wwPDB EM Validation Summary Report

Jun 10, 2025 – 06:59 PM JST

PDB ID	:	8K96 / pdb_00008k96
EMDB ID	:	EMD-36976
Title	:	CryoEM structure of LonC protease hepatmer with Bortezomib
Authors	:	Li, M.; Hsieh, K.; Liu, H.; Zhang, S.; Gao, Y.; Gong, Q.; Zhang, K.; Chang, C.; Li, S.
Deposited on	:	2023-07-31
Resolution	:	2.89 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

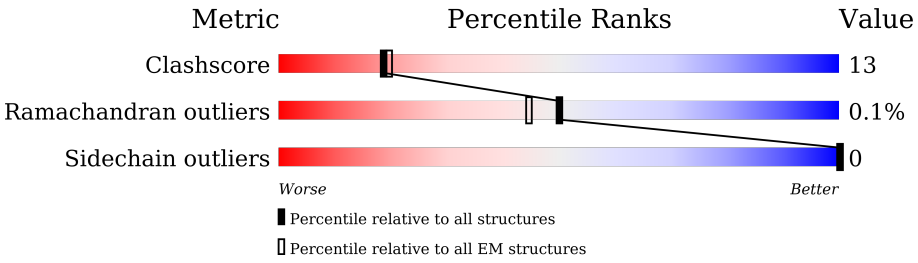
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 2.89 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	732	7% 69% 30%
1	B	732	7% 69% 29%
1	C	732	7% 70% 28%
1	D	732	7% 69% 29%
1	E	732	7% 70% 28%
1	F	732	7% 70% 28%
1	G	732	7% 70% 29%

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
2	PO4	A	801	-	-	X	-
2	PO4	B	801	-	-	X	-
2	PO4	C	801	-	-	X	-
2	PO4	D	801	-	-	X	-
2	PO4	E	801	-	-	X	-
2	PO4	F	801	-	-	X	-
2	PO4	G	801	-	-	X	-
3	BO2	A	802	-	-	X	-
3	BO2	B	802	-	-	X	-
3	BO2	C	802	-	-	X	-
3	BO2	E	802	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 39263 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 endopeptidase La.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	719	Total	C	N	O	S	0	0
			5576	3525	1000	1044	7		
1	A	719	Total	C	N	O	S	0	0
			5576	3525	1000	1044	7		
1	G	719	Total	C	N	O	S	0	0
			5576	3525	1000	1044	7		
1	F	719	Total	C	N	O	S	0	0
			5576	3525	1000	1044	7		
1	E	719	Total	C	N	O	S	0	0
			5576	3525	1000	1044	7		
1	D	719	Total	C	N	O	S	0	0
			5576	3525	1000	1044	7		
1	C	719	Total	C	N	O	S	0	0
			5576	3525	1000	1044	7		

There are 91 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	720	LYS	-	expression tag	UNP C9DRU9
B	721	LEU	-	expression tag	UNP C9DRU9
B	722	ALA	-	expression tag	UNP C9DRU9
B	723	ALA	-	expression tag	UNP C9DRU9
B	724	ALA	-	expression tag	UNP C9DRU9
B	725	LEU	-	expression tag	UNP C9DRU9
B	726	GLU	-	expression tag	UNP C9DRU9
B	727	HIS	-	expression tag	UNP C9DRU9
B	728	HIS	-	expression tag	UNP C9DRU9
B	729	HIS	-	expression tag	UNP C9DRU9
B	730	HIS	-	expression tag	UNP C9DRU9
B	731	HIS	-	expression tag	UNP C9DRU9
B	732	HIS	-	expression tag	UNP C9DRU9
A	720	LYS	-	expression tag	UNP C9DRU9
A	721	LEU	-	expression tag	UNP C9DRU9
A	722	ALA	-	expression tag	UNP C9DRU9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	723	ALA	-	expression tag	UNP C9DRU9
A	724	ALA	-	expression tag	UNP C9DRU9
A	725	LEU	-	expression tag	UNP C9DRU9
A	726	GLU	-	expression tag	UNP C9DRU9
A	727	HIS	-	expression tag	UNP C9DRU9
A	728	HIS	-	expression tag	UNP C9DRU9
A	729	HIS	-	expression tag	UNP C9DRU9
A	730	HIS	-	expression tag	UNP C9DRU9
A	731	HIS	-	expression tag	UNP C9DRU9
A	732	HIS	-	expression tag	UNP C9DRU9
G	720	LYS	-	expression tag	UNP C9DRU9
G	721	LEU	-	expression tag	UNP C9DRU9
G	722	ALA	-	expression tag	UNP C9DRU9
G	723	ALA	-	expression tag	UNP C9DRU9
G	724	ALA	-	expression tag	UNP C9DRU9
G	725	LEU	-	expression tag	UNP C9DRU9
G	726	GLU	-	expression tag	UNP C9DRU9
G	727	HIS	-	expression tag	UNP C9DRU9
G	728	HIS	-	expression tag	UNP C9DRU9
G	729	HIS	-	expression tag	UNP C9DRU9
G	730	HIS	-	expression tag	UNP C9DRU9
G	731	HIS	-	expression tag	UNP C9DRU9
G	732	HIS	-	expression tag	UNP C9DRU9
F	720	LYS	-	expression tag	UNP C9DRU9
F	721	LEU	-	expression tag	UNP C9DRU9
F	722	ALA	-	expression tag	UNP C9DRU9
F	723	ALA	-	expression tag	UNP C9DRU9
F	724	ALA	-	expression tag	UNP C9DRU9
F	725	LEU	-	expression tag	UNP C9DRU9
F	726	GLU	-	expression tag	UNP C9DRU9
F	727	HIS	-	expression tag	UNP C9DRU9
F	728	HIS	-	expression tag	UNP C9DRU9
F	729	HIS	-	expression tag	UNP C9DRU9
F	730	HIS	-	expression tag	UNP C9DRU9
F	731	HIS	-	expression tag	UNP C9DRU9
F	732	HIS	-	expression tag	UNP C9DRU9
E	720	LYS	-	expression tag	UNP C9DRU9
E	721	LEU	-	expression tag	UNP C9DRU9
E	722	ALA	-	expression tag	UNP C9DRU9
E	723	ALA	-	expression tag	UNP C9DRU9
E	724	ALA	-	expression tag	UNP C9DRU9
E	725	LEU	-	expression tag	UNP C9DRU9

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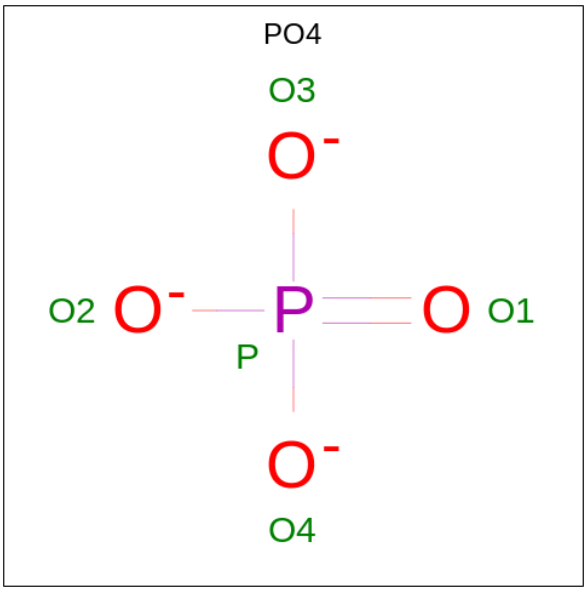
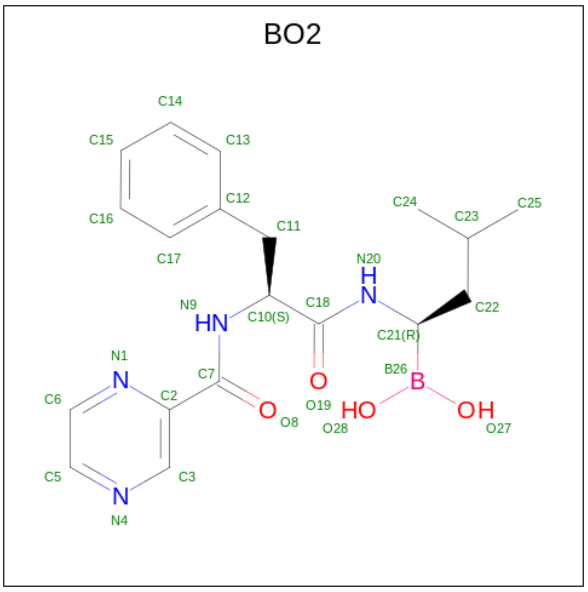
Chain	Residue	Modelled	Actual	Comment	Reference
E	726	GLU	-	expression tag	UNP C9DRU9
E	727	HIS	-	expression tag	UNP C9DRU9
E	728	HIS	-	expression tag	UNP C9DRU9
E	729	HIS	-	expression tag	UNP C9DRU9
E	730	HIS	-	expression tag	UNP C9DRU9
E	731	HIS	-	expression tag	UNP C9DRU9
E	732	HIS	-	expression tag	UNP C9DRU9
D	720	LYS	-	expression tag	UNP C9DRU9
D	721	LEU	-	expression tag	UNP C9DRU9
D	722	ALA	-	expression tag	UNP C9DRU9
D	723	ALA	-	expression tag	UNP C9DRU9
D	724	ALA	-	expression tag	UNP C9DRU9
D	725	LEU	-	expression tag	UNP C9DRU9
D	726	GLU	-	expression tag	UNP C9DRU9
D	727	HIS	-	expression tag	UNP C9DRU9
D	728	HIS	-	expression tag	UNP C9DRU9
D	729	HIS	-	expression tag	UNP C9DRU9
D	730	HIS	-	expression tag	UNP C9DRU9
D	731	HIS	-	expression tag	UNP C9DRU9
D	732	HIS	-	expression tag	UNP C9DRU9
C	720	LYS	-	expression tag	UNP C9DRU9
C	721	LEU	-	expression tag	UNP C9DRU9
C	722	ALA	-	expression tag	UNP C9DRU9
C	723	ALA	-	expression tag	UNP C9DRU9
C	724	ALA	-	expression tag	UNP C9DRU9
C	725	LEU	-	expression tag	UNP C9DRU9
C	726	GLU	-	expression tag	UNP C9DRU9
C	727	HIS	-	expression tag	UNP C9DRU9
C	728	HIS	-	expression tag	UNP C9DRU9
C	729	HIS	-	expression tag	UNP C9DRU9
C	730	HIS	-	expression tag	UNP C9DRU9
C	731	HIS	-	expression tag	UNP C9DRU9
C	732	HIS	-	expression tag	UNP C9DRU9

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is N-[(1R)-1-(DIHYDROXYBORYL)-3-METHYLBUTYL]-N-(PYRAZIN-2-YLCARBONYL)-L-PHENYLALANINAMIDE (CCD ID: BO2) (formula: $C_{19}H_{25}BN_4O_4$) (labeled as "Ligand of Interest" by depositor).

