



# Full wwPDB EM Validation Report ⓘ

Oct 13, 2024 – 04:03 PM EDT

PDB ID : 7URC  
EMDB ID : EMD-26708  
Title : Human PORCN in complex with LGK974  
Authors : Liu, Y.; Qi, X.; Li, X.  
Deposited on : 2022-04-21  
Resolution : 3.14 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

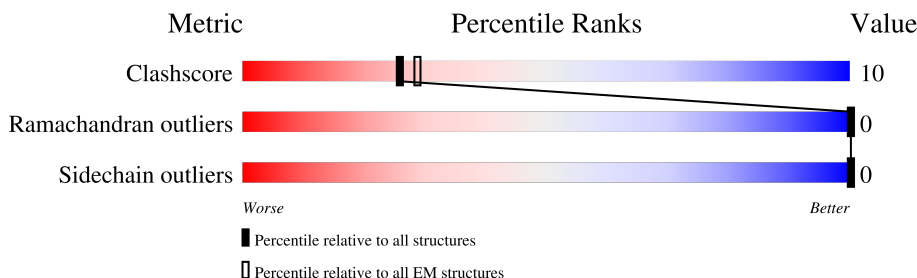
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.14 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	464	
2	L	234	
3	H	250	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	AJP	A	511	X	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5561 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 Protein-serine O-palmitoleoyltransferase porcupine.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	432	Total	C	N	O	S	0	0
			3449	2291	573	562	23		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP Q9H237
A	-6	ASP	-	expression tag	UNP Q9H237
A	-5	TYR	-	expression tag	UNP Q9H237
A	-4	LYS	-	expression tag	UNP Q9H237
A	-3	ASP	-	expression tag	UNP Q9H237
A	-2	ASP	-	expression tag	UNP Q9H237
A	-1	ASP	-	expression tag	UNP Q9H237
A	0	ASP	-	expression tag	UNP Q9H237
A	1	LYS	-	expression tag	UNP Q9H237

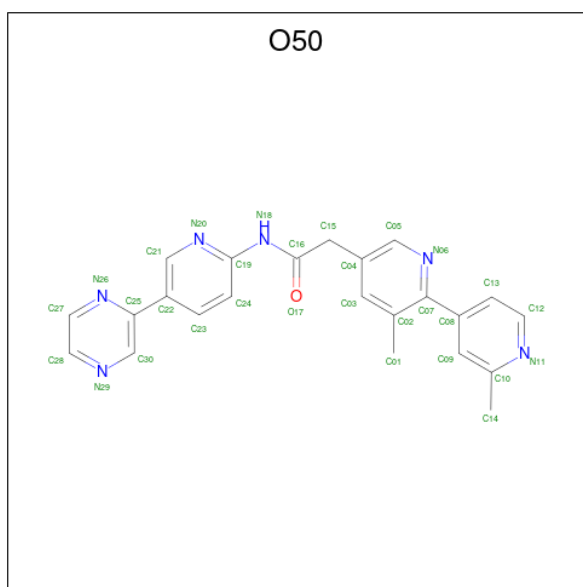
- Molecule 2 is a protein called 2C11 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L	107	Total	C	N	O	S	0	0
			829	527	137	162	3		

- Molecule 3 is a protein called 2C11 heavy chain.

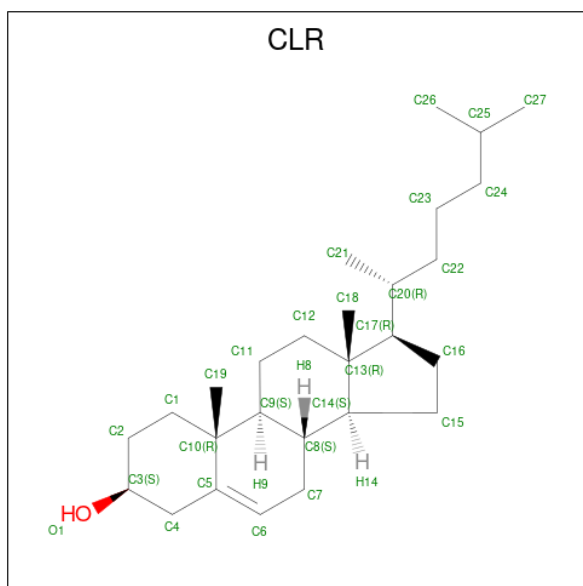
Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	119	Total	C	N	O	S	0	0
			926	584	152	185	5		

- Molecule 4 is 2-[(2P)-2',3-dimethyl[2,4'-bipyridin]-5-yl]-N-[(5P)-5-(pyrazin-2-yl)pyridin-2-yl]acetamide (three-letter code: O50) (formula: C<sub>23</sub>H<sub>20</sub>N<sub>6</sub>O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			30	23	6	1	

- Molecule 5 is CHOLESTEROL (three-letter code: CLR) (formula:  $C_{27}H_{46}O$ ).



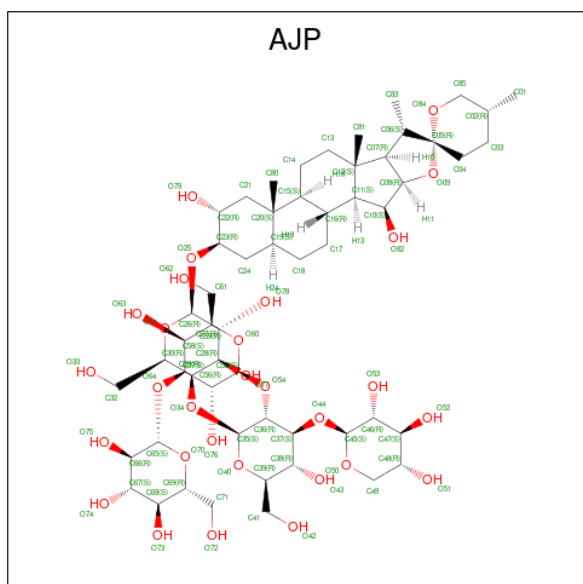
Mol	Chain	Residues	Atoms				AltConf
5	A	1	Total	C	O		0
			28	27	1		
5	A	1	Total	C	O		0
			28	27	1		
5	A	1	Total	C	O		0
			28	27	1		

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Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	
5	A	1	Total	C	O	0
			28	27	1	

- Molecule 6 is Digitonin (three-letter code: AJP) (formula:  $C_{56}H_{92}O_{29}$ ).



Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total	C	O	0
			74	50	24	

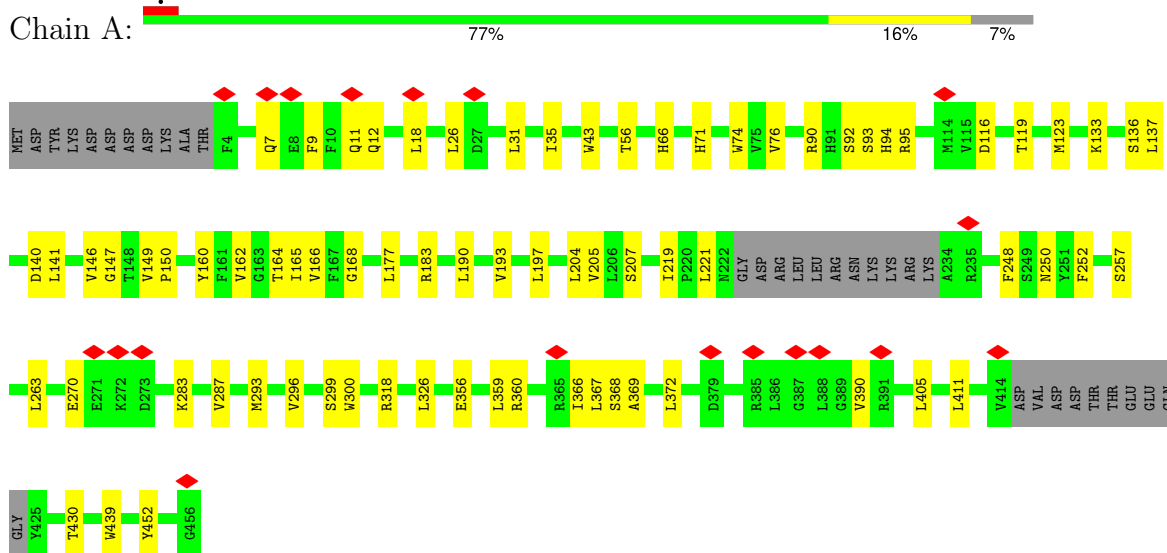
- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Zn	0
			1	1	

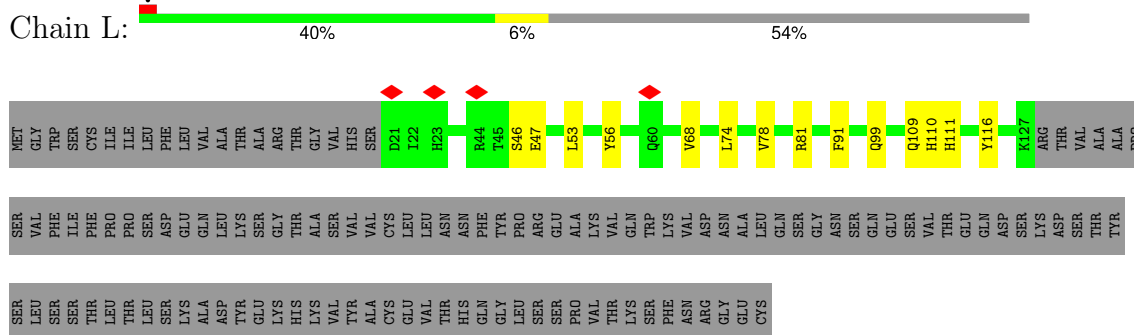
### 3 Residue-property plots

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.

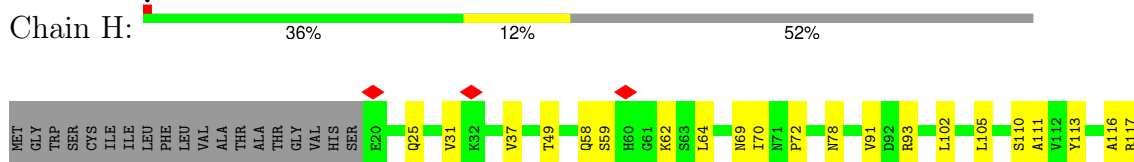
- Molecule 1: Isoform 2 of Protein-serine O-palmitoleyltransferase porcupine



- Molecule 2: 2C11 light chain



- Molecule 3: 2C11 heavy chain



HIS	THR	S118
HIS	SER	Y119
HIS	GLY	
HIS	VAL	F125
HIS	HIS	A126
HIS	THR	Y127
HIS	PRO	
	PRO	G131
	ALA	
	VAL	V134
	LEU	T135
	GLN	V136
	SER	S137
	SER	S138
	GLY	ALA
	LEU	SER
	TYR	THR
	SER	LYS
	LEU	GLY
	SER	PRO
	PRO	ALA
	SER	PRO
	SER	SER
	SER	SER
	LEU	LYS
	GLY	SER
	THR	THR
	GLN	SER
	THR	GLY
	TYR	GLY
	ILE	THR
	CYS	ALA
	ASN	ALA
	VAL	LEU
	ASN	GLY
	HIS	CYS
	LYS	LEU
	PRO	VAL
	SER	LYS
	ASN	ASP
	THR	TYR
	LYS	PRO
	VAL	ASP
	ARG	GLU
	VAL	VAL
	PRO	SER
	LYS	THR
	SER	ASN
	CYS	SER
	ASP	GLY
	LYS	ALA
	THR	LEU

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	100636	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	8.5	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.717	Depositor
Minimum map value	-1.808	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.068	Depositor
Recommended contour level	0.5	Depositor
Map size ( $\text{\AA}$ )	232.4, 232.4, 232.4	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.83, 0.83, 0.83	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: CLR, O50, ZN, AJP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.29	0/3555	0.40	0/4840
2	L	0.29	0/851	0.45	0/1152
3	H	0.30	0/949	0.45	0/1286
All	All	0.29	0/5355	0.42	0/7278

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	3449	0	3462	45	0
2	L	829	0	794	9	0
3	H	926	0	873	18	0
4	A	30	0	0	0	0
5	A	252	0	414	18	0
6	A	74	0	0	28	0
7	A	1	0	0	0	0
All	All	5561	0	5543	111	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 10.

