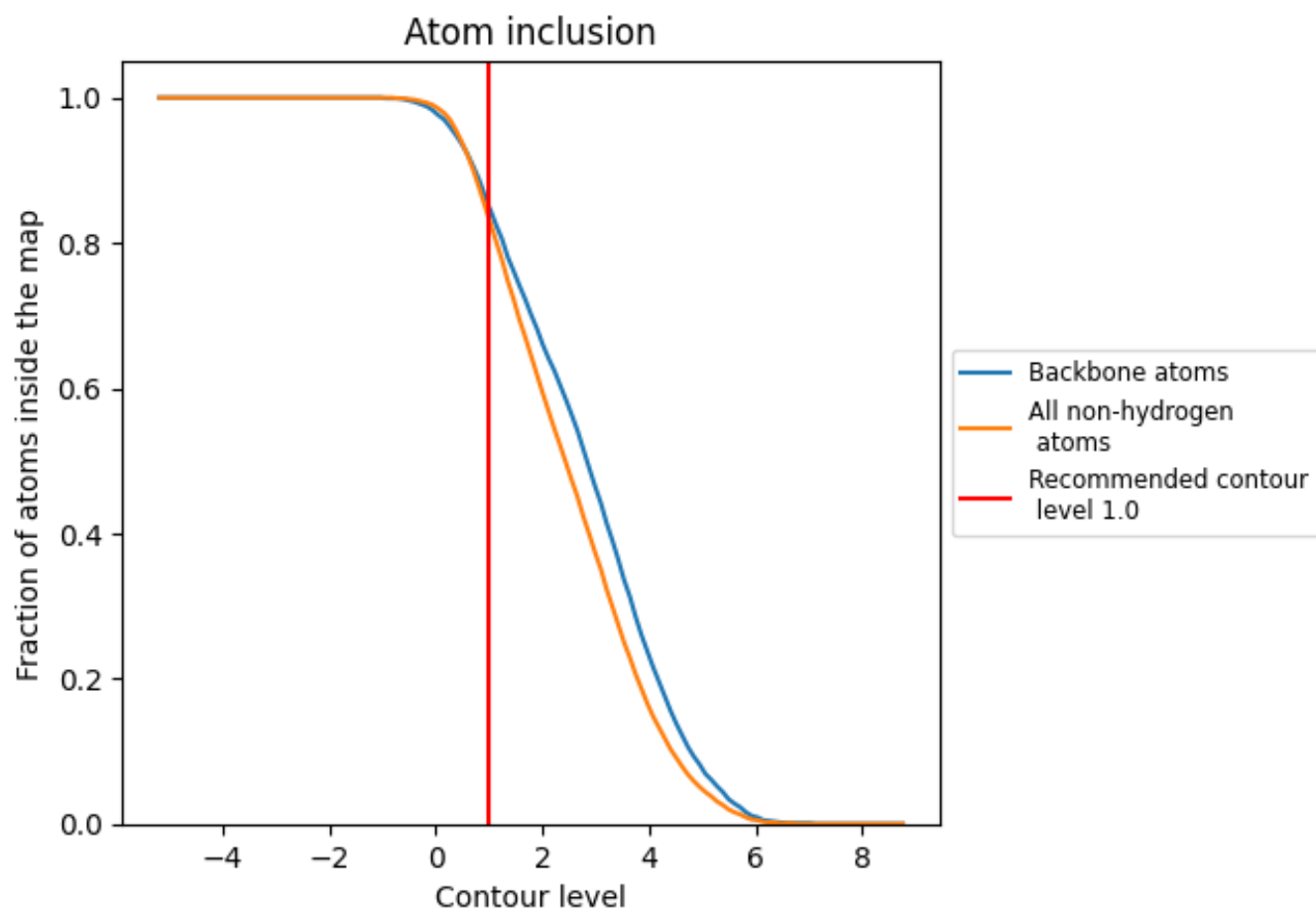
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.0).



















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 83% 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 (1.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8320	 0.5480
A	 0.8150	 0.5430
B	 0.8530	 0.5550
C	 0.8120	 0.5420
D	 0.8470	 0.5560
E	 0.8540	 0.5570
F	 0.8120	 0.5380
G	 0.8480	 0.5540
H	 0.8130	 0.5400