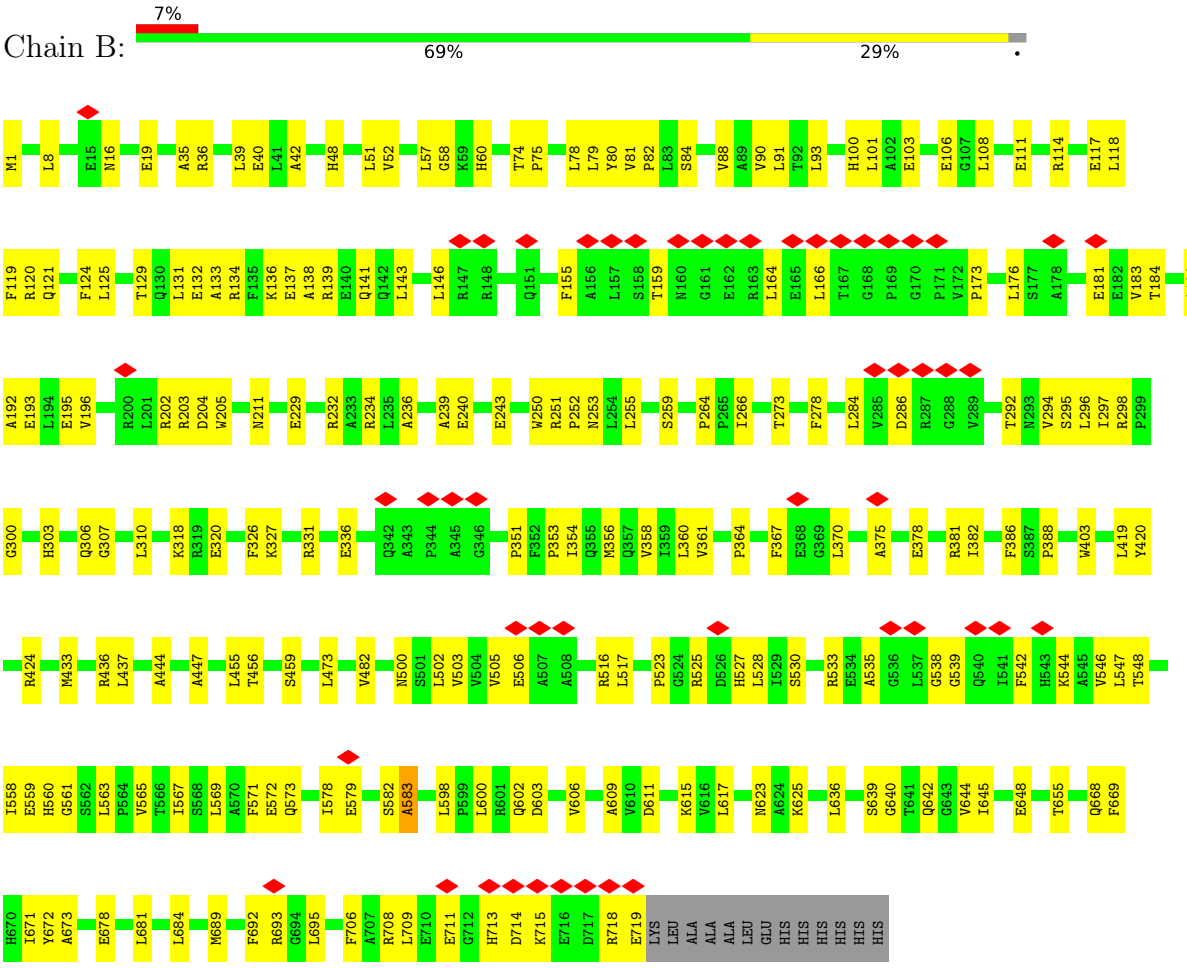


Mol	Chain	Residues	Atoms					AltConf
3	B	1	Total	B	C	N	O	0
			28	1	19	4	4	
3	A	1	Total	B	C	N	O	0
			28	1	19	4	4	
3	G	1	Total	B	C	N	O	0
			28	1	19	4	4	
3	F	1	Total	B	C	N	O	0
			28	1	19	4	4	
3	E	1	Total	B	C	N	O	0
			28	1	19	4	4	
3	D	1	Total	B	C	N	O	0
			28	1	19	4	4	
3	C	1	Total	B	C	N	O	0
			28	1	19	4	4	

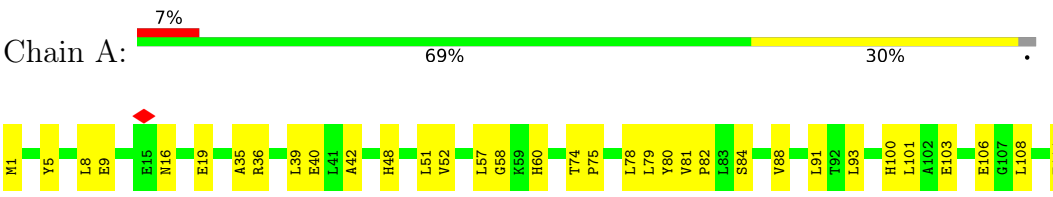
3 Residue-property plots (i)

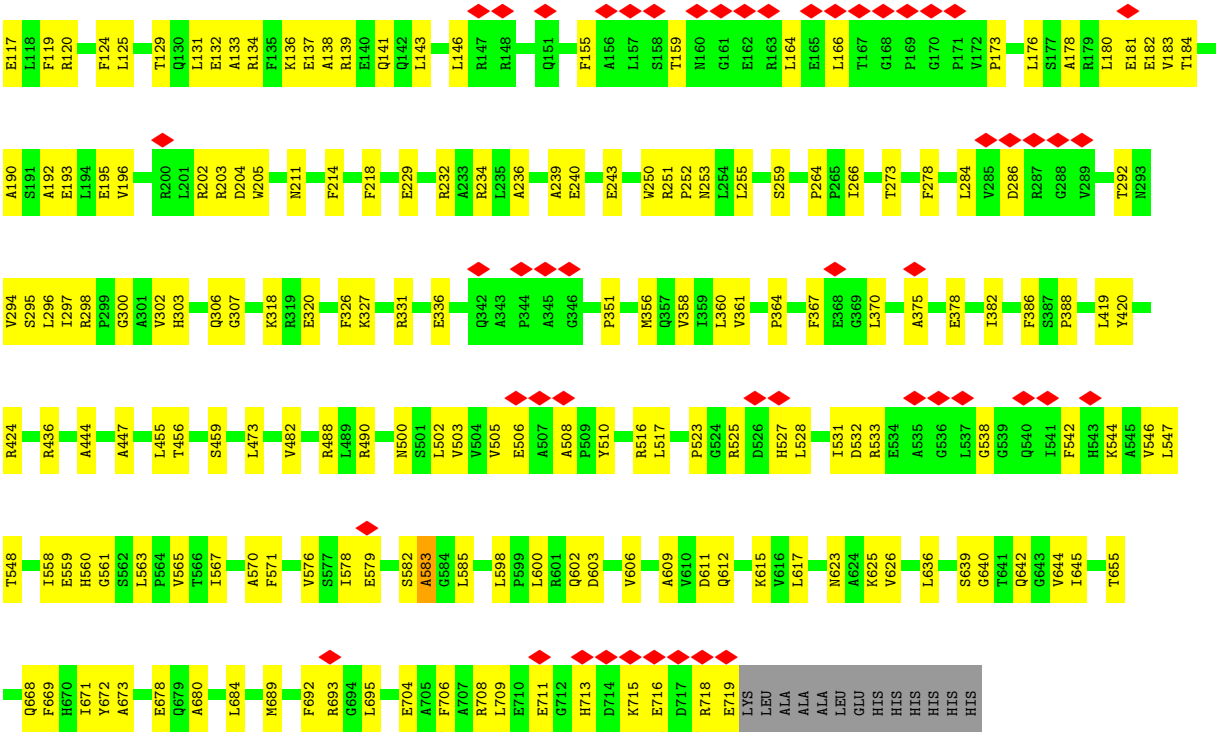
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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