All (111) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:511:AJP:C15	6:A:511:AJP:C16	1.75	1.56
6:A:511:AJP:C12	6:A:511:AJP:C11	1.80	1.55
6:A:511:AJP:C02	6:A:511:AJP:C01	1.94	1.43
6:A:511:AJP:C08	6:A:511:AJP:C07	1.98	1.40
6:A:511:AJP:O09	6:A:511:AJP:C05	1.79	1.30
6:A:511:AJP:C08	6:A:511:AJP:C05	2.21	1.18
6:A:511:AJP:C11	6:A:511:AJP:C07	2.26	1.12
6:A:511:AJP:C01	6:A:511:AJP:C03	2.54	0.86
6:A:511:AJP:C12	6:A:511:AJP:C08	2.49	0.83
6:A:511:AJP:C08	6:A:511:AJP:C06	2.56	0.82
6:A:511:AJP:C01	6:A:511:AJP:C85	2.58	0.81
6:A:511:AJP:C07	6:A:511:AJP:C10	2.60	0.80
6:A:511:AJP:C16	6:A:511:AJP:C20	2.61	0.78
6:A:511:AJP:C15	6:A:511:AJP:C11	2.61	0.78
1:A:318:ARG:NH2	6:A:511:AJP:O76	2.18	0.77
6:A:511:AJP:C08	6:A:511:AJP:C81	2.63	0.76
6:A:511:AJP:C11	6:A:511:AJP:C81	2.64	0.76
6:A:511:AJP:C08	6:A:511:AJP:C04	2.64	0.75
1:A:296:VAL:HG11	1:A:405:LEU:HD21	1.71	0.72
3:H:49:THR:HG21	3:H:93:ARG:HD3	1.68	0.72
3:H:113:TYR:O	3:H:131:GLY:HA2	1.89	0.71
6:A:511:AJP:C15	6:A:511:AJP:C17	2.64	0.70
3:H:58:GLN:HB2	3:H:64:LEU:HD23	1.74	0.68
6:A:511:AJP:C12	6:A:511:AJP:C10	2.71	0.66
1:A:168:GLY:HA2	1:A:257:SER:HB2	1.77	0.65
3:H:49:THR:HA	3:H:72:PRO:HB2	1.81	0.62
1:A:164:THR:HA	1:A:168:GLY:HA3	1.83	0.61
1:A:183:ARG:NH1	1:A:270:GLU:OE1	2.31	0.61
3:H:110:SER:HA	3:H:134:VAL:O	2.01	0.61
2:L:109:GLN:HE21	2:L:116:TYR:HB3	1.66	0.61
1:A:360:ARG:NH1	1:A:372:LEU:O	2.33	0.60
6:A:511:AJP:C16	6:A:511:AJP:C80	2.79	0.59
2:L:109:GLN:NE2	2:L:110:HIS:O	2.38	0.57
3:H:116:ALA:HB1	3:H:125:PHE:HB3	1.87	0.57
1:A:287:VAL:HG13	1:A:296:VAL:HG13	1.88	0.55
3:H:59:SER:HB2	3:H:62:LYS:HB2	1.88	0.55
6:A:511:AJP:C11	6:A:511:AJP:C13	2.74	0.54
1:A:366:ILE:HG22	1:A:367:LEU:HD23	1.90	0.54
1:A:9:PHE:HA	1:A:12:GLN:HE21	1.73	0.54
1:A:133:LYS:O	1:A:136:SER:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:511:AJP:C81	6:A:511:AJP:C83	2.85	0.54
6:A:511:AJP:O63	6:A:511:AJP:O62	2.25	0.53
6:A:511:AJP:O43	6:A:511:AJP:O42	2.26	0.52
1:A:147:GLY:HA3	2:L:111:HIS:O	2.10	0.52
3:H:49:THR:CG2	3:H:93:ARG:HD3	2.37	0.52
6:A:511:AJP:C16	6:A:511:AJP:C14	2.82	0.52
2:L:56:TYR:HE1	2:L:109:GLN:HB3	1.75	0.51
5:A:503:CLR:H193	6:A:511:AJP:C18	2.41	0.51
1:A:165:ILE:HG23	1:A:166:VAL:HG23	1.93	0.51
1:A:90:ARG:O	1:A:95:ARG:NH1	2.45	0.50
1:A:193:VAL:HG11	1:A:263:LEU:HD13	1.94	0.50
1:A:18:LEU:HD13	1:A:205:VAL:HG21	1.95	0.49
1:A:411:LEU:HD11	1:A:430:THR:HA	1.95	0.49
1:A:369:ALA:HB1	1:A:390:VAL:HG22	1.95	0.48
2:L:53:LEU:HD13	2:L:91:PHE:CD1	2.48	0.48
1:A:293:MET:N	1:A:356:GLU:OE1	2.43	0.48
1:A:92:SER:HG	1:A:94:HIS:HD1	1.61	0.47
1:A:207:SER:HB2	1:A:248:PHE:HB3	1.95	0.47
1:A:71:HIS:CD2	1:A:119:THR:HG21	2.50	0.47
3:H:25:GLN:NE2	3:H:113:TYR:O	2.44	0.47
1:A:219:ILE:HG22	1:A:221:LEU:H	1.80	0.47
1:A:35:ILE:HG22	1:A:162:VAL:HG21	1.97	0.46
1:A:204:LEU:HB2	1:A:252:PHE:CD1	2.50	0.46
1:A:250:ASN:ND2	1:A:300:TRP:CE2	2.84	0.46
3:H:69:ASN:OD1	3:H:78:ASN:HB3	2.15	0.46
2:L:81:ARG:CZ	2:L:99:GLN:HG3	2.44	0.46
5:A:502:CLR:H222	5:A:502:CLR:H162	1.82	0.46
5:A:508:CLR:H162	5:A:508:CLR:H221	1.52	0.45
1:A:190:LEU:HD22	5:A:508:CLR:C15	2.47	0.45
1:A:7:GLN:O	1:A:11:GLN:HG2	2.18	0.44
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.86	0.44
5:A:504:CLR:H222	5:A:504:CLR:H25	1.73	0.44
3:H:70:ILE:HD13	3:H:91:VAL:HG13	2.00	0.44
1:A:31:LEU:HD23	1:A:66:HIS:CG	2.53	0.43
1:A:116:ASP:N	1:A:116:ASP:OD1	2.50	0.43
1:A:190:LEU:HD22	5:A:508:CLR:H151	2.00	0.43
1:A:137:LEU:HD21	1:A:150:PRO:HG2	2.00	0.43
5:A:508:CLR:H183	5:A:508:CLR:H20	1.69	0.43
1:A:197:LEU:HD23	1:A:197:LEU:HA	1.92	0.43
5:A:504:CLR:H17	5:A:504:CLR:H231	1.77	0.42
1:A:43:TRP:HZ2	1:A:56:THR:HB	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:37:VAL:HG12	3:H:102:LEU:HB2	2.01	0.42
3:H:31:VAL:HG21	3:H:105:LEU:HD12	2.02	0.42
5:A:506:CLR:H211	5:A:506:CLR:H231	1.77	0.42
5:A:510:CLR:H263	5:A:510:CLR:H231	1.84	0.42
2:L:46:SER:OG	2:L:47:GLU:N	2.53	0.42
2:L:68:VAL:HG22	2:L:74:LEU:HD13	2.01	0.42
1:A:141:LEU:HD13	1:A:149:VAL:HG22	2.02	0.41
5:A:509:CLR:H183	5:A:509:CLR:H20	1.85	0.41
1:A:74:TRP:HD1	1:A:123:MET:HE1	1.84	0.41
1:A:283:LYS:HB2	1:A:299:SER:OG	2.19	0.41
1:A:368:SER:OG	1:A:368:SER:O	2.38	0.41
1:A:439:TRP:CZ2	5:A:505:CLR:H122	2.55	0.41
3:H:117:ARG:HE	3:H:127:TYR:HD2	1.68	0.41
5:A:508:CLR:H182	5:A:508:CLR:H8	1.75	0.41
2:L:74:LEU:HD12	2:L:78:VAL:HG11	2.02	0.41
1:A:92:SER:OG	1:A:93:SER:N	2.54	0.41
1:A:140:ASP:HB3	1:A:146:VAL:HG23	2.02	0.41
1:A:326:LEU:HD23	5:A:502:CLR:H181	2.01	0.41
1:A:359:LEU:HD13	1:A:452:TYR:HB2	2.03	0.41
3:H:119:TYR:HD1	3:H:126:ALA:HB2	1.86	0.41
5:A:506:CLR:H222	5:A:506:CLR:H162	1.77	0.41
6:A:511:AJP:C10	6:A:511:AJP:C81	2.99	0.41
5:A:507:CLR:H162	5:A:507:CLR:H222	1.59	0.40
1:A:76:VAL:HA	1:A:160:TYR:OH	2.22	0.40
5:A:509:CLR:H162	5:A:509:CLR:H222	1.53	0.40
3:H:58:GLN:O	3:H:111:ALA:HB1	2.21	0.40
3:H:138:SER:O	3:H:138:SER:OG	2.35	0.40
1:A:26:LEU:HD23	1:A:26:LEU:HA	1.86	0.40
5:A:503:CLR:H222	5:A:503:CLR:H162	1.78	0.40
3:H:31:VAL:HG23	3:H:136:VAL:HG22	2.03	0.40

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	426/464 (92%)	414 (97%)	12 (3%)	0	100	100
2	L	105/234 (45%)	100 (95%)	5 (5%)	0	100	100
3	H	117/250 (47%)	111 (95%)	6 (5%)	0	100	100
All	All	648/948 (68%)	625 (96%)	23 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 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	365/398 (92%)	365 (100%)	0	100	100
2	L	92/204 (45%)	92 (100%)	0	100	100
3	H	102/215 (47%)	102 (100%)	0	100	100
All	All	559/817 (68%)	559 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	24	GLN
1	A	121	HIS
1	A	247	HIS
2	L	111	HIS
3	H	52	ASN
3	H	78	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 ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	AJP	A	511	-	83,83,95	7.32	36 (43%)	126,131,149	2.49	33 (26%)
4	O50	A	501	-	33,33,33	1.58	5 (15%)	45,45,45	2.12	18 (40%)
5	CLR	A	509	-	31,31,31	0.66	1 (3%)	48,48,48	1.61	9 (18%)
5	CLR	A	503	-	31,31,31	0.69	1 (3%)	48,48,48	1.52	8 (16%)
5	CLR	A	506	-	31,31,31	0.69	1 (3%)	48,48,48	1.60	10 (20%)
5	CLR	A	510	-	31,31,31	0.67	1 (3%)	48,48,48	1.55	8 (16%)
5	CLR	A	502	-	31,31,31	0.67	1 (3%)	48,48,48	1.58	9 (18%)
5	CLR	A	507	-	31,31,31	0.66	1 (3%)	48,48,48	1.57	8 (16%)
5	CLR	A	508	-	31,31,31	0.84	2 (6%)	48,48,48	1.60	7 (14%)
5	CLR	A	505	-	31,31,31	0.71	1 (3%)	48,48,48	1.53	8 (16%)
5	CLR	A	504	-	31,31,31	0.67	1 (3%)	48,48,48	1.49	11 (22%)

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	AJP	A	511	-	29/29/33/38	12/22/194/220	1/10/10/11
4	O50	A	501	-	-	2/16/16/16	0/4/4/4
5	CLR	A	509	-	-	5/10/68/68	0/4/4/4
5	CLR	A	503	-	-	7/10/68/68	0/4/4/4
5	CLR	A	506	-	-	5/10/68/68	0/4/4/4
5	CLR	A	510	-	-	5/10/68/68	0/4/4/4
5	CLR	A	502	-	-	5/10/68/68	0/4/4/4
5	CLR	A	507	-	-	7/10/68/68	0/4/4/4
5	CLR	A	508	-	-	4/10/68/68	0/4/4/4
5	CLR	A	505	-	-	5/10/68/68	0/4/4/4
5	CLR	A	504	-	-	4/10/68/68	0/4/4/4

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	511	AJP	C07-C08	27.12	1.98	1.53
6	A	511	AJP	O09-C08	-25.50	0.99	1.43
6	A	511	AJP	O84-C05	-23.21	1.08	1.42
6	A	511	AJP	C12-C07	-19.90	1.19	1.56
6	A	511	AJP	C04-C05	-17.91	1.24	1.51
6	A	511	AJP	O09-C05	17.68	1.79	1.42
6	A	511	AJP	C03-C02	-14.29	1.14	1.52
6	A	511	AJP	C01-C02	13.38	1.94	1.52
6	A	511	AJP	C12-C11	13.20	1.80	1.56
6	A	511	AJP	C85-C02	-12.99	1.23	1.51
6	A	511	AJP	C16-C15	11.62	1.75	1.53
6	A	511	AJP	C10-C08	-9.81	1.31	1.53
6	A	511	AJP	C11-C10	9.27	1.71	1.53
6	A	511	AJP	O84-C85	7.85	1.55	1.43
6	A	511	AJP	C13-C12	-6.82	1.42	1.54
6	A	511	AJP	C14-C15	6.54	1.64	1.53
6	A	511	AJP	C16-C11	-5.73	1.46	1.54
6	A	511	AJP	C20-C15	-5.62	1.46	1.56
6	A	511	AJP	C07-C06	-5.03	1.40	1.54
4	A	501	O50	C08-C07	4.91	1.54	1.49
4	A	501	O50	C16-N18	4.76	1.45	1.35
6	A	511	AJP	C18-C19	4.71	1.64	1.53
6	A	511	AJP	O25-C23	-4.34	1.36	1.44
6	A	511	AJP	C24-C23	4.24	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	511	AJP	C17-C16	-3.51	1.47	1.53
6	A	511	AJP	O50-C49	3.32	1.49	1.43
6	A	511	AJP	C18-C17	3.16	1.60	1.52
6	A	511	AJP	C48-C47	-3.13	1.47	1.52
6	A	511	AJP	O40-C35	2.86	1.49	1.41
6	A	511	AJP	O50-C45	2.84	1.47	1.41
6	A	511	AJP	O64-C57	2.61	1.49	1.43
6	A	511	AJP	O79-C22	-2.60	1.37	1.43
4	A	501	O50	C22-C25	2.52	1.52	1.49
4	A	501	O50	C19-N18	2.51	1.46	1.40
6	A	511	AJP	C58-C57	-2.44	1.46	1.52
5	A	504	CLR	C10-C9	-2.35	1.52	1.56
6	A	511	AJP	O60-C55	2.35	1.47	1.41
5	A	506	CLR	C10-C9	-2.35	1.52	1.56
6	A	511	AJP	C28-C29	-2.34	1.45	1.52
4	A	501	O50	O17-C16	-2.34	1.18	1.23
5	A	505	CLR	C10-C9	-2.31	1.52	1.56
6	A	511	AJP	C37-C36	-2.26	1.47	1.52
6	A	511	AJP	O44-C37	2.25	1.49	1.43
5	A	510	CLR	C10-C9	-2.24	1.52	1.56
5	A	503	CLR	C10-C9	-2.20	1.52	1.56
5	A	508	CLR	C10-C9	-2.17	1.52	1.56
5	A	509	CLR	C10-C9	-2.17	1.52	1.56
5	A	508	CLR	C13-C14	-2.13	1.51	1.55
5	A	507	CLR	C10-C9	-2.12	1.52	1.56
5	A	502	CLR	C10-C9	-2.05	1.52	1.56
6	A	511	AJP	C22-C23	2.05	1.55	1.52

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	511	AJP	O84-C05-C04	11.63	120.89	110.76
6	A	511	AJP	C03-C02-C85	10.71	121.58	108.59
6	A	511	AJP	C13-C12-C07	7.83	126.51	115.36
6	A	511	AJP	O09-C08-C10	7.28	124.94	110.20
6	A	511	AJP	C81-C12-C13	-5.89	101.93	110.61
6	A	511	AJP	C21-C20-C19	5.36	112.35	107.23
4	A	501	O50	C02-C07-N06	-5.34	118.62	123.08
5	A	506	CLR	C13-C17-C20	-5.14	111.56	119.50
5	A	508	CLR	C13-C17-C20	-5.01	111.77	119.50
5	A	509	CLR	C13-C17-C20	-4.88	111.95	119.50
5	A	507	CLR	C13-C17-C20	-4.85	112.01	119.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	505	CLR	C13-C17-C20	-4.57	112.44	119.50
5	A	502	CLR	C13-C17-C20	-4.56	112.45	119.50
5	A	508	CLR	C13-C14-C8	-4.44	108.11	114.41
6	A	511	AJP	C06-C07-C08	-4.42	97.18	104.28
6	A	511	AJP	C13-C12-C11	4.40	116.70	108.11
5	A	504	CLR	C19-C10-C9	-4.15	107.00	111.66
6	A	511	AJP	O40-C35-C36	4.13	117.52	109.49
5	A	510	CLR	C13-C17-C20	-4.05	113.25	119.50
5	A	503	CLR	C13-C17-C20	-4.01	113.31	119.50
5	A	510	CLR	C19-C10-C9	-3.97	107.20	111.66
5	A	503	CLR	C19-C10-C9	-3.94	107.24	111.66
5	A	506	CLR	C19-C10-C9	-3.89	107.29	111.66
6	A	511	AJP	C05-C06-C07	3.86	109.05	103.37
5	A	505	CLR	C19-C10-C9	-3.82	107.37	111.66
6	A	511	AJP	C20-C15-C16	-3.80	108.58	112.43
6	A	511	AJP	C35-O34-C29	-3.79	108.98	117.98
6	A	511	AJP	C13-C14-C15	-3.78	106.72	113.14
4	A	501	O50	C08-C09-C10	-3.72	118.58	120.19
5	A	508	CLR	C17-C13-C14	3.70	104.35	100.10
5	A	502	CLR	C19-C10-C9	-3.65	107.56	111.66
5	A	507	CLR	C19-C10-C9	-3.62	107.60	111.66
5	A	509	CLR	C19-C10-C9	-3.58	107.64	111.66
4	A	501	O50	C24-C23-C22	-3.50	116.63	121.12
6	A	511	AJP	C12-C11-C16	3.46	118.72	113.90
6	A	511	AJP	C81-C12-C11	-3.44	104.10	111.58
6	A	511	AJP	C21-C20-C15	3.39	114.66	110.10
4	A	501	O50	C05-N06-C07	3.39	123.87	118.01
4	A	501	O50	C21-N20-C19	3.38	121.00	117.83
4	A	501	O50	C13-C12-N11	-3.33	119.90	123.97
6	A	511	AJP	O09-C05-C06	-3.29	100.19	104.56
6	A	511	AJP	C26-O25-C23	-3.25	109.83	115.27
6	A	511	AJP	C12-C07-C06	3.19	129.94	120.50
5	A	502	CLR	C13-C14-C8	-3.18	109.90	114.41
5	A	506	CLR	C13-C14-C8	-3.16	109.93	114.41
5	A	502	CLR	C9-C10-C5	3.10	114.19	109.65
5	A	509	CLR	C13-C14-C8	-3.10	110.01	114.41
4	A	501	O50	C09-C08-C07	3.10	125.69	120.09
6	A	511	AJP	C20-C21-C22	-3.08	109.11	114.17
5	A	503	CLR	C13-C14-C8	-3.04	110.10	114.41
5	A	507	CLR	C13-C14-C8	-3.02	110.13	114.41
6	A	511	AJP	C01-C02-C85	-2.99	106.42	111.03
4	A	501	O50	C02-C03-C04	-2.95	118.90	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	503	CLR	C9-C10-C5	2.95	113.97	109.65
5	A	510	CLR	C13-C14-C8	-2.91	110.28	114.41
6	A	511	AJP	C11-C12-C07	-2.82	95.90	100.16
5	A	508	CLR	C11-C12-C13	-2.80	108.01	112.74
5	A	504	CLR	C13-C14-C8	-2.75	110.51	114.41
5	A	504	CLR	C15-C14-C8	-2.71	114.78	119.10
4	A	501	O50	C04-C05-N06	-2.67	120.03	123.99
5	A	509	CLR	C9-C10-C5	2.61	113.48	109.65
5	A	507	CLR	C9-C10-C5	2.61	113.47	109.65
5	A	505	CLR	C13-C14-C8	-2.59	110.74	114.41
4	A	501	O50	C19-N18-C16	-2.55	123.55	128.22
5	A	502	CLR	C8-C7-C6	-2.54	109.25	112.76
5	A	504	CLR	C18-C13-C14	-2.53	107.08	111.68
6	A	511	AJP	C04-C03-C02	2.52	116.69	111.67
6	A	511	AJP	C45-O44-C37	-2.49	112.06	117.98
6	A	511	AJP	C35-C36-C37	2.49	115.58	110.74
5	A	502	CLR	C21-C20-C17	-2.49	109.15	112.88
5	A	509	CLR	C3-C4-C5	-2.48	108.10	112.05
5	A	507	CLR	C3-C4-C5	-2.46	108.14	112.05
6	A	511	AJP	C85-O84-C05	2.43	117.89	113.69
5	A	506	CLR	C21-C20-C17	-2.38	109.31	112.88
4	A	501	O50	C03-C04-C05	2.36	119.09	116.90
5	A	504	CLR	C3-C4-C5	-2.36	108.30	112.05
4	A	501	O50	C13-C08-C07	-2.34	116.82	120.62
5	A	508	CLR	C4-C5-C10	2.33	119.41	116.42
5	A	510	CLR	C4-C5-C6	-2.33	117.41	120.57
4	A	501	O50	N18-C19-N20	2.32	121.82	114.87
5	A	504	CLR	C16-C17-C20	-2.30	108.69	112.18
5	A	510	CLR	C3-C4-C5	-2.30	108.39	112.05
5	A	506	CLR	C3-C4-C5	-2.25	108.47	112.05
5	A	504	CLR	C9-C10-C5	2.24	112.93	109.65
5	A	505	CLR	C4-C5-C6	-2.23	117.55	120.57
5	A	502	CLR	C3-C4-C5	-2.23	108.50	112.05
4	A	501	O50	C03-C02-C07	2.22	119.49	117.16
6	A	511	AJP	C03-C04-C05	2.22	115.42	111.93
5	A	506	CLR	C23-C22-C20	-2.22	108.87	115.08
5	A	509	CLR	C8-C7-C6	-2.22	109.69	112.76
5	A	506	CLR	C9-C10-C5	2.21	112.89	109.65
5	A	504	CLR	C4-C5-C6	-2.19	117.59	120.57
5	A	505	CLR	C9-C10-C5	2.19	112.86	109.65
4	A	501	O50	C30-C25-C22	-2.18	119.19	122.10
5	A	506	CLR	C11-C9-C10	-2.17	110.41	113.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	511	AJP	C80-C20-C19	-2.17	106.81	110.44
5	A	505	CLR	C21-C20-C17	-2.17	109.63	112.88
5	A	510	CLR	C15-C14-C13	-2.16	101.30	103.84
5	A	505	CLR	C14-C8-C9	-2.16	106.27	109.09
6	A	511	AJP	C04-C05-C06	-2.15	111.77	115.66
5	A	506	CLR	C4-C5-C6	-2.14	117.67	120.57
5	A	503	CLR	C14-C8-C9	-2.13	106.30	109.09
6	A	511	AJP	C14-C13-C12	-2.13	109.14	112.74
5	A	509	CLR	C4-C5-C6	-2.13	117.68	120.57
5	A	503	CLR	C15-C14-C13	-2.13	101.34	103.84
5	A	508	CLR	C10-C9-C8	-2.12	109.61	112.71
5	A	510	CLR	C9-C10-C5	2.12	112.75	109.65
6	A	511	AJP	O84-C05-O09	-2.10	104.87	109.88
5	A	509	CLR	C21-C20-C17	-2.10	109.73	112.88
5	A	507	CLR	C21-C20-C17	-2.10	109.73	112.88
4	A	501	O50	C27-C28-N29	-2.09	119.36	121.96
5	A	504	CLR	C8-C7-C6	-2.08	109.88	112.76
4	A	501	O50	C15-C16-N18	2.08	118.62	114.73
5	A	503	CLR	C3-C4-C5	-2.08	108.75	112.05
4	A	501	O50	C28-N29-C30	2.07	120.49	116.85
5	A	505	CLR	C15-C14-C13	-2.07	101.41	103.84
5	A	507	CLR	C4-C5-C6	-2.06	117.77	120.57
6	A	511	AJP	C41-C39-C38	-2.06	107.96	113.02
5	A	507	CLR	C23-C22-C20	-2.06	109.32	115.08
6	A	511	AJP	O31-C30-C32	2.05	111.51	106.44
5	A	502	CLR	C15-C14-C8	-2.04	115.84	119.10
5	A	503	CLR	C8-C7-C6	-2.04	109.94	112.76
5	A	502	CLR	C4-C5-C6	-2.04	117.81	120.57
5	A	504	CLR	C13-C17-C20	-2.03	116.35	119.50
5	A	506	CLR	C15-C14-C13	-2.03	101.45	103.84
5	A	509	CLR	C15-C14-C8	-2.02	115.87	119.10
5	A	504	CLR	C11-C9-C10	-2.01	110.60	113.08
5	A	510	CLR	C18-C13-C14	-2.01	108.03	111.68
5	A	508	CLR	C7-C6-C5	-2.00	121.64	125.02

All (29) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	511	AJP	C07
6	A	511	AJP	C48
6	A	511	AJP	C26
6	A	511	AJP	C02

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Mol	Chain	Res	Type	Atom
6	A	511	AJP	C28
6	A	511	AJP	C39
6	A	511	AJP	C56
6	A	511	AJP	C05
6	A	511	AJP	C11
6	A	511	AJP	C45
6	A	511	AJP	C12
6	A	511	AJP	C36
6	A	511	AJP	C37
6	A	511	AJP	C16
6	A	511	AJP	C20
6	A	511	AJP	C35
6	A	511	AJP	C57
6	A	511	AJP	C19
6	A	511	AJP	C46
6	A	511	AJP	C27
6	A	511	AJP	C59
6	A	511	AJP	C15
6	A	511	AJP	C22
6	A	511	AJP	C30
6	A	511	AJP	C38
6	A	511	AJP	C55
6	A	511	AJP	C23
6	A	511	AJP	C10
6	A	511	AJP	C47

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	504	CLR	C17-C20-C22-C23
6	A	511	AJP	O60-C55-O54-C36
6	A	511	AJP	O50-C45-O44-C37
5	A	508	CLR	C13-C17-C20-C21
5	A	508	CLR	C16-C17-C20-C21
6	A	511	AJP	C30-C29-O34-C35
5	A	508	CLR	C13-C17-C20-C22
5	A	505	CLR	C13-C17-C20-C21
5	A	507	CLR	C13-C17-C20-C21
5	A	510	CLR	C17-C20-C22-C23
5	A	510	CLR	C21-C20-C22-C23
5	A	506	CLR	C13-C17-C20-C21
5	A	507	CLR	C21-C20-C22-C23