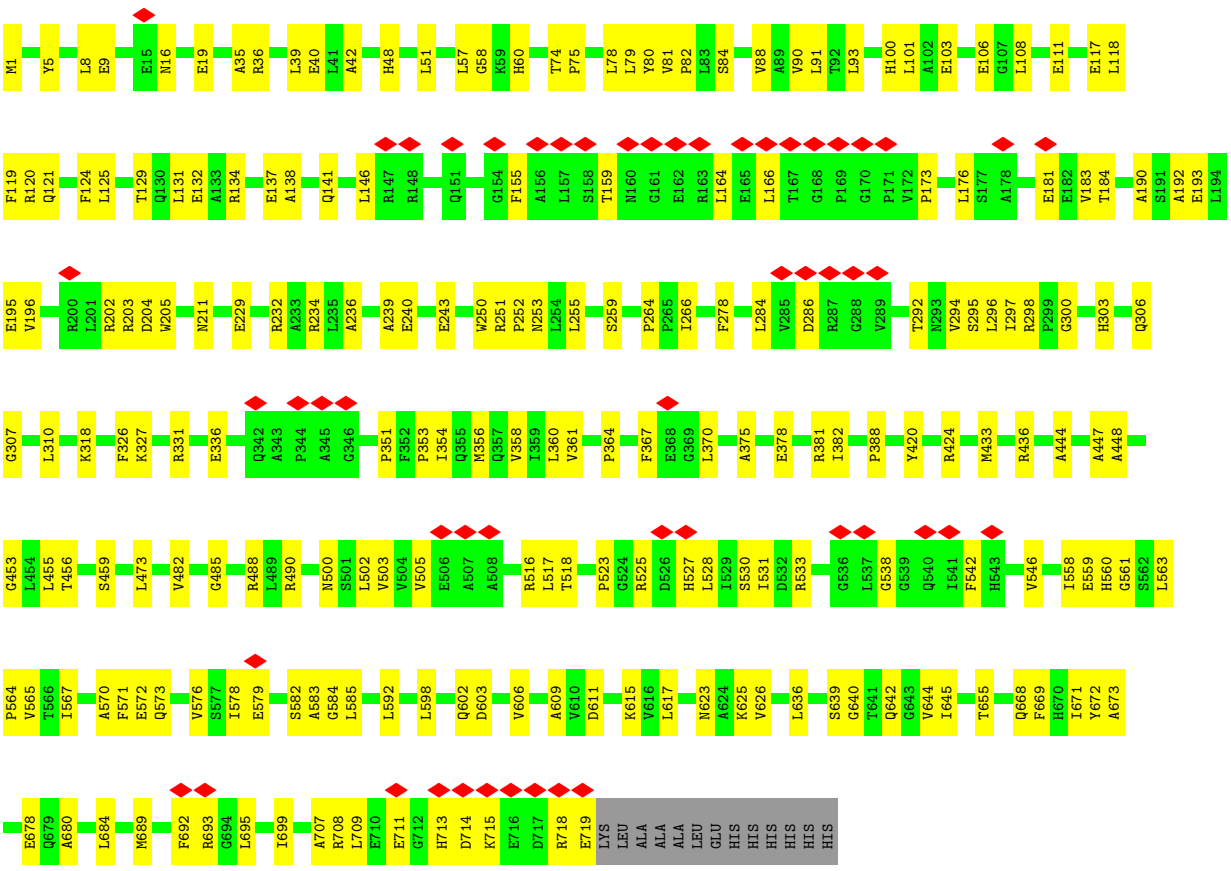
• Molecule 1: endopeptidase La





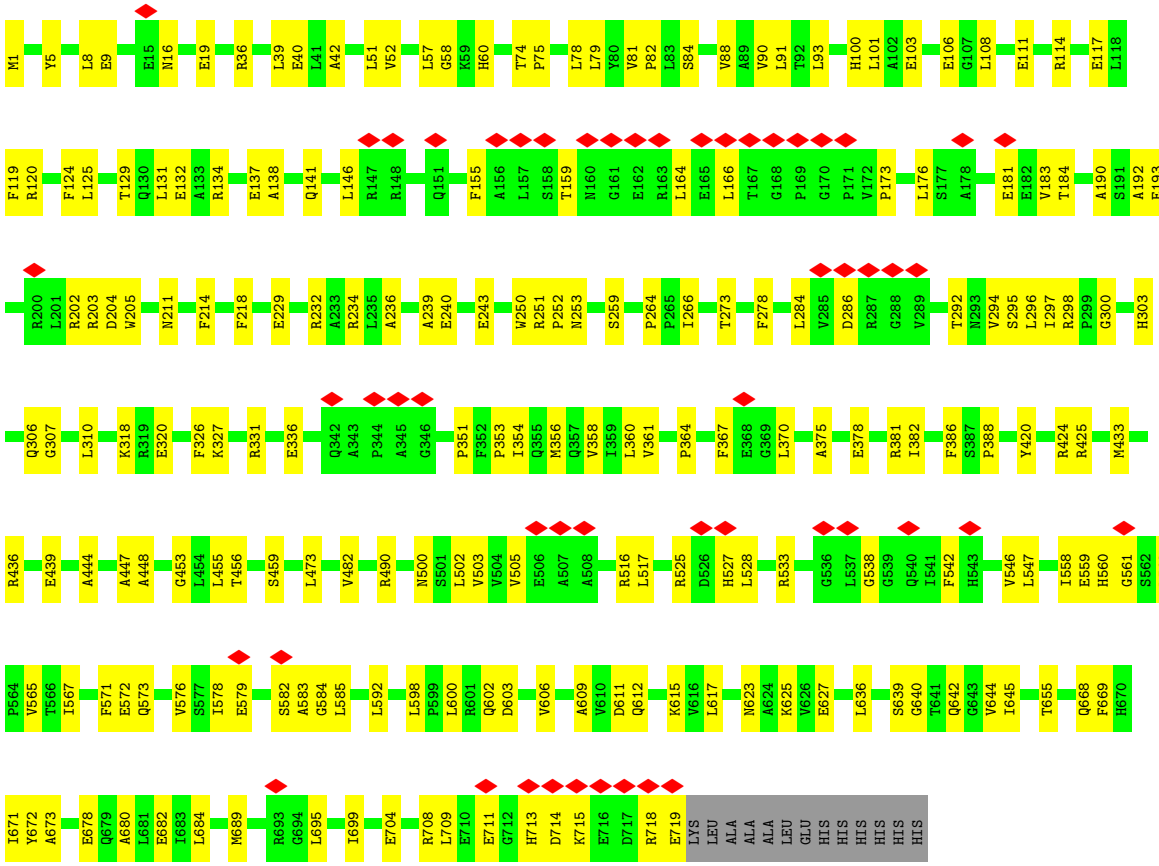
• Molecule 1: endopeptidase La

Chain G:



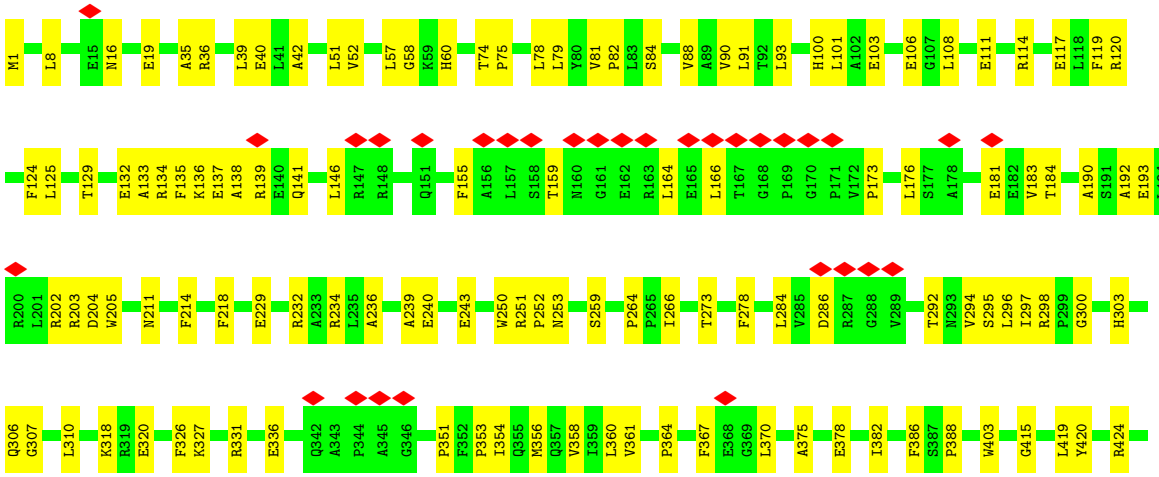
• Molecule 1: endopeptidase La

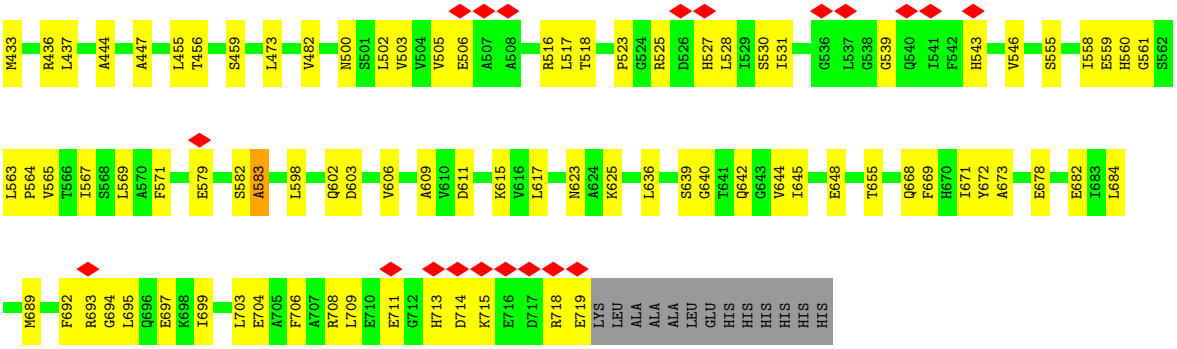
Chain F:



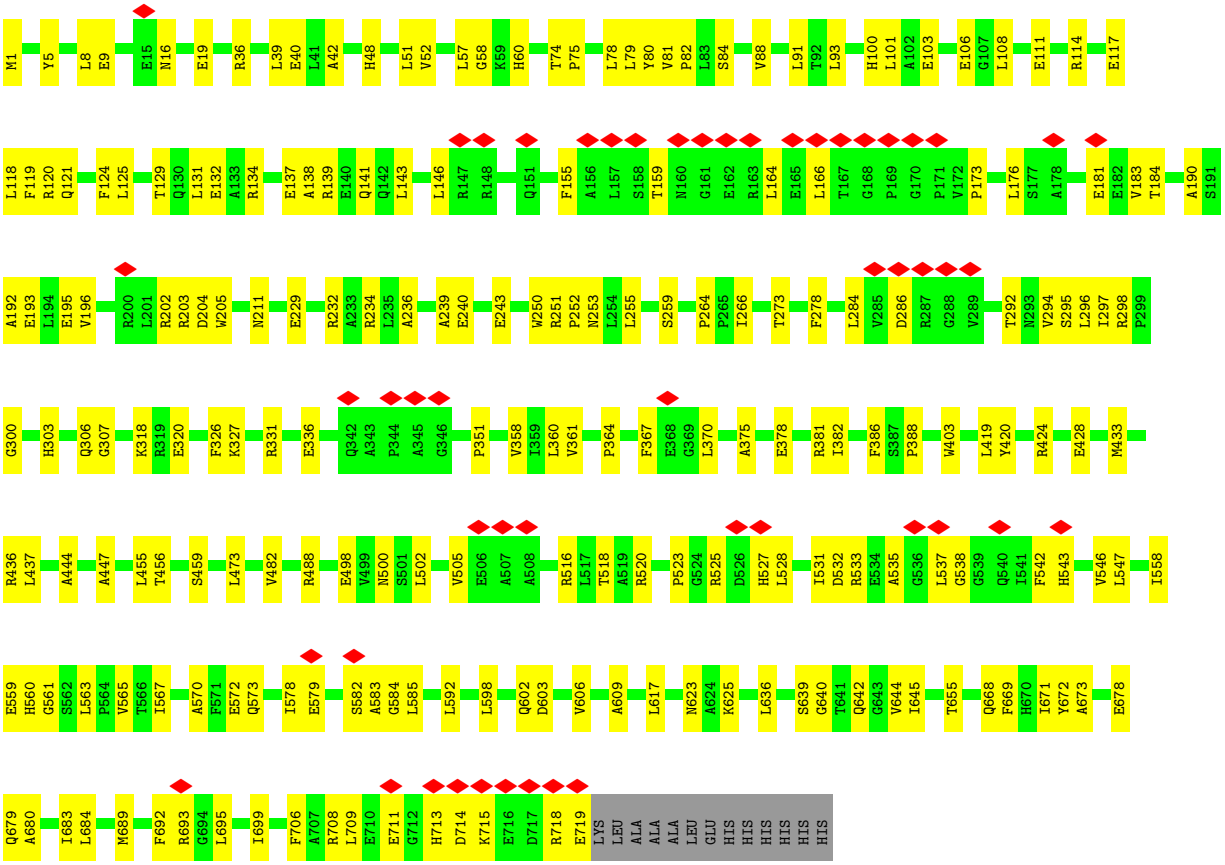
• Molecule 1: endopeptidase La

Chain E:

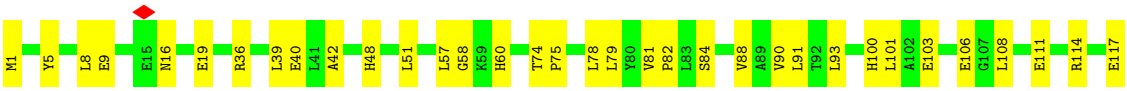


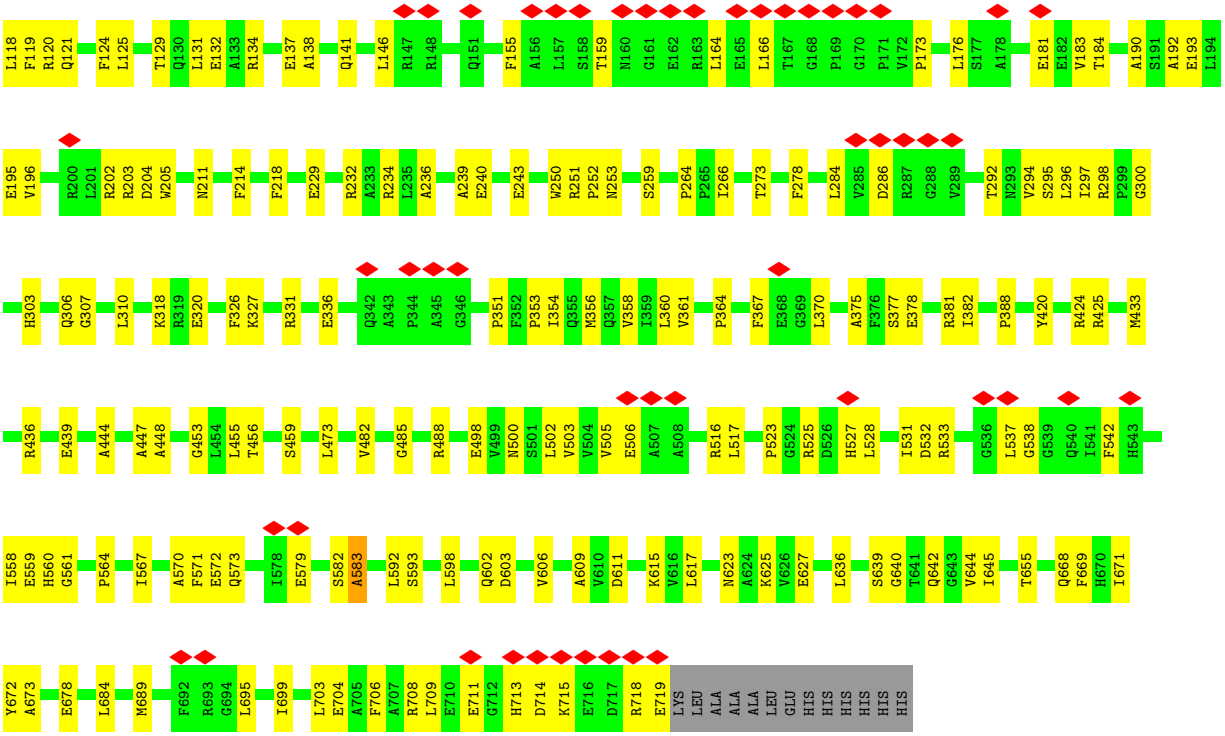


• Molecule 1: endopeptidase La



• Molecule 1: endopeptidase La




L118 F119 R120 Q121 F124 L125 T129 Q130 L131 E132 A133 R134 E137 A138 Q141 L146 R147 R148 Q151 F155 A156 L157 S158 T159 N160 G161 E162 R163 L164 E165 L166 T167 G168 P169 G170 P171 V172 P173 L176 S177 A178 E181 E182 V183 T184 A190 S191 A192 E193 L194
E195 V196 R200 L201 R202 R203 D204 W205 N211 F214 F218 E229 R232 A233 R234 L235 A236 A239 E240 E243 W250 R251 P252 N253 S259 P264 P265 I266 T273 F278 L284 V285 D286 R287 G288 V289 T292 N293 V294 S295 L296 T297 R298 P299 G300
H303 Q306 G307 L310 K318 R319 E320 F326 K327 R331 E336 Q342 A343 P344 A345 G346 P351 F352 P353 I354 Q355 M356 Q357 V358 I359 L360 V361 P364 F367 E368 G369 L370 A375 F376 S377 E378 R381 I382 P388 Y420 R424 R425 M433
R436 E439 A444 A447 A448 G453 L454 L455 T456 S459 L473 V482 G485 R488 E498 V499 N500 S501 L502 V503 V504 V505 E506 A507 A508 R516 L517 P523 G524 R525 D526 H527 L528 I531 D532 R533 G536 L537 G538 G539 Q540 I541 F542 H543
I558 E559 H560 G561 P564 I567 A570 F571 E572 Q573 I578 E579 S582 A583 L592 S593 L598 Q602 D603 V606 A609 V610 D611 K615 V616 L617 N623 A624 K625 V626 E627 L636 S639 G640 T641 Q642 G643 V644 I645 T655 Q668 F669 H670 I671
Y672 A673 E678 L684 M689 F692 R693 G694 L695 I699 L703 E704 A705 F706 A707 R708 L709 E710 E711 G712 H713 D714 K715 E716 D717 R718 E719 LYS LEU ALA ALA ALA LEU GLU HIS HIS HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	154341	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.472	Depositor
Minimum map value	-1.036	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	275.52, 275.52, 275.52	wwPDB
Map dimensions	336, 336, 336	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, BO2

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	0.11	0/5687	0.30	0/7721
1	B	0.11	0/5687	0.30	0/7721
1	C	0.11	0/5687	0.30	0/7721
1	D	0.11	0/5687	0.29	0/7721
1	E	0.11	0/5687	0.29	0/7721
1	F	0.11	0/5687	0.29	0/7721
1	G	0.11	0/5687	0.30	0/7721
All	All	0.11	0/39809	0.30	0/54047

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

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	5576	0	5588	156	0
1	B	5576	0	5588	153	0
1	C	5576	0	5588	150	0
1	D	5576	0	5588	149	0
1	E	5576	0	5588	151	0
1	F	5576	0	5588	144	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	5576	0	5588	149	0
2	A	5	0	0	2	0
2	B	5	0	0	2	0
2	C	5	0	0	2	0
2	D	5	0	0	2	0
2	E	5	0	0	2	0
2	F	5	0	0	2	0
2	G	5	0	0	2	0
3	A	28	0	25	9	0
3	B	28	0	25	9	0
3	C	28	0	25	9	0
3	D	28	0	24	7	0
3	E	28	0	25	9	0
3	F	28	0	24	7	0
3	G	28	0	24	7	0
All	All	39263	0	39288	998	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 13.