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Mol	Chain	Res	Type	Atoms
6	A	511	AJP	O31-C30-C32-O33
5	A	502	CLR	C13-C17-C20-C21
5	A	505	CLR	C13-C17-C20-C22
6	A	511	AJP	C46-C45-O44-C37
5	A	507	CLR	C17-C20-C22-C23
5	A	508	CLR	C16-C17-C20-C22
5	A	503	CLR	C20-C22-C23-C24
5	A	507	CLR	C20-C22-C23-C24
6	A	511	AJP	O60-C59-C61-O62
5	A	509	CLR	C13-C17-C20-C21
5	A	507	CLR	C13-C17-C20-C22
5	A	502	CLR	C13-C17-C20-C22
5	A	506	CLR	C13-C17-C20-C22
6	A	511	AJP	O31-C26-O25-C23
5	A	505	CLR	C21-C20-C22-C23
6	A	511	AJP	O40-C39-C41-O42
4	A	501	O50	N20-C19-N18-C16
4	A	501	O50	C24-C19-N18-C16
5	A	505	CLR	C16-C17-C20-C21
5	A	507	CLR	C16-C17-C20-C21
6	A	511	AJP	C29-C30-C32-O33
5	A	509	CLR	C13-C17-C20-C22
5	A	502	CLR	C16-C17-C20-C21
5	A	506	CLR	C16-C17-C20-C21
5	A	509	CLR	C16-C17-C20-C21
5	A	503	CLR	C22-C23-C24-C25
6	A	511	AJP	C56-C55-O54-C36
6	A	511	AJP	C28-C29-O34-C35
5	A	510	CLR	C22-C23-C24-C25
5	A	509	CLR	C20-C22-C23-C24
5	A	503	CLR	C23-C24-C25-C27
5	A	503	CLR	C13-C17-C20-C21
5	A	510	CLR	C13-C17-C20-C21
5	A	505	CLR	C16-C17-C20-C22
5	A	507	CLR	C16-C17-C20-C22
5	A	503	CLR	C23-C24-C25-C26
5	A	502	CLR	C16-C17-C20-C22
5	A	504	CLR	C20-C22-C23-C24
5	A	506	CLR	C16-C17-C20-C22
5	A	502	CLR	C21-C20-C22-C23
5	A	509	CLR	C16-C17-C20-C22
5	A	503	CLR	C13-C17-C20-C22

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	A	510	CLR	C13-C17-C20-C22
5	A	504	CLR	C22-C23-C24-C25
5	A	504	CLR	C21-C20-C22-C23
5	A	506	CLR	C23-C24-C25-C26
5	A	503	CLR	C16-C17-C20-C21
6	A	511	AJP	C27-C26-O25-C23

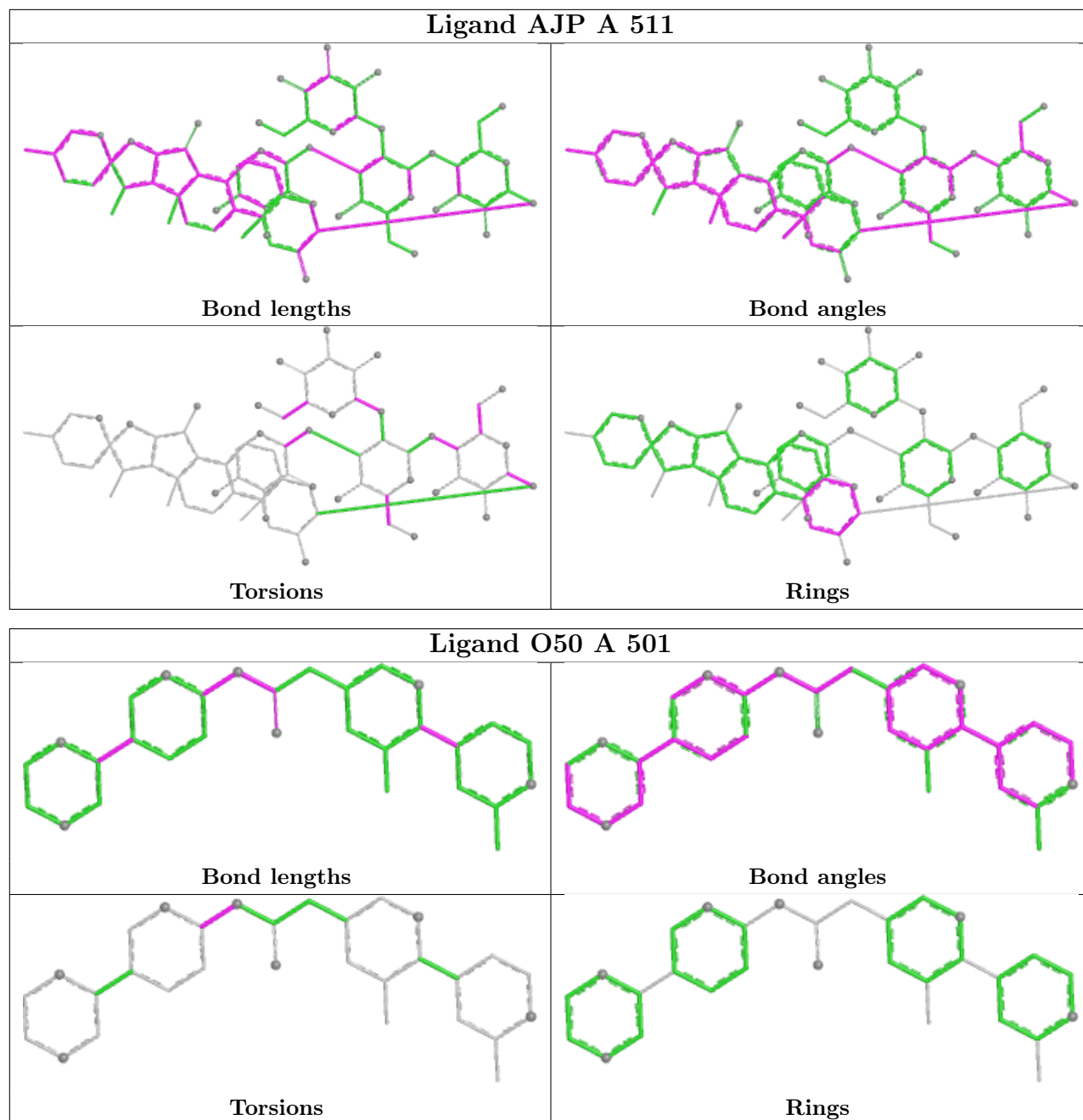
All (1) ring outliers are listed below:

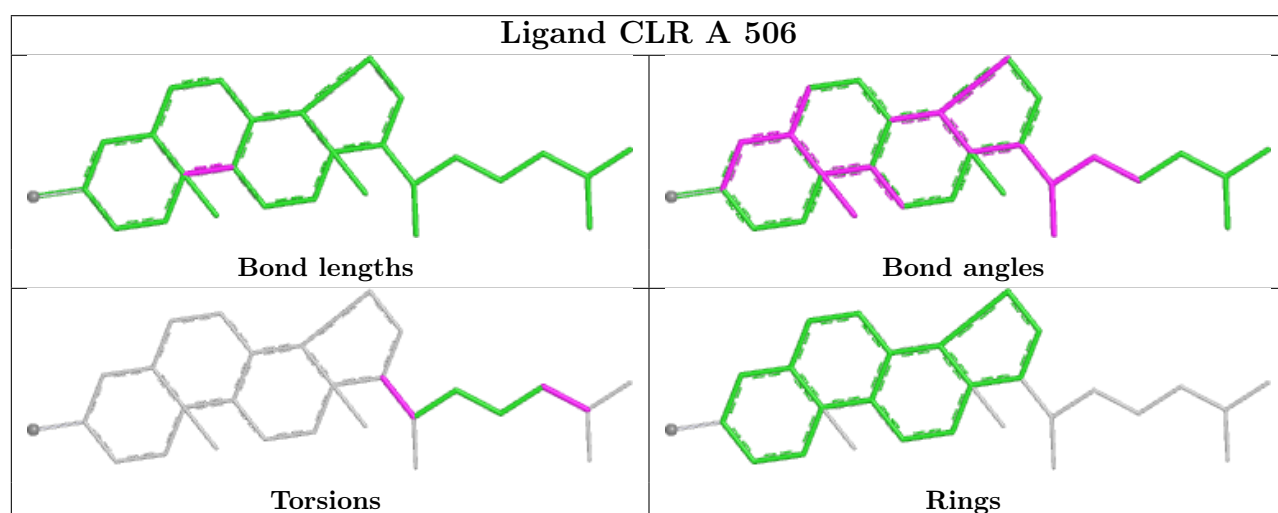
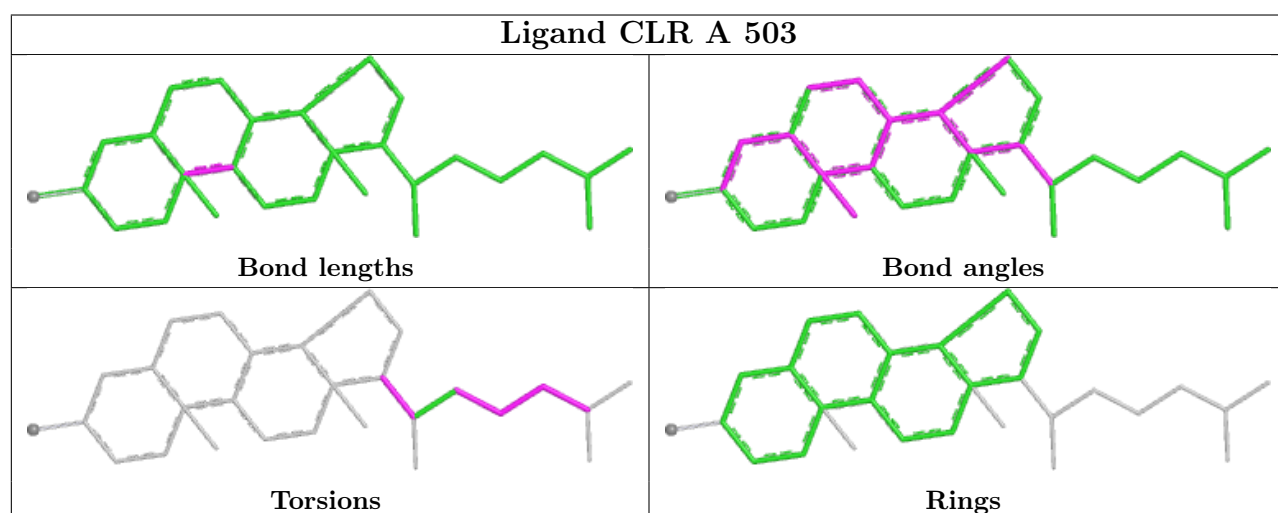
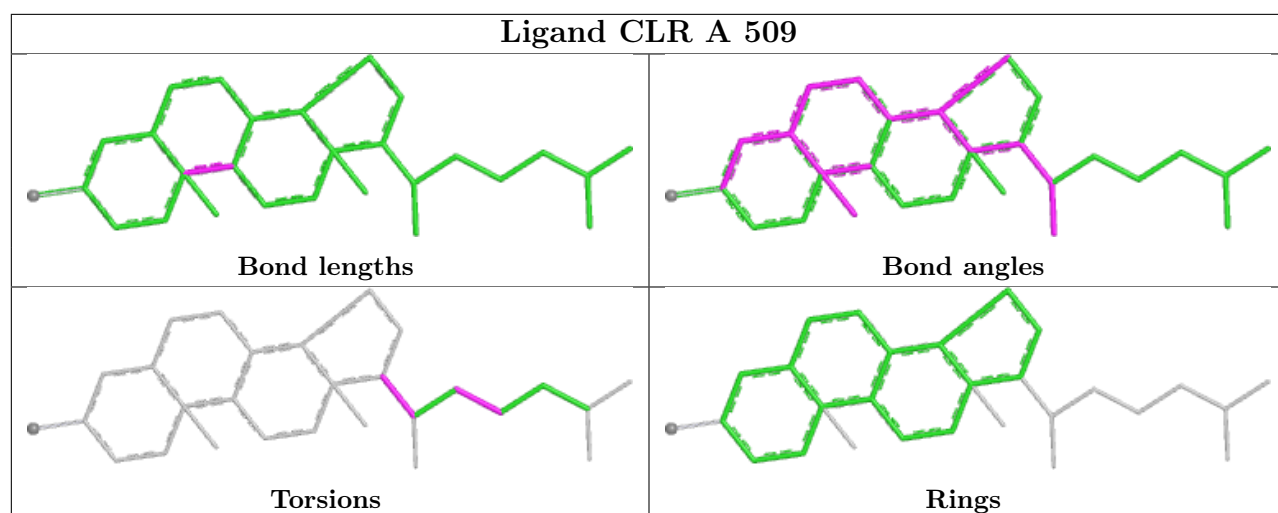
Mol	Chain	Res	Type	Atoms
6	A	511	AJP	C19-C20-C21-C22-C23-C24