The worst 5 of 998 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:F:561:GLY:H	1:E:713:HIS:HB2	1.49	0.78
1:A:561:GLY:H	1:G:713:HIS:HB2	1.49	0.78
1:B:713:HIS:HB2	1:C:561:GLY:H	1.49	0.77
1:E:561:GLY:H	1:D:713:HIS:HB2	1.48	0.76
1:B:561:GLY:H	1:A:713:HIS:HB2	1.48	0.76

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	717/732 (98%)	696 (97%)	20 (3%)	1 (0%)	48	77
1	B	717/732 (98%)	695 (97%)	21 (3%)	1 (0%)	48	77
1	C	717/732 (98%)	697 (97%)	19 (3%)	1 (0%)	48	77
1	D	717/732 (98%)	698 (97%)	18 (2%)	1 (0%)	48	77
1	E	717/732 (98%)	695 (97%)	21 (3%)	1 (0%)	48	77
1	F	717/732 (98%)	697 (97%)	19 (3%)	1 (0%)	48	77
1	G	717/732 (98%)	695 (97%)	21 (3%)	1 (0%)	48	77
All	All	5019/5124 (98%)	4873 (97%)	139 (3%)	7 (0%)	50	77

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	583	ALA
1	F	583	ALA
1	D	583	ALA
1	B	583	ALA
1	A	583	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	568/578 (98%)	568 (100%)	0	100	100
1	B	568/578 (98%)	568 (100%)	0	100	100
1	C	568/578 (98%)	568 (100%)	0	100	100
1	D	568/578 (98%)	568 (100%)	0	100	100
1	E	568/578 (98%)	568 (100%)	0	100	100
1	F	568/578 (98%)	568 (100%)	0	100	100
1	G	568/578 (98%)	568 (100%)	0	100	100
All	All	3976/4046 (98%)	3976 (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. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	303	HIS
1	D	303	HIS
1	E	396	ASN
1	E	668	GLN
1	D	396	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

14 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	E	801	-	4,4,4	6.88	2 (50%)	6,6,6	0.50	0
2	PO4	F	801	-	4,4,4	6.87	2 (50%)	6,6,6	0.51	0
2	PO4	C	801	-	4,4,4	6.86	2 (50%)	6,6,6	0.50	0
3	BO2	B	802	1	25,29,29	0.20	0	32,38,38	0.45	0
3	BO2	G	802	1	25,29,29	0.20	0	32,38,38	0.50	1 (3%)
3	BO2	F	802	1	25,29,29	0.20	0	32,38,38	0.51	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	BO2	A	802	1	25,29,29	0.20	0	32,38,38	0.45	0
2	PO4	G	801	-	4,4,4	6.88	2 (50%)	6,6,6	0.50	0
2	PO4	B	801	-	4,4,4	6.87	2 (50%)	6,6,6	0.50	0
2	PO4	A	801	-	4,4,4	6.87	2 (50%)	6,6,6	0.50	0
2	PO4	D	801	-	4,4,4	6.88	2 (50%)	6,6,6	0.49	0
3	BO2	E	802	1	25,29,29	0.19	0	32,38,38	0.47	0
3	BO2	C	802	1	25,29,29	0.20	0	32,38,38	0.45	0
3	BO2	D	802	1	25,29,29	0.20	0	32,38,38	0.50	1 (3%)

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
3	BO2	G	802	1	-	11/22/28/28	0/2/2/2
3	BO2	B	802	1	-	8/22/28/28	0/2/2/2
3	BO2	F	802	1	-	11/22/28/28	0/2/2/2
3	BO2	A	802	1	-	8/22/28/28	0/2/2/2
3	BO2	E	802	1	-	8/22/28/28	0/2/2/2
3	BO2	C	802	1	-	7/22/28/28	0/2/2/2
3	BO2	D	802	1	-	11/22/28/28	0/2/2/2

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	801	PO4	P-O4	13.55	1.95	1.54
2	G	801	PO4	P-O4	13.55	1.95	1.54
2	D	801	PO4	P-O4	13.55	1.95	1.54
2	A	801	PO4	P-O4	13.54	1.95	1.54
2	B	801	PO4	P-O4	13.54	1.95	1.54

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	802	BO2	C18-C10-N9	2.03	116.69	111.16
3	D	802	BO2	C18-C10-N9	2.02	116.66	111.16
3	F	802	BO2	C18-C10-N9	2.02	116.65	111.16

There are no chirality outliers.

5 of 64 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	802	BO2	C3-C2-C7-O8
3	G	802	BO2	C3-C2-C7-O8
3	G	802	BO2	C3-C2-C7-N9
3	G	802	BO2	C2-C7-N9-C10
3	F	802	BO2	C3-C2-C7-O8

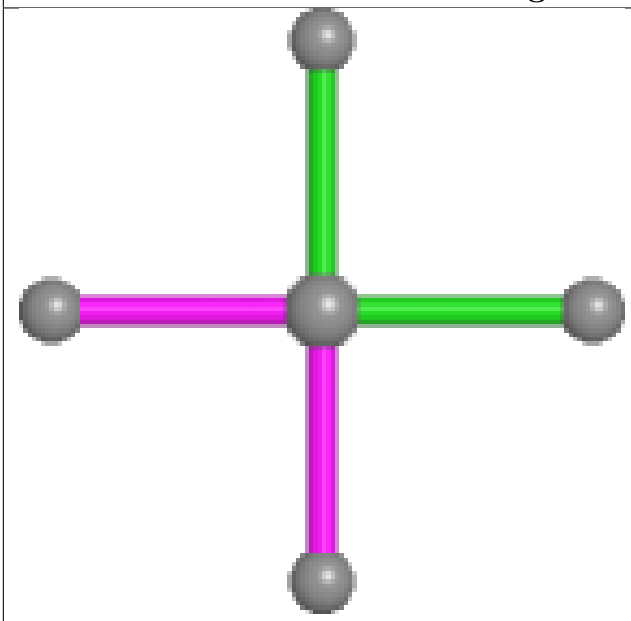
There are no ring outliers.

14 monomers are involved in 71 short contacts:

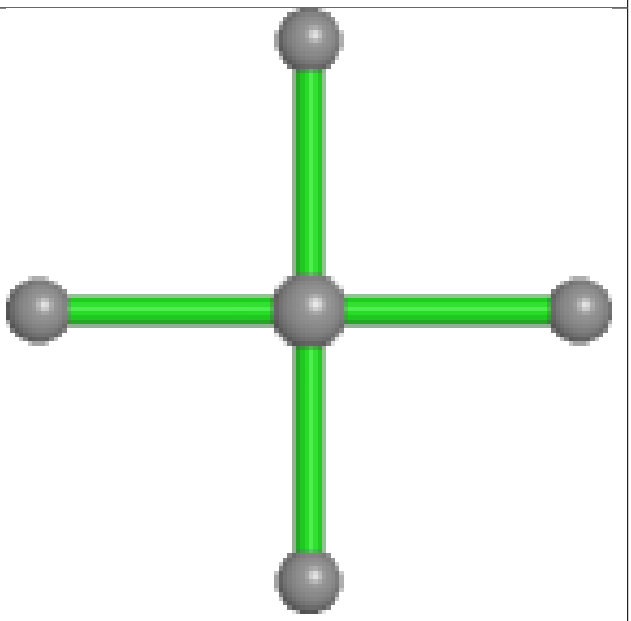
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	801	PO4	2	0
2	F	801	PO4	2	0
2	C	801	PO4	2	0
3	B	802	BO2	9	0
3	G	802	BO2	7	0
3	F	802	BO2	7	0
3	A	802	BO2	9	0
2	G	801	PO4	2	0
2	B	801	PO4	2	0
2	A	801	PO4	2	0
2	D	801	PO4	2	0
3	E	802	BO2	9	0
3	C	802	BO2	9	0
3	D	802	BO2	7	0

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 then 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.