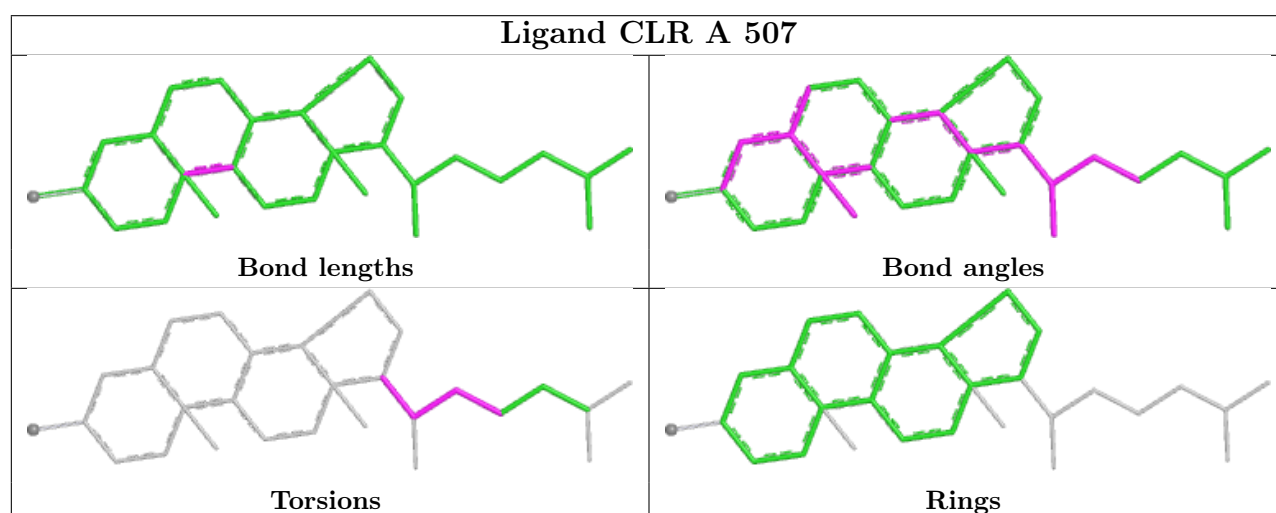
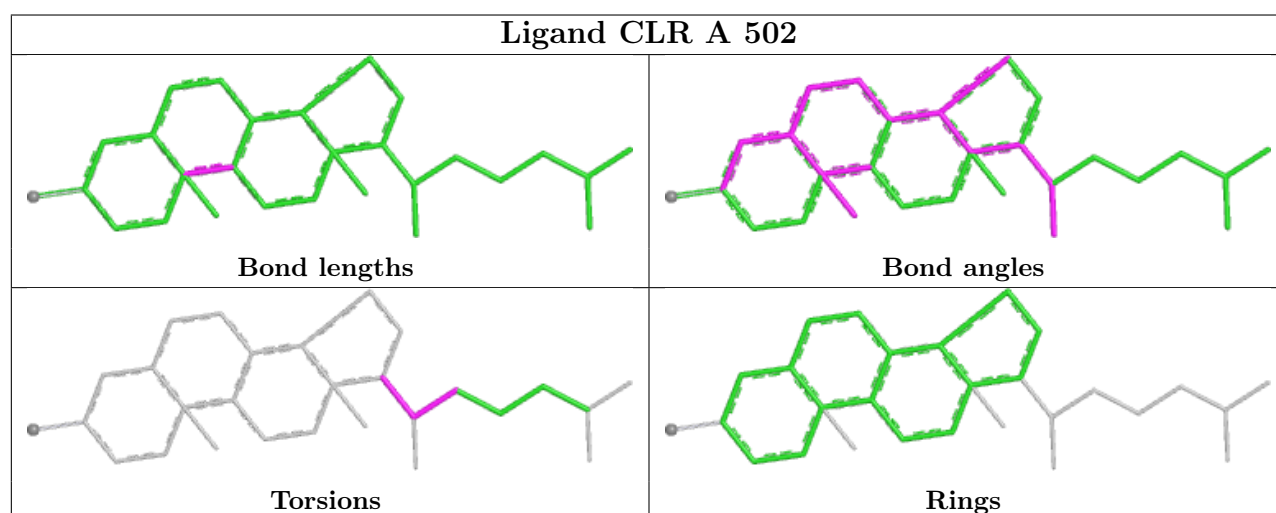
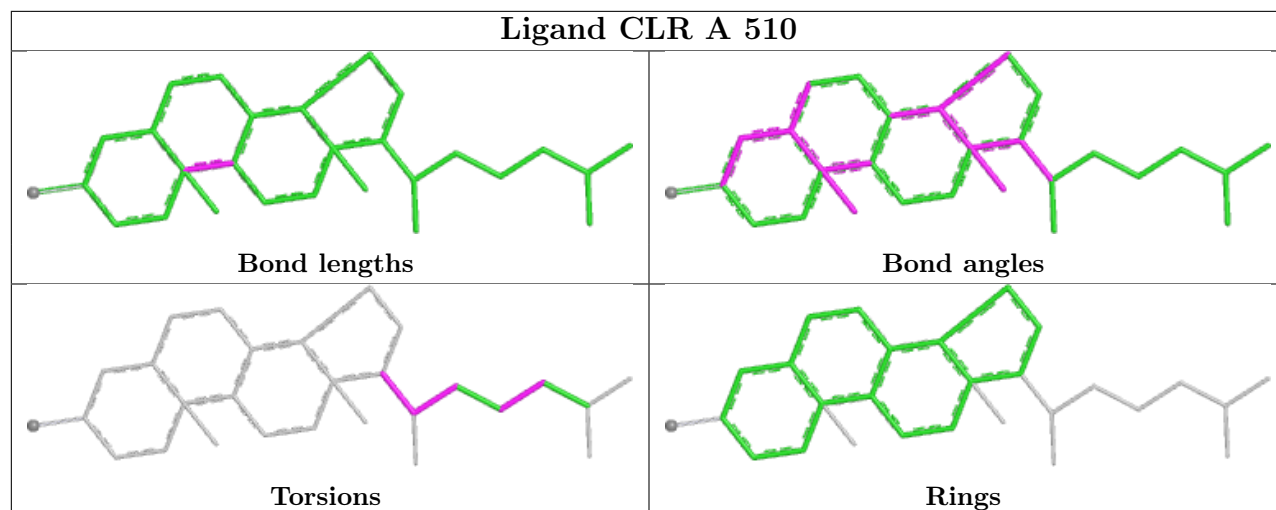
10 monomers are involved in 45 short contacts:

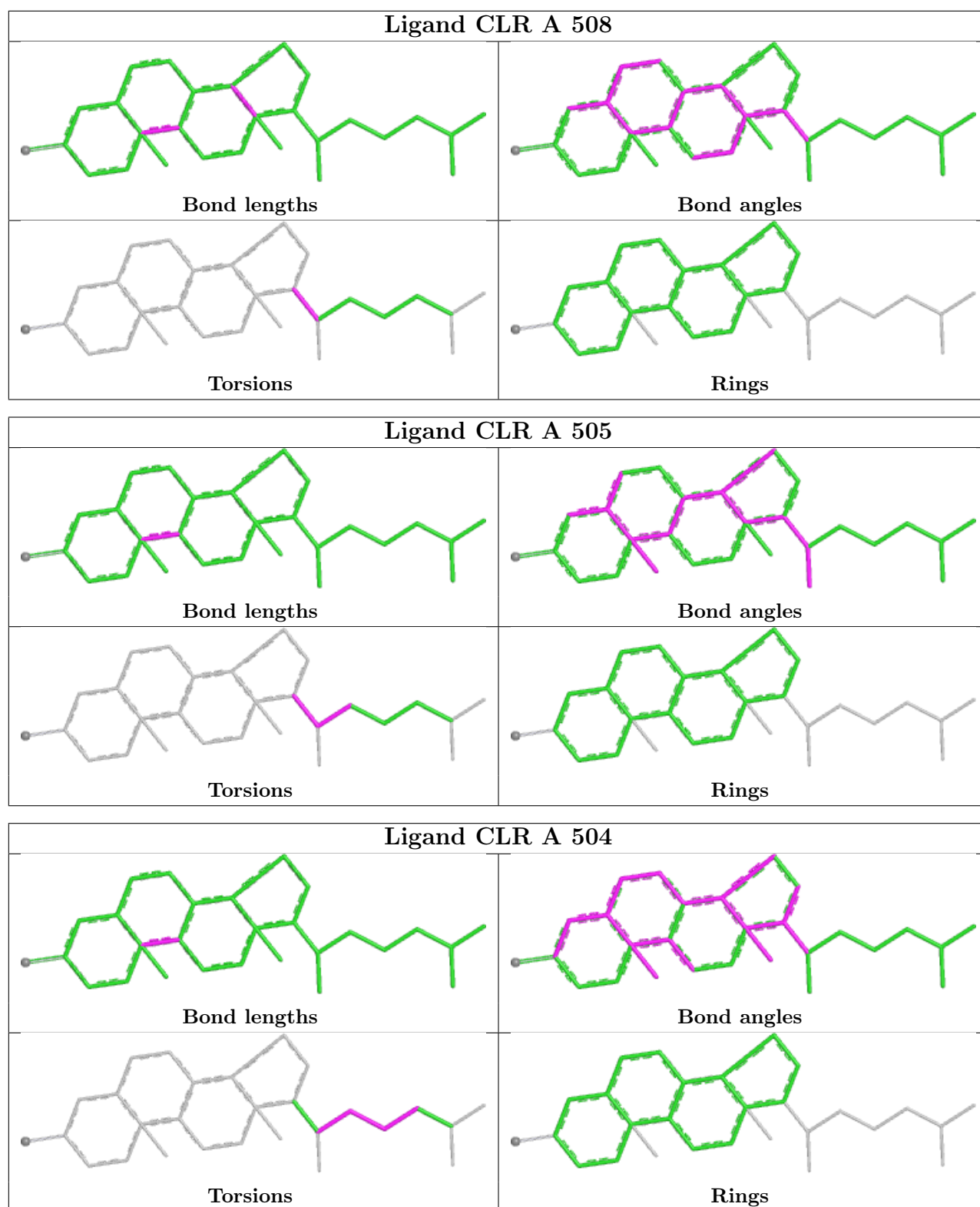
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	511	AJP	28	0
5	A	509	CLR	2	0
5	A	503	CLR	2	0
5	A	506	CLR	2	0
5	A	510	CLR	1	0
5	A	502	CLR	2	0
5	A	507	CLR	1	0
5	A	508	CLR	5	0
5	A	505	CLR	1	0
5	A	504	CLR	2	0

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 ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

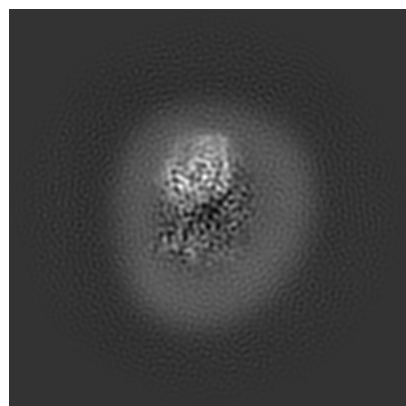
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26708. These allow visual inspection of the internal detail of the map and identification of artifacts.