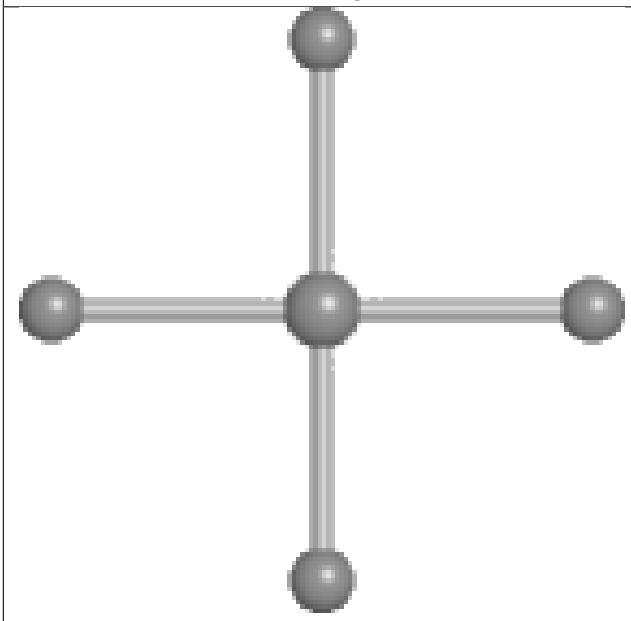
Ligand PO4 E 801



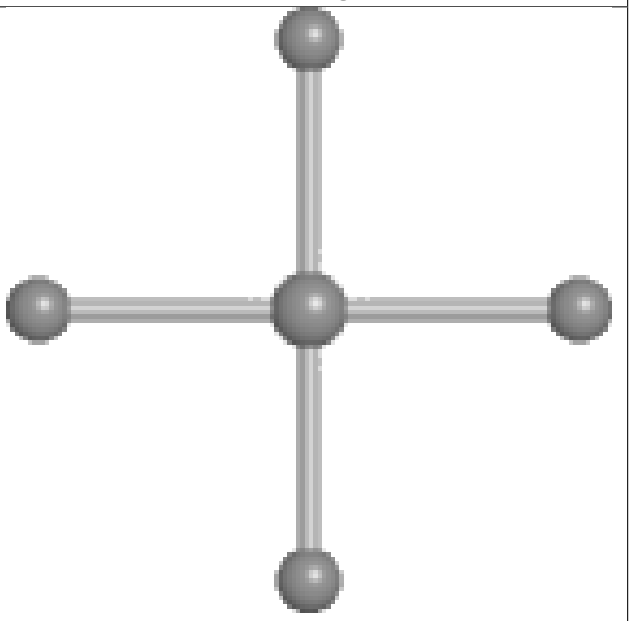
Bond lengths



Bond angles

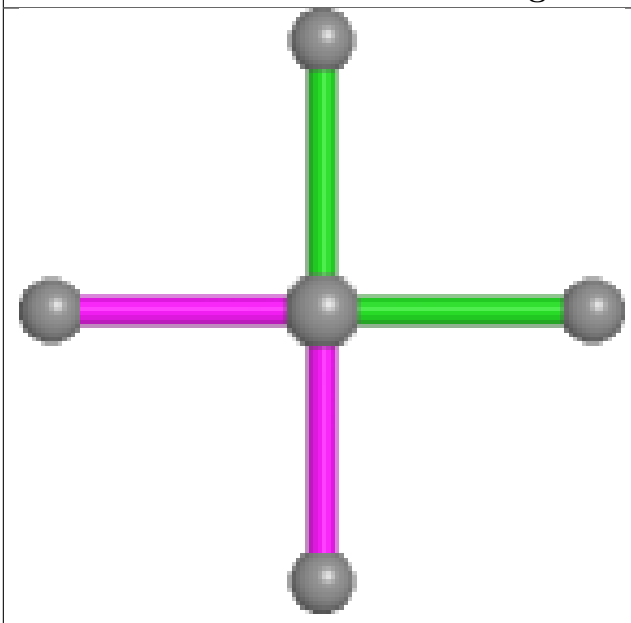


Torsions



Rings

Ligand PO4 F 801



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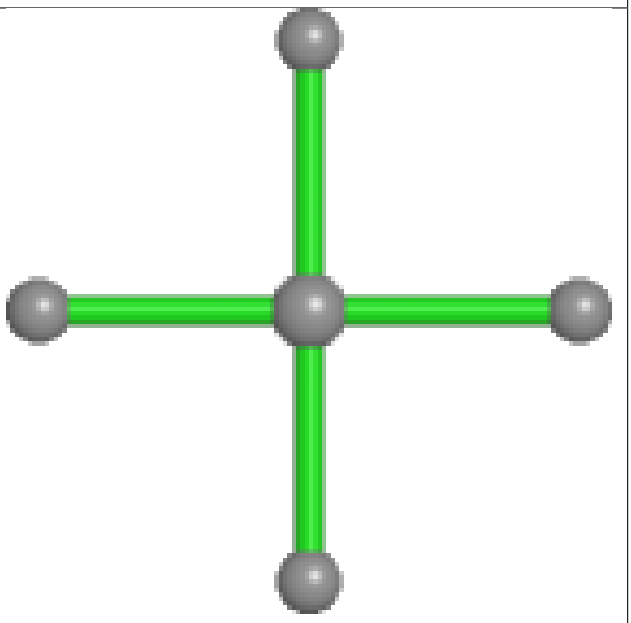

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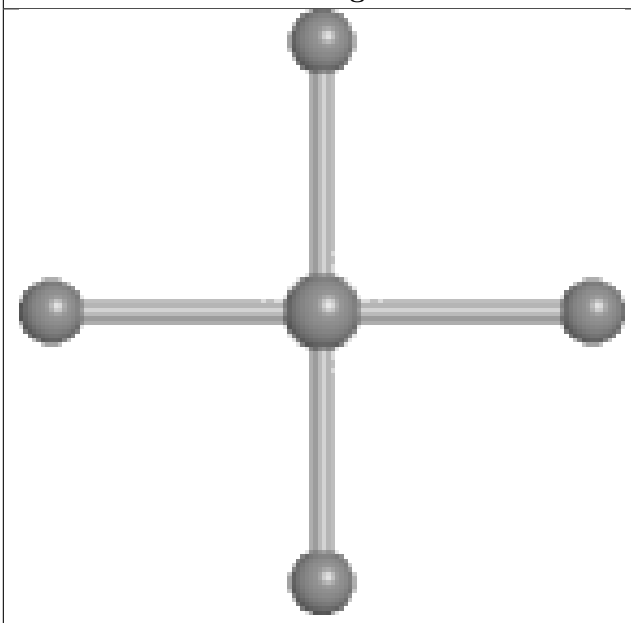

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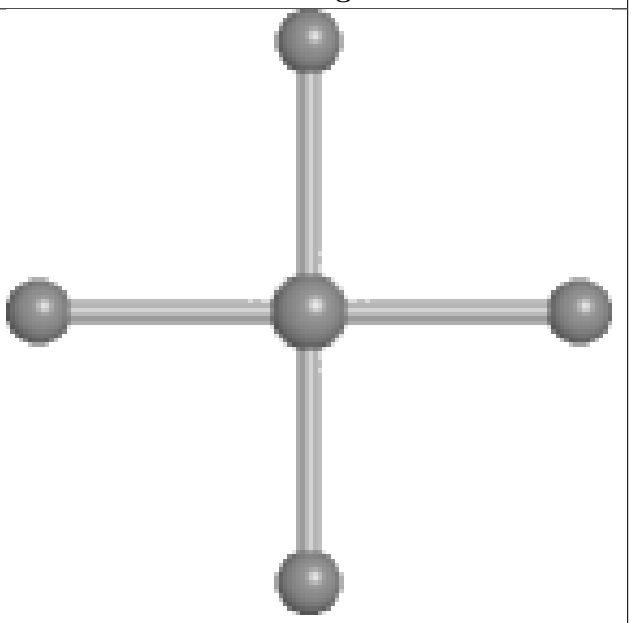
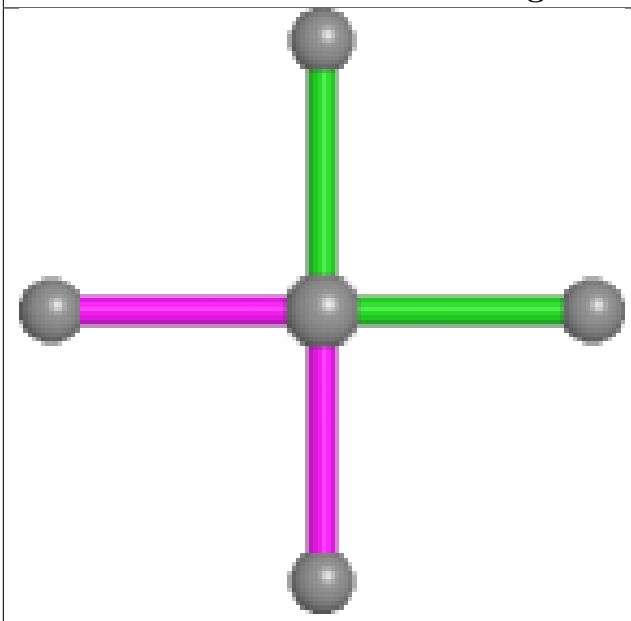


Rings

Ligand PO4 C 801



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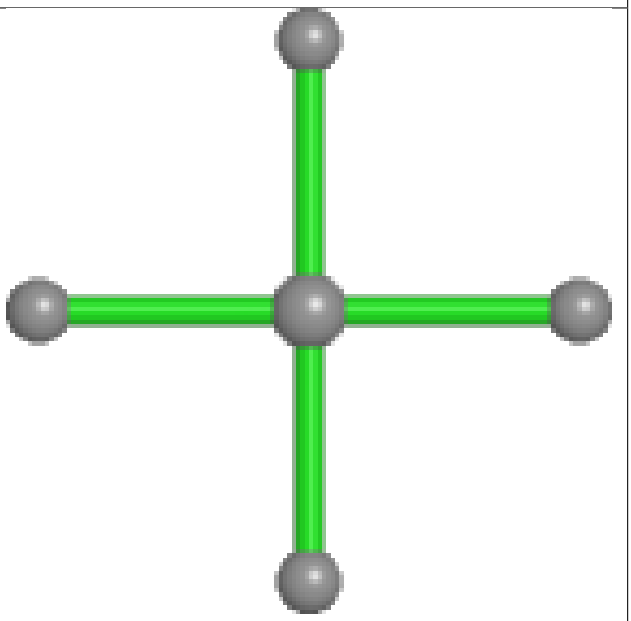
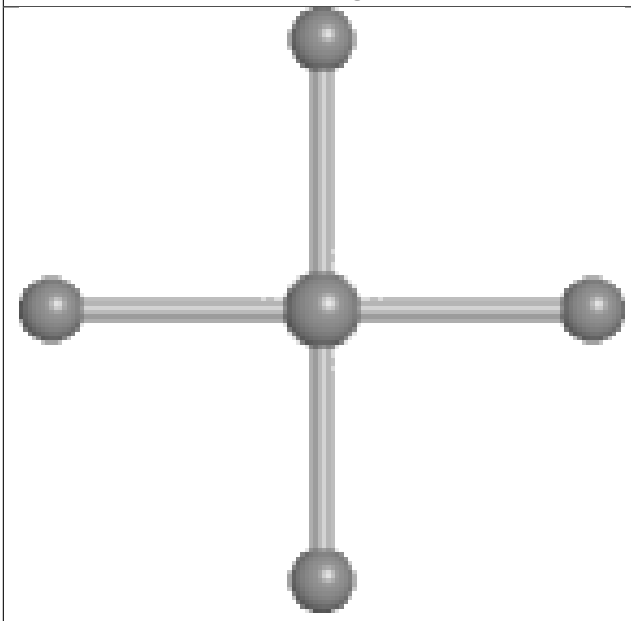


Bond angles



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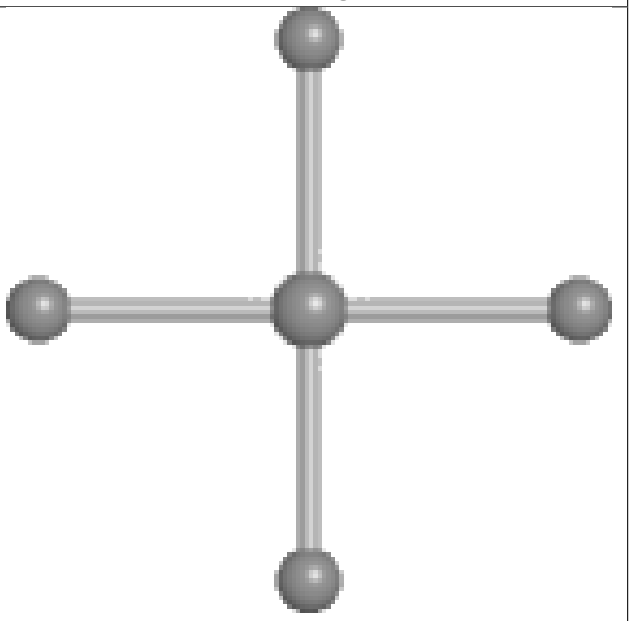
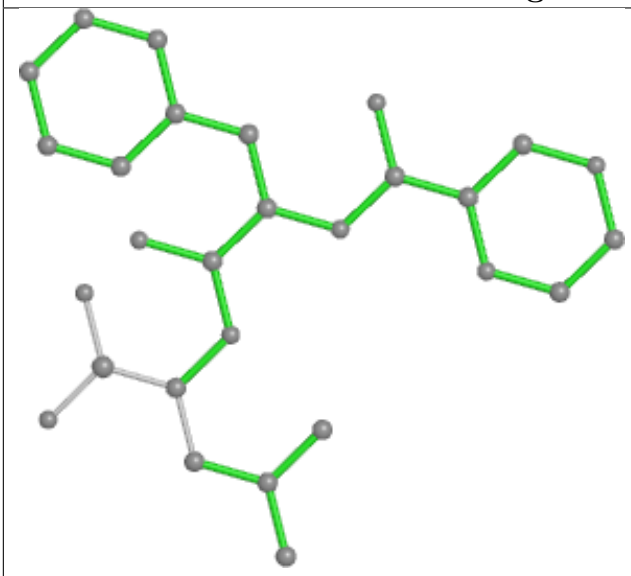


Rings

Ligand BO2 B 802



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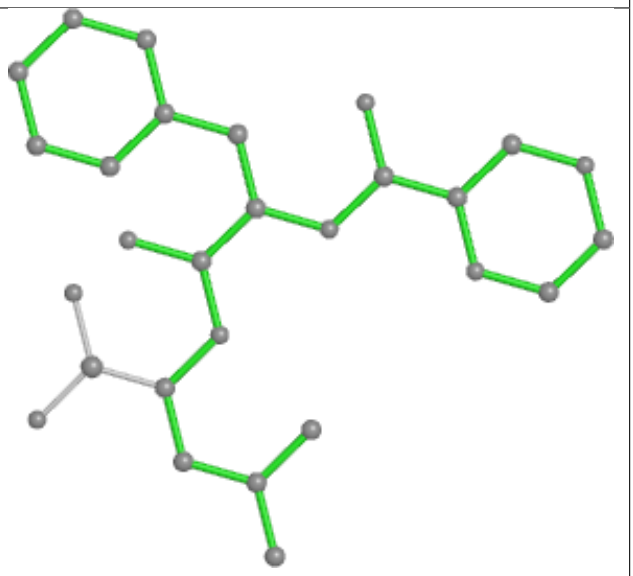

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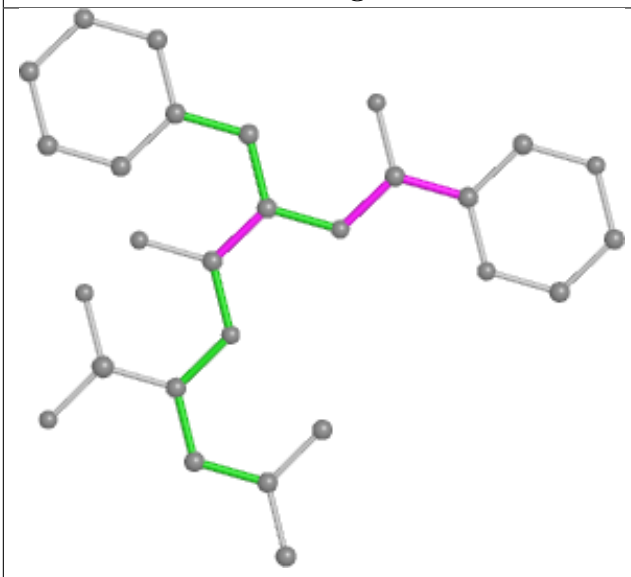

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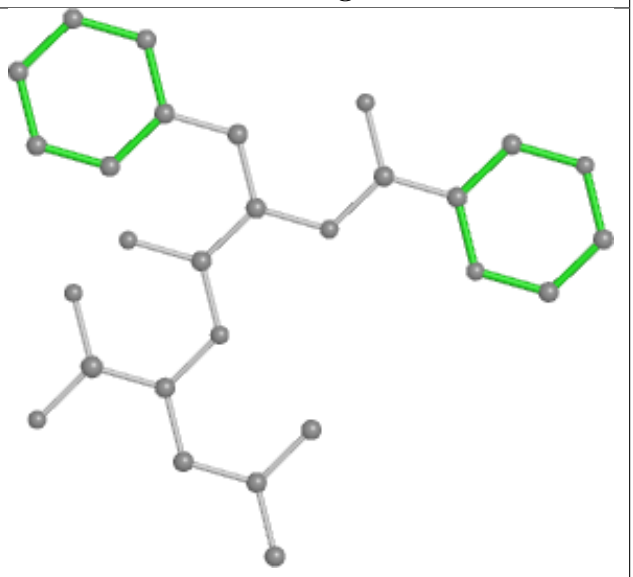
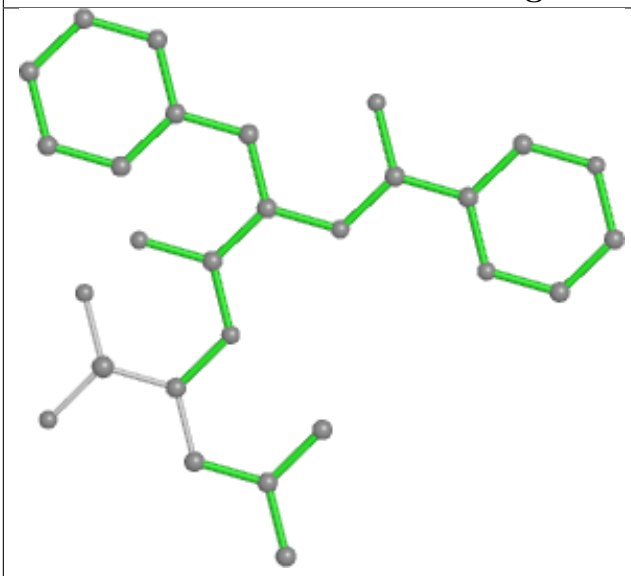


Rings

Ligand BO2 G 802



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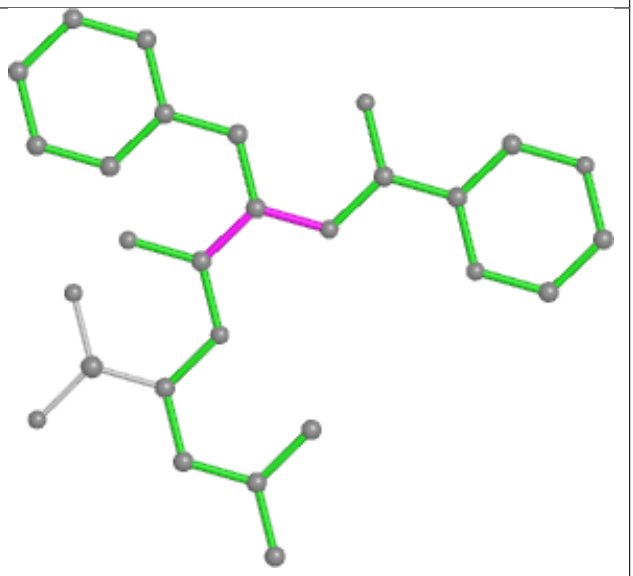

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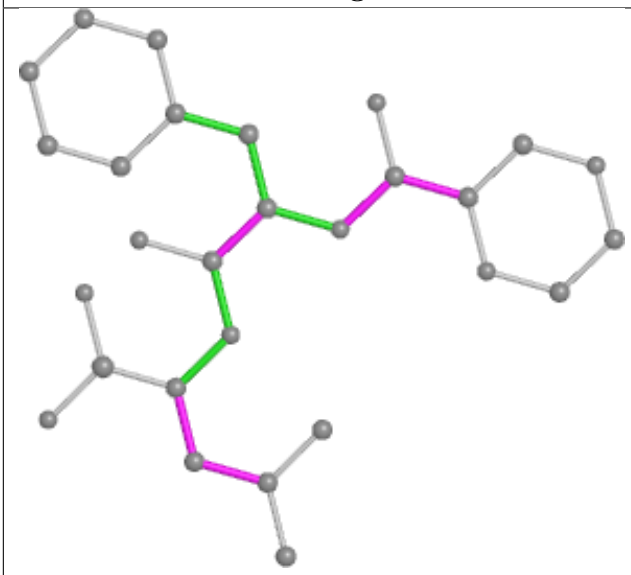