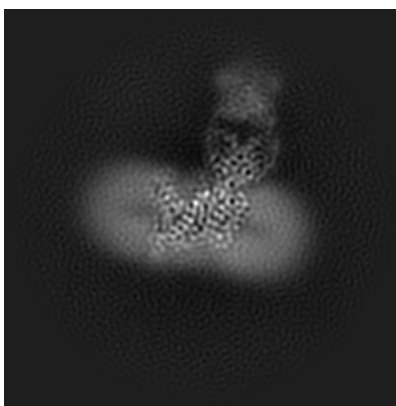
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

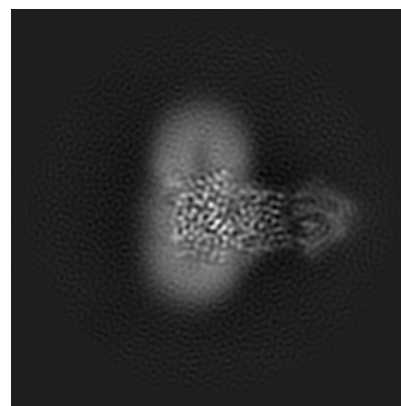
#### 6.1.1 Primary map



X

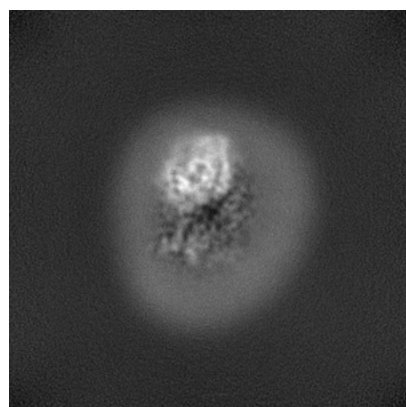


Y

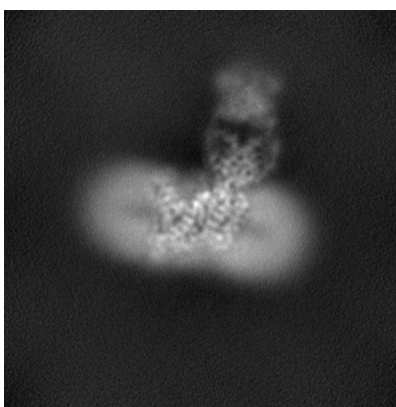


Z

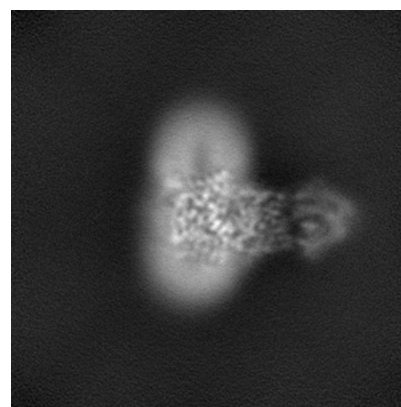
#### 6.1.2 Raw map



X



Y

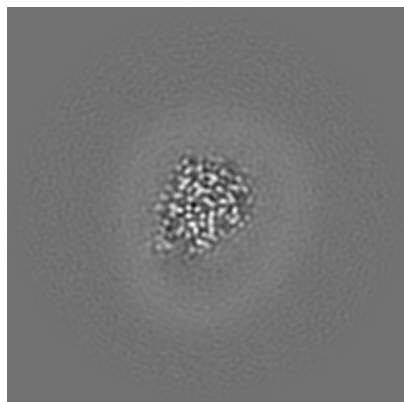


Z

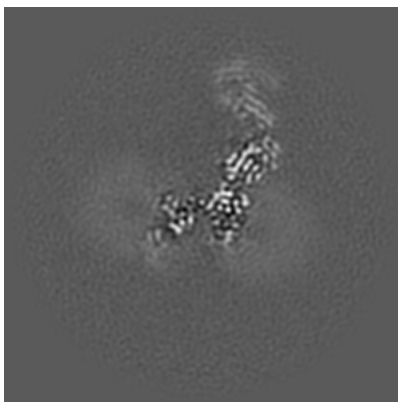
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

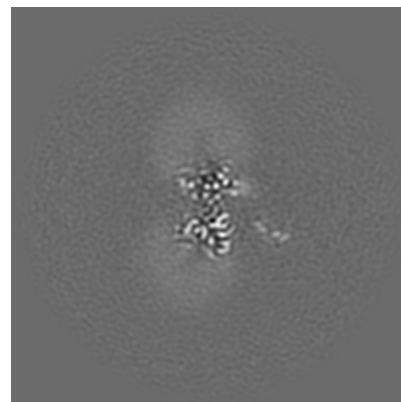
### 6.2.1 Primary map



X Index: 140

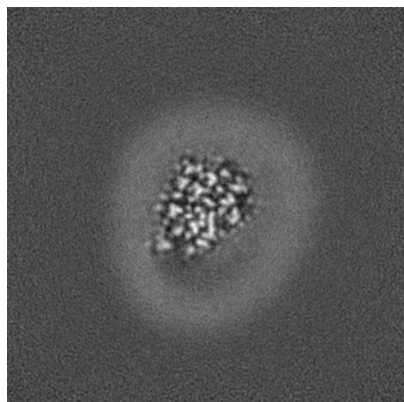


Y Index: 140

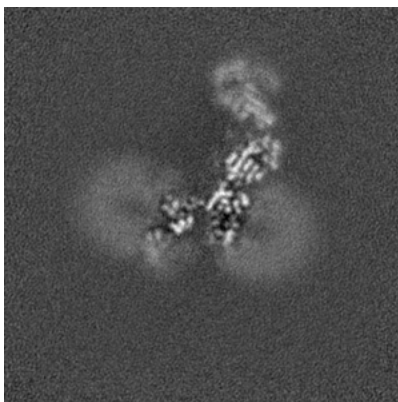


Z Index: 140

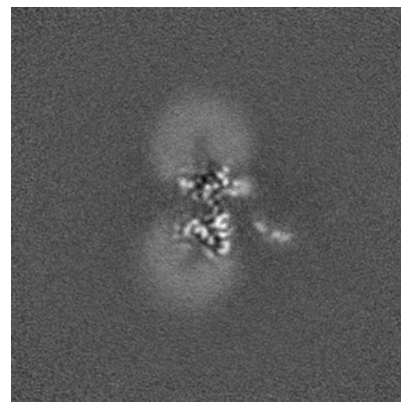
### 6.2.2 Raw map



X Index: 140



Y Index: 140

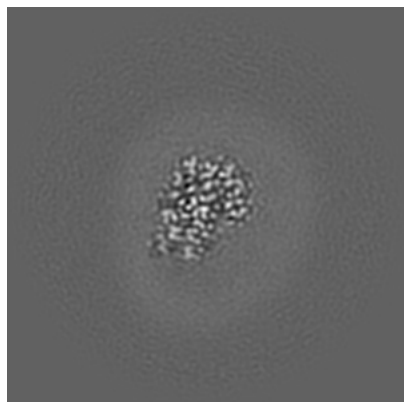


Z Index: 140

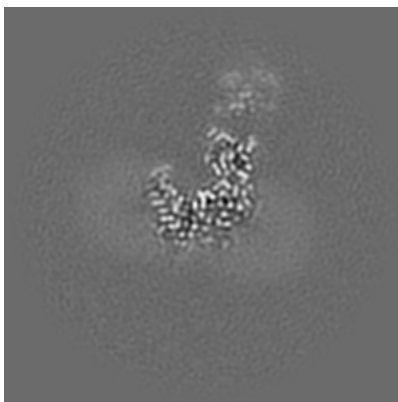
The images above show central slices of the map in three orthogonal directions.

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

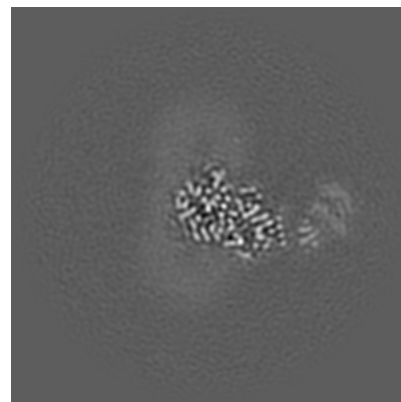
### 6.3.1 Primary map



X Index: 143

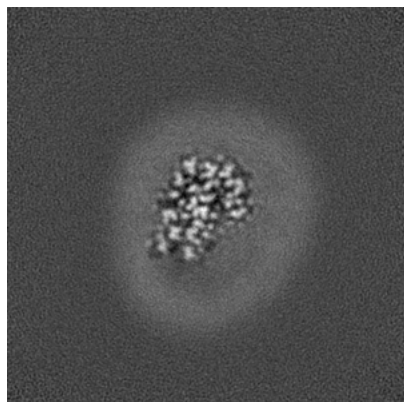


Y Index: 126

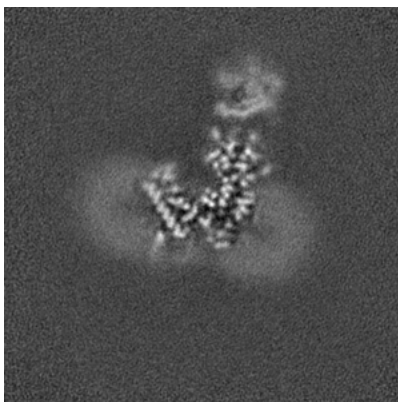


Z Index: 157

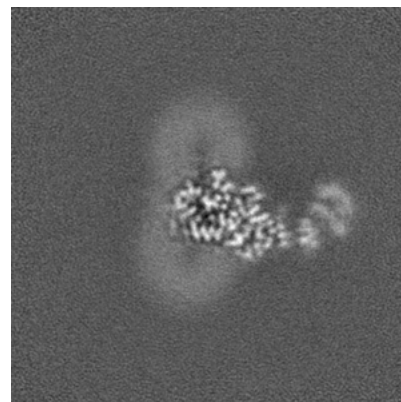
### 6.3.2 Raw map



X Index: 143



Y Index: 129

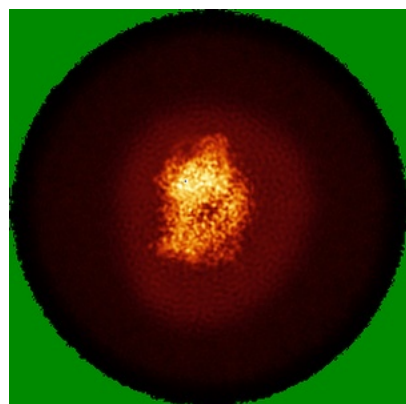


Z Index: 156

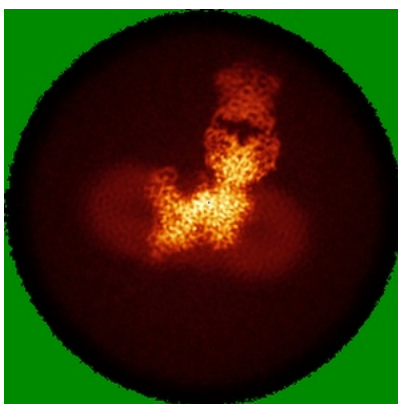
The images above show the largest variance slices of the map in three orthogonal directions.

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

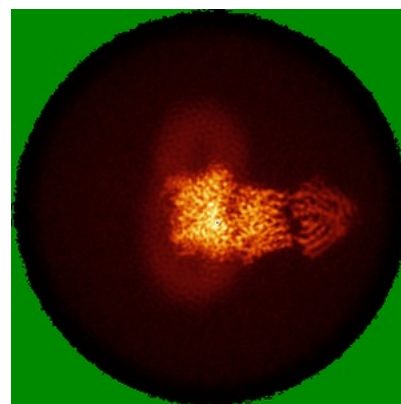
### 6.4.1 Primary map



X

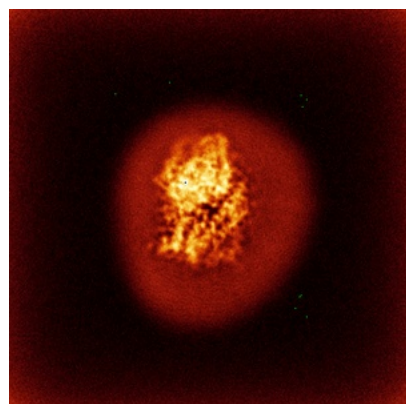


Y

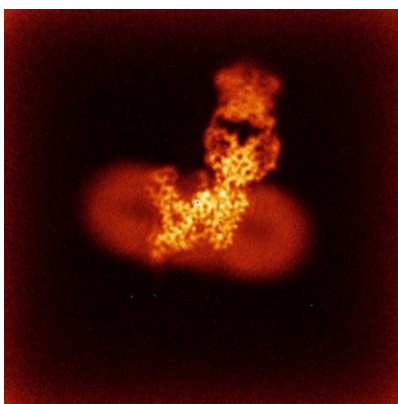


Z

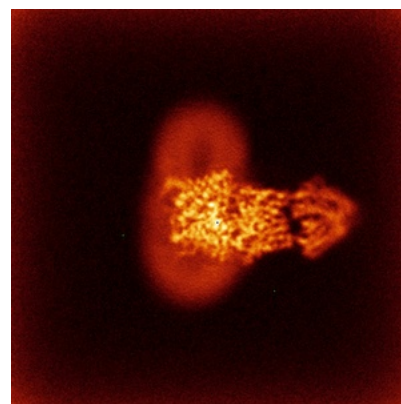
### 6.4.2 Raw map



X



Y

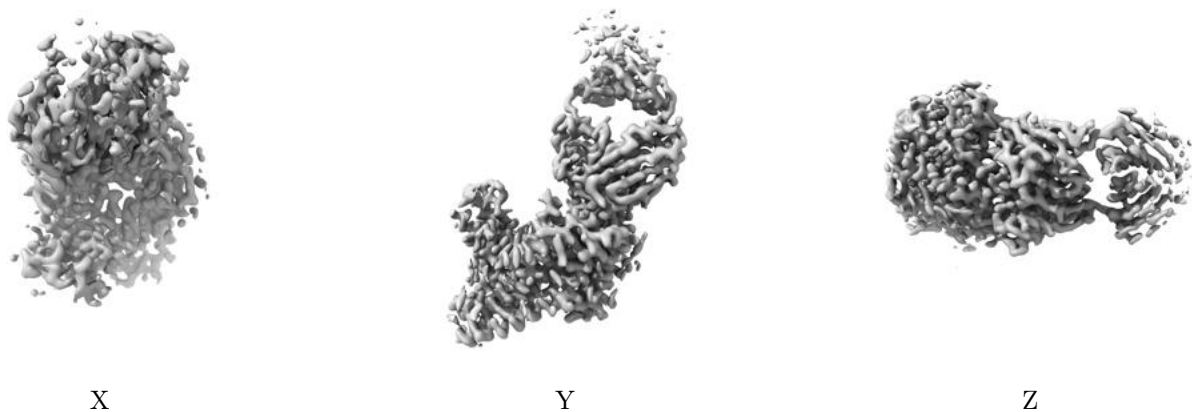


Z

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.

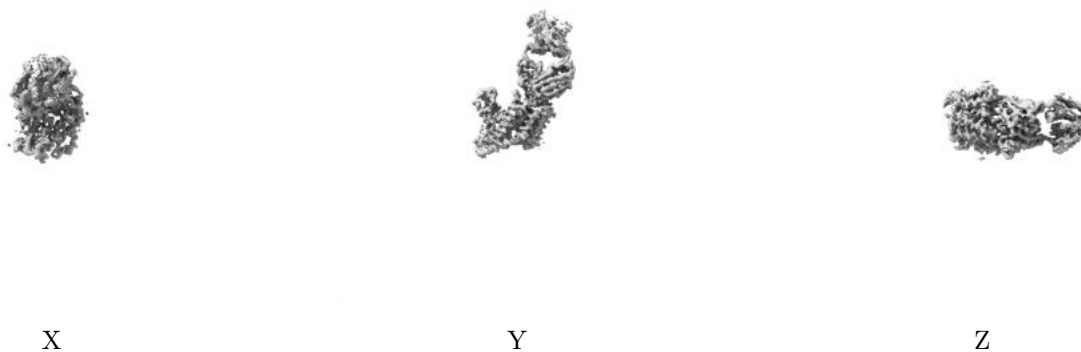
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

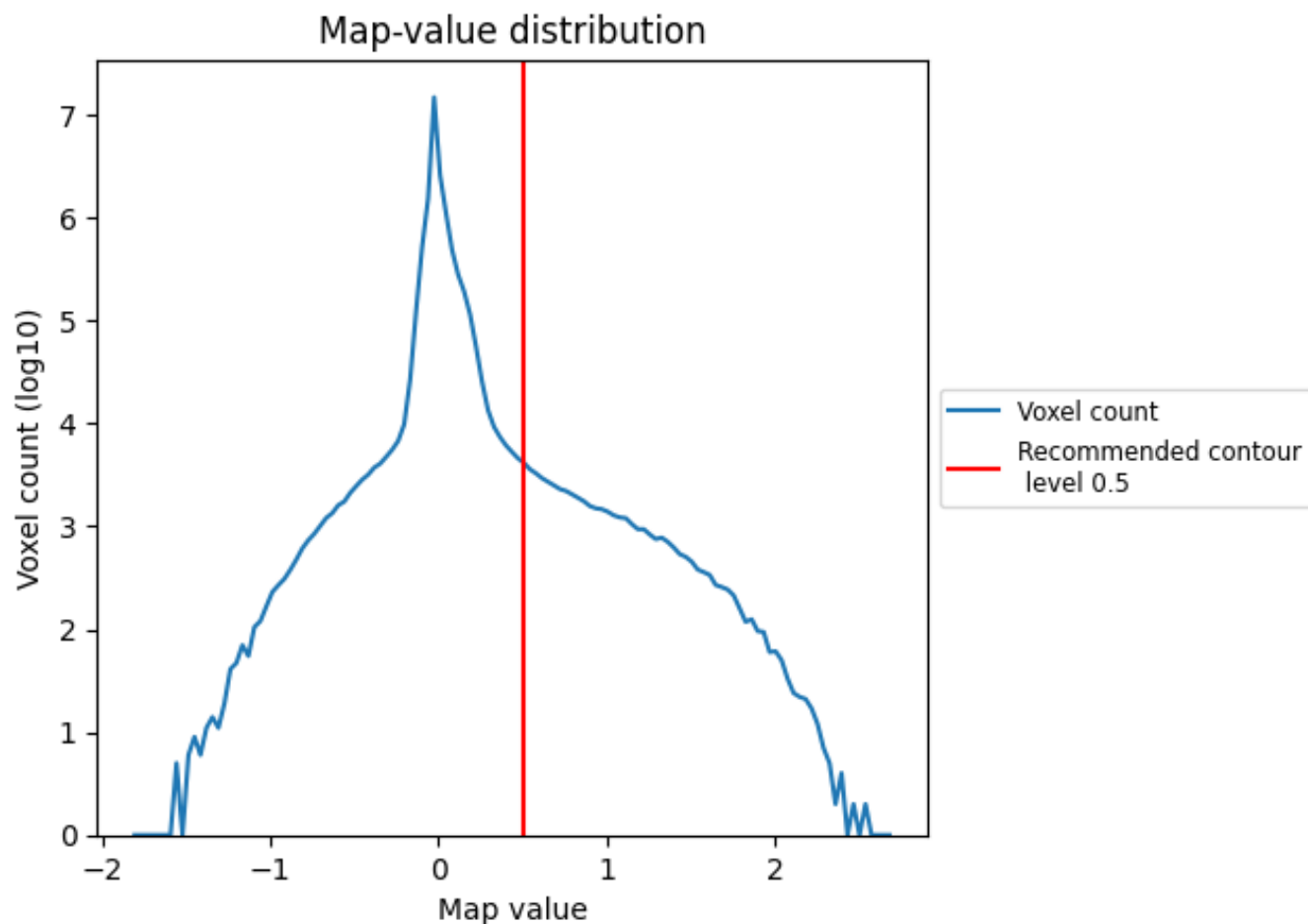
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

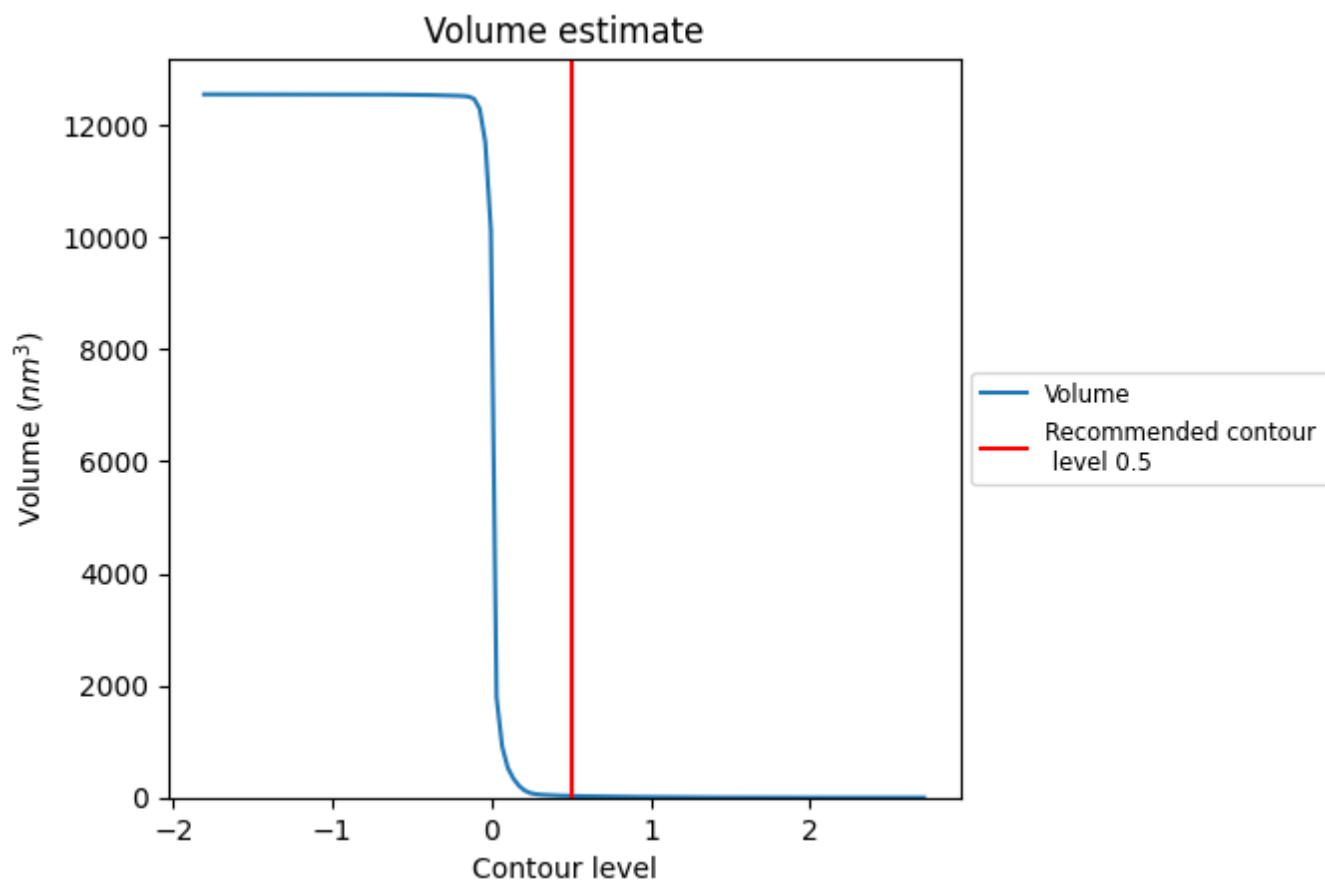
This section contains the results of statistical analysis of the map.

### 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.

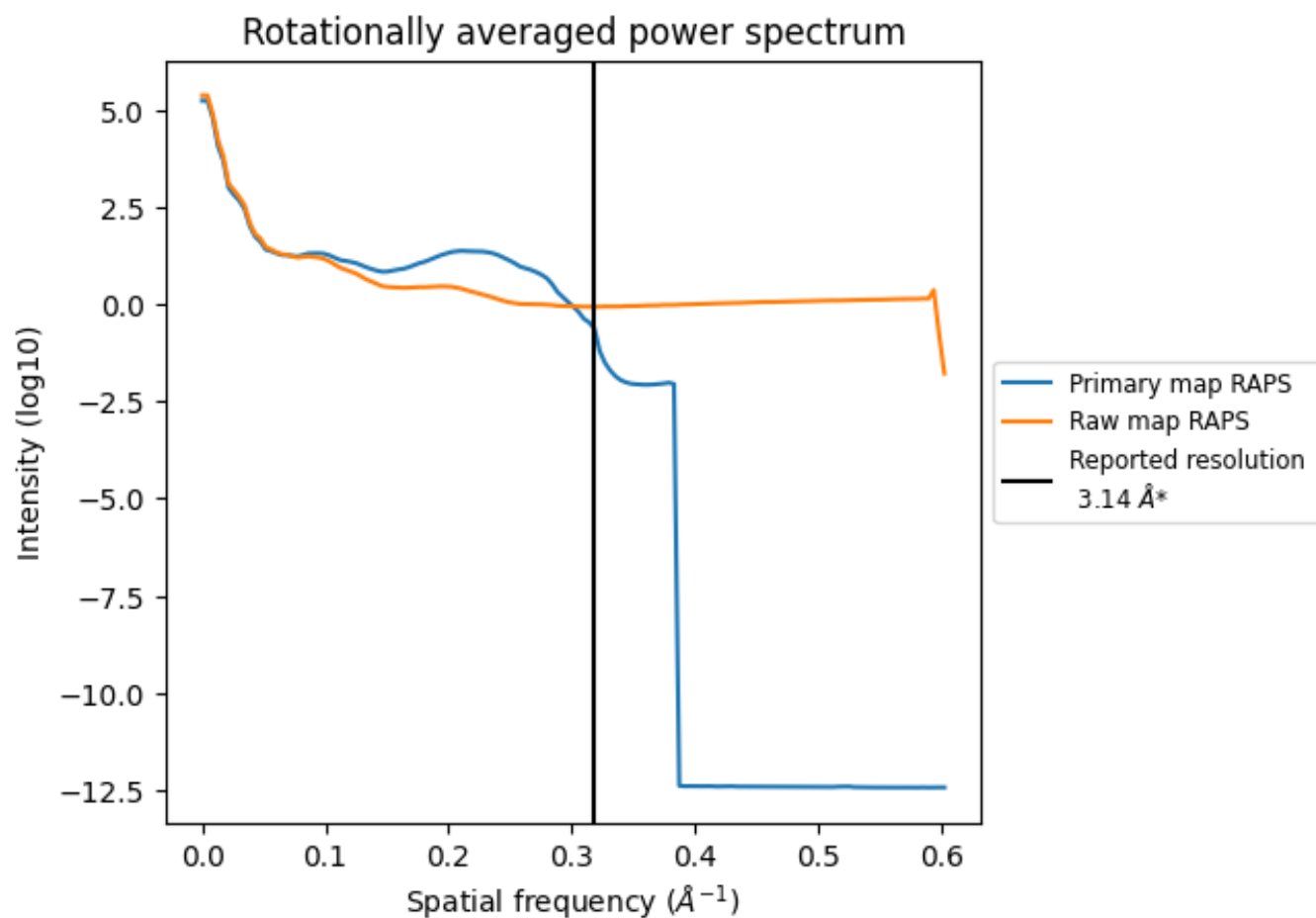
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 29 nm<sup>3</sup>; this corresponds to an approximate mass of 26 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 ⓘ

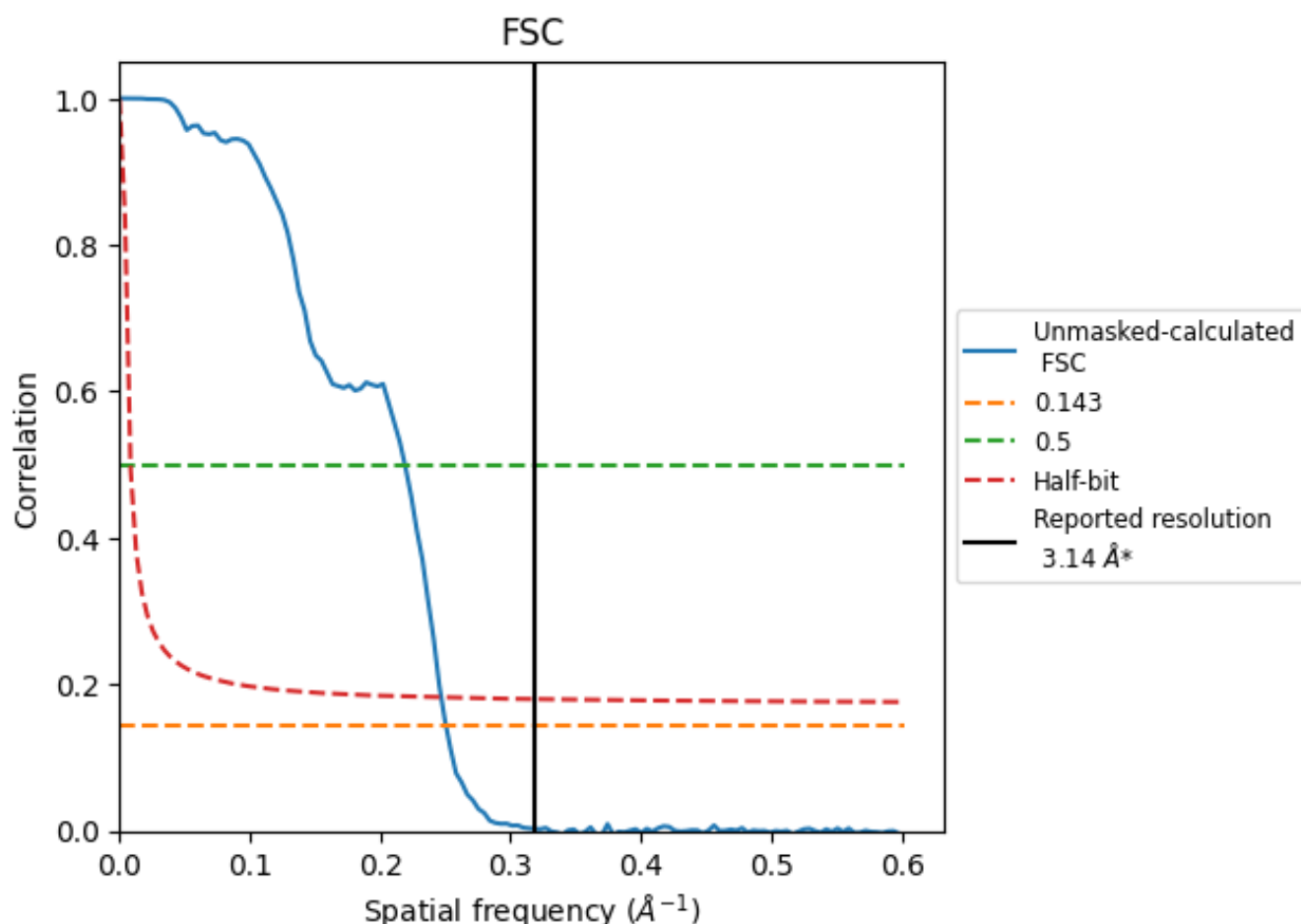


\*Reported resolution corresponds to spatial frequency of 0.318 Å<sup>-1</sup>

## 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 0.318  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

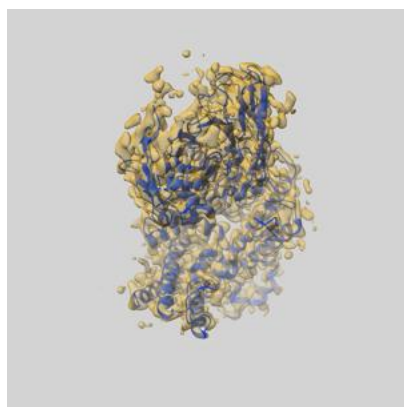
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.14	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.99	4.57	4.05

\*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 3.99 differs from the reported value 3.14 by more than 10 %

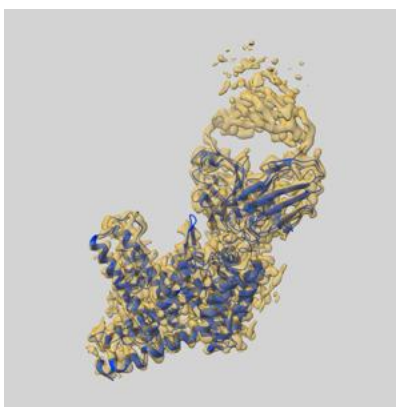
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-26708 and PDB model 7URC. Per-residue inclusion information can be found in section [3](#) on page [6](#).

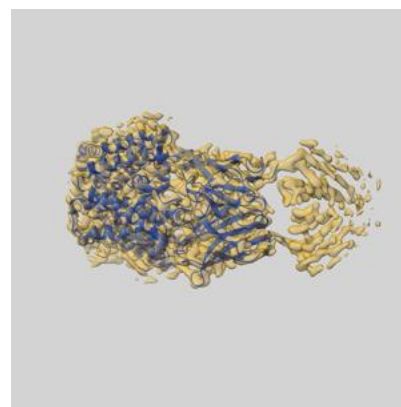
### 9.1 Map-model overlay [i](#)



X



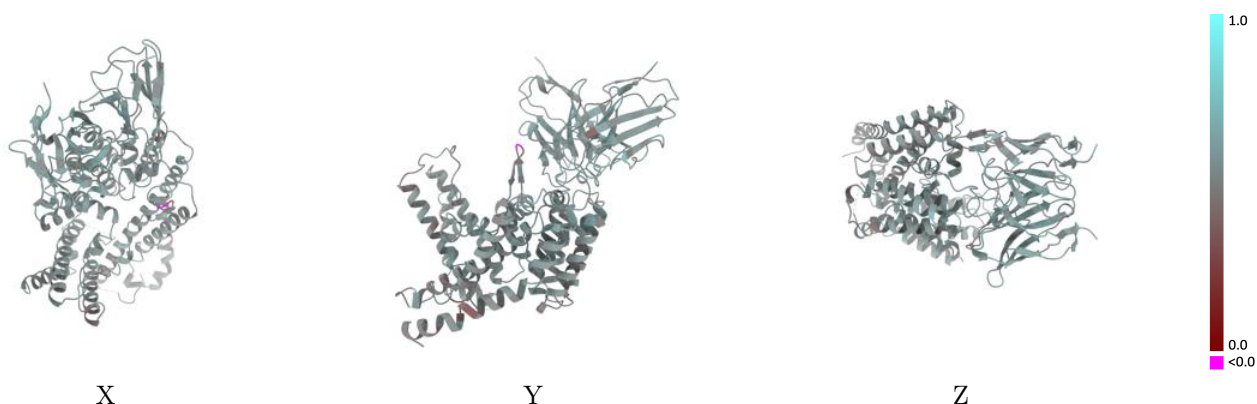
Y



Z

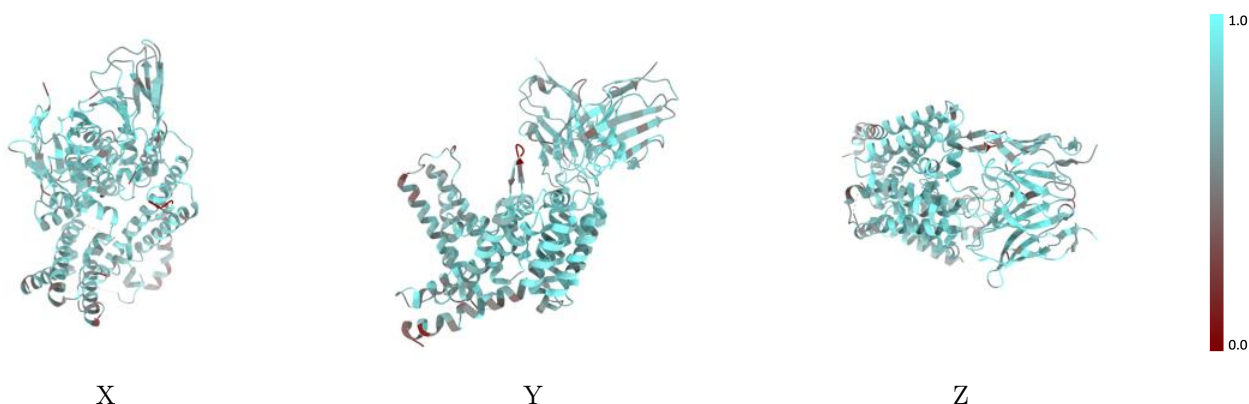
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



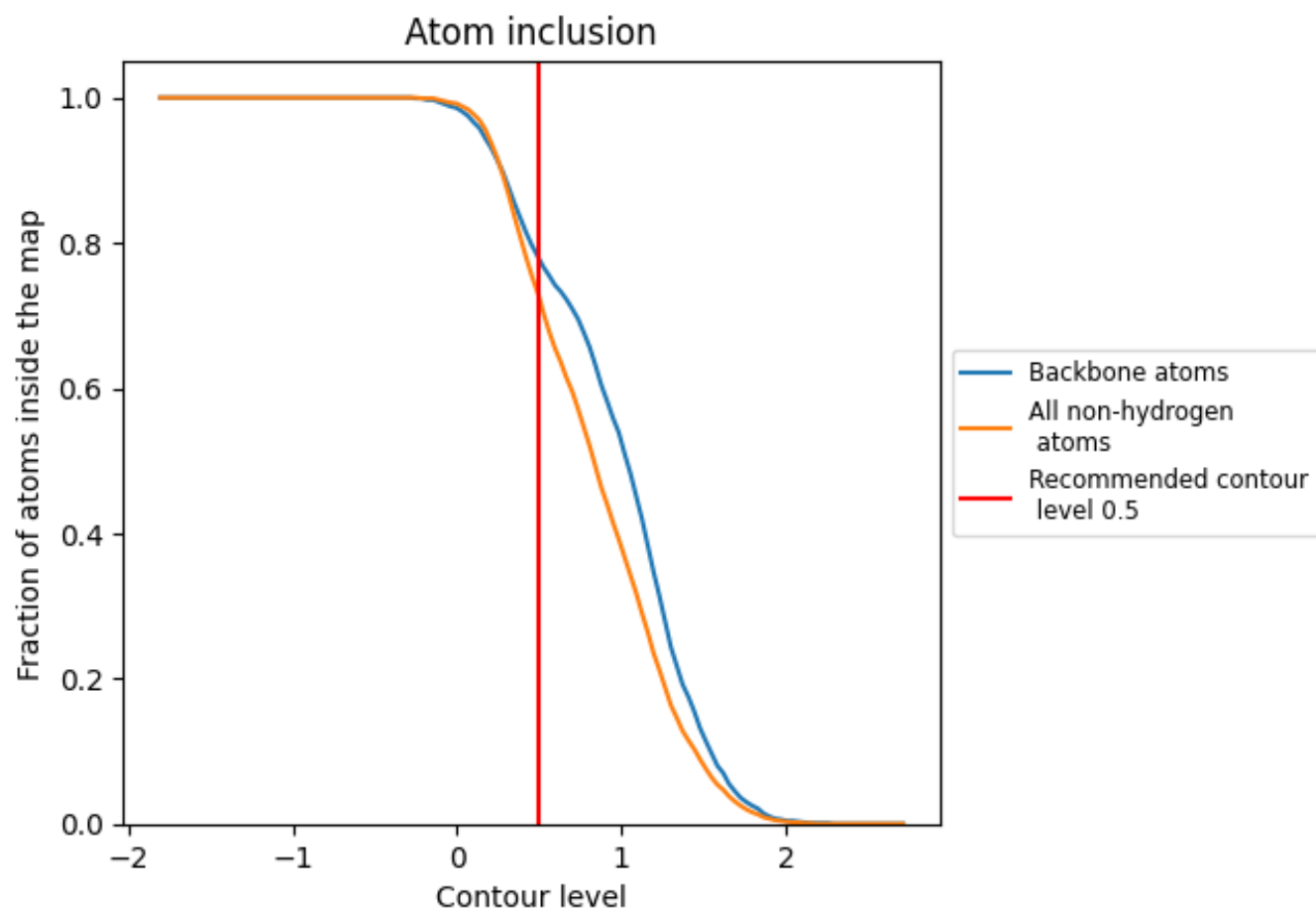
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 72% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.7250	<div><div></div></div> 0.5320
A	<div><div></div></div> 0.7170	<div><div></div></div> 0.5220
H	<div><div></div></div> 0.7580	<div><div></div></div> 0.5580
L	<div><div></div></div> 0.7270	<div><div></div></div> 0.5480