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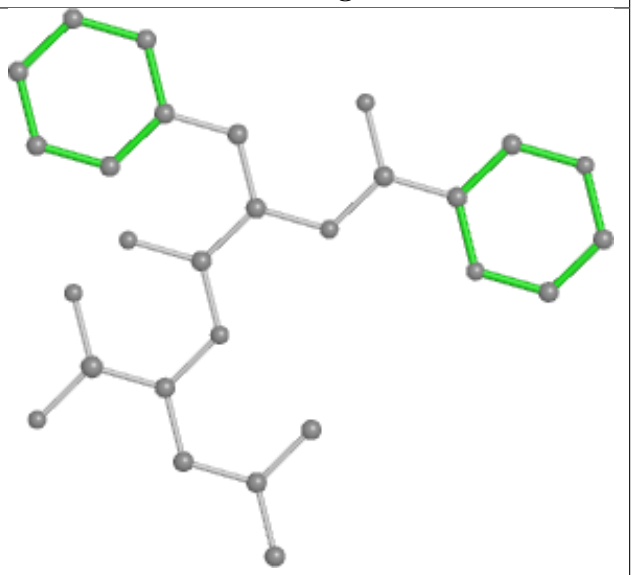
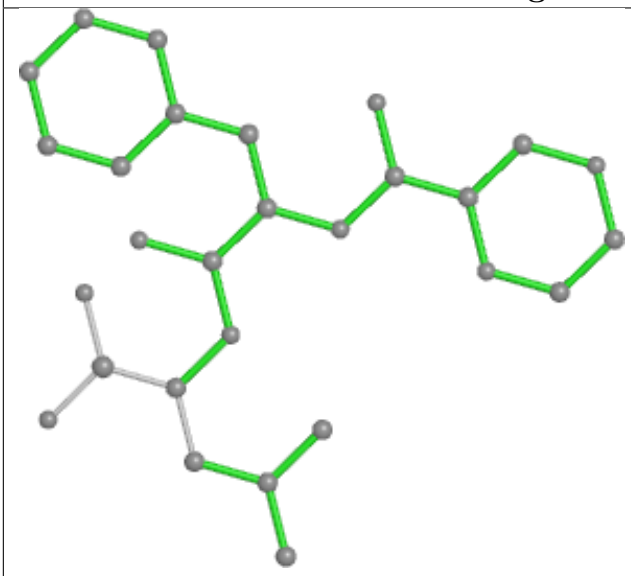


Rings

Ligand BO2 F 802



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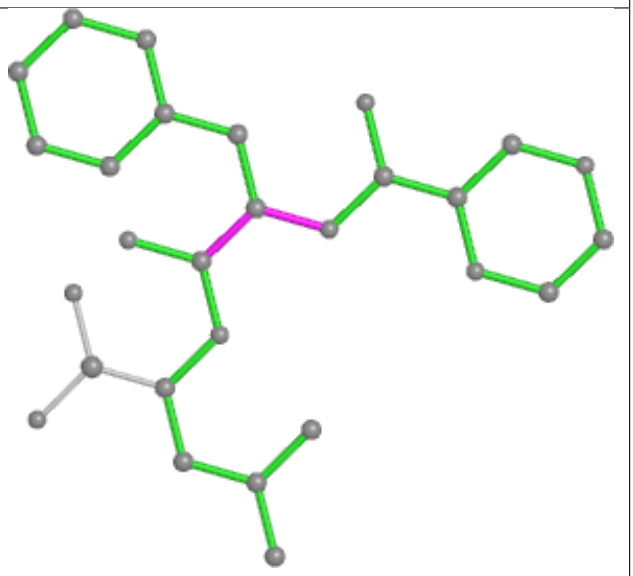

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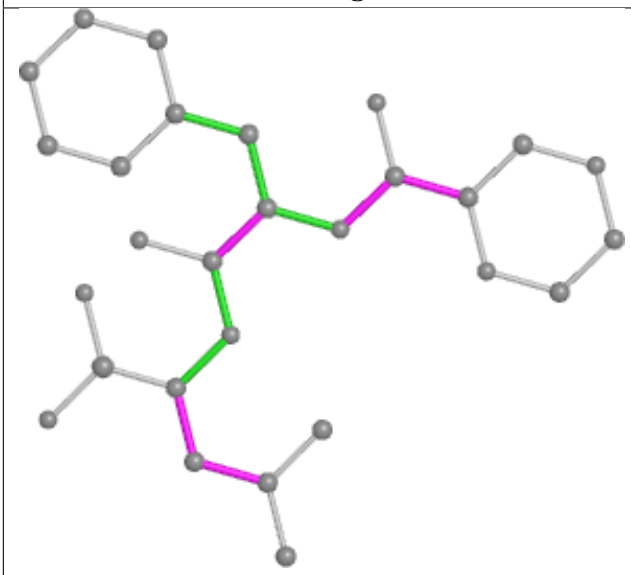

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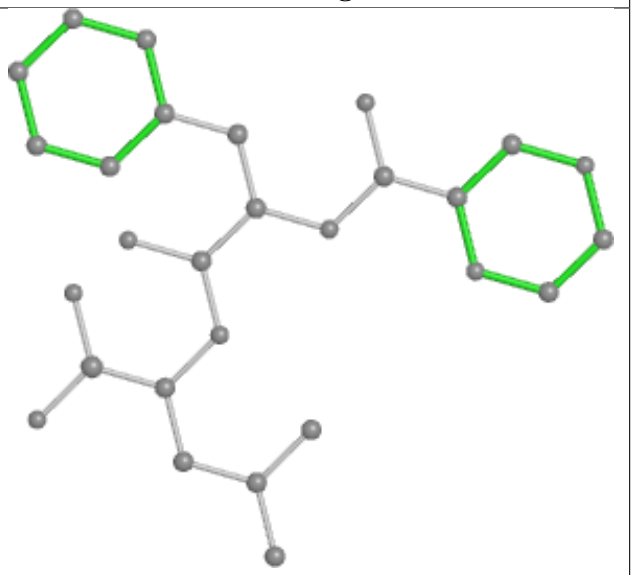
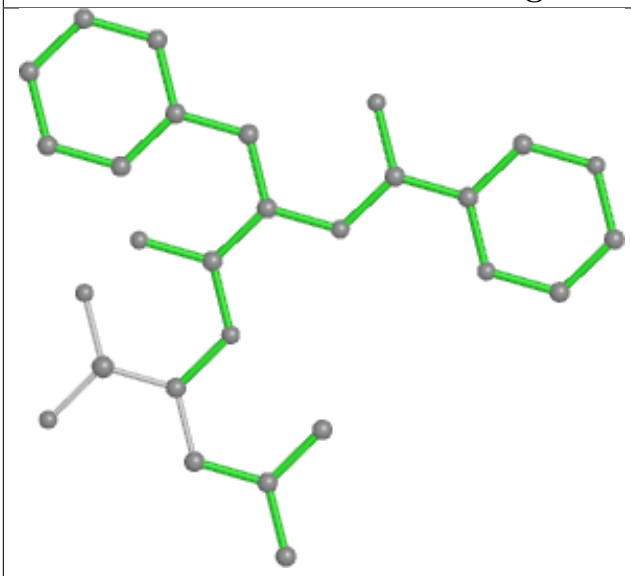


Rings

Ligand BO2 A 802



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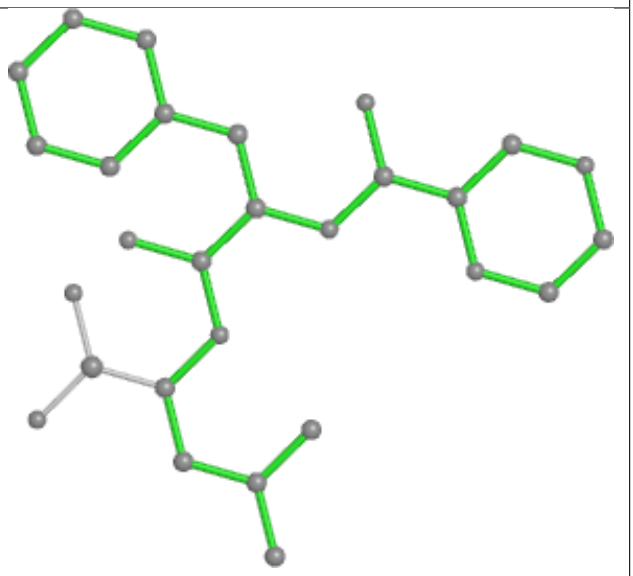

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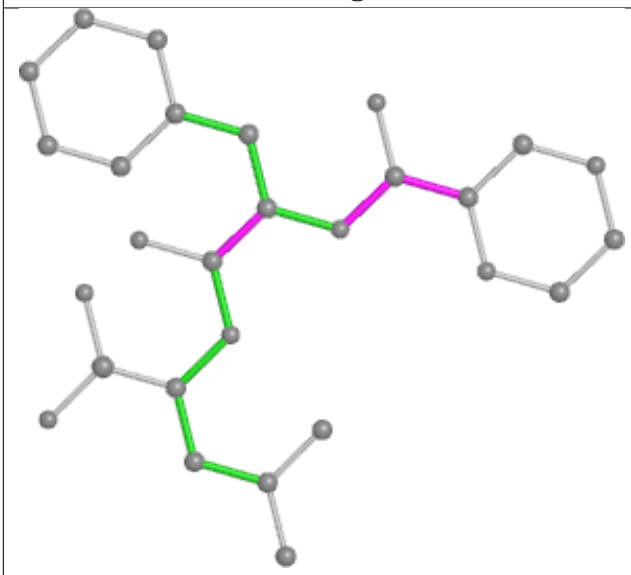

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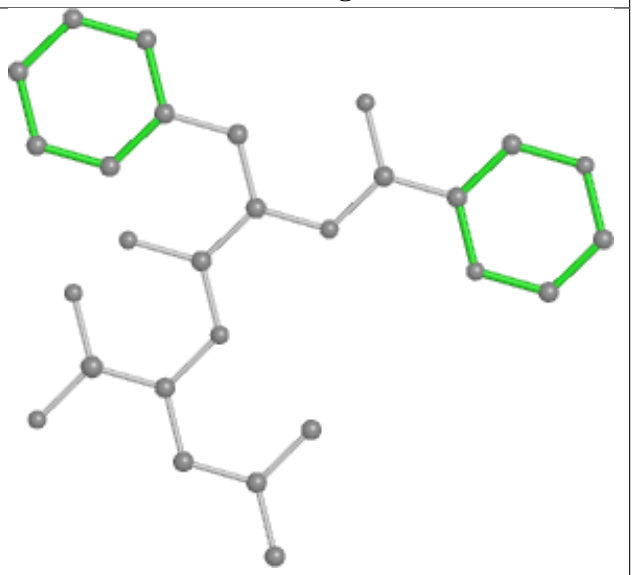
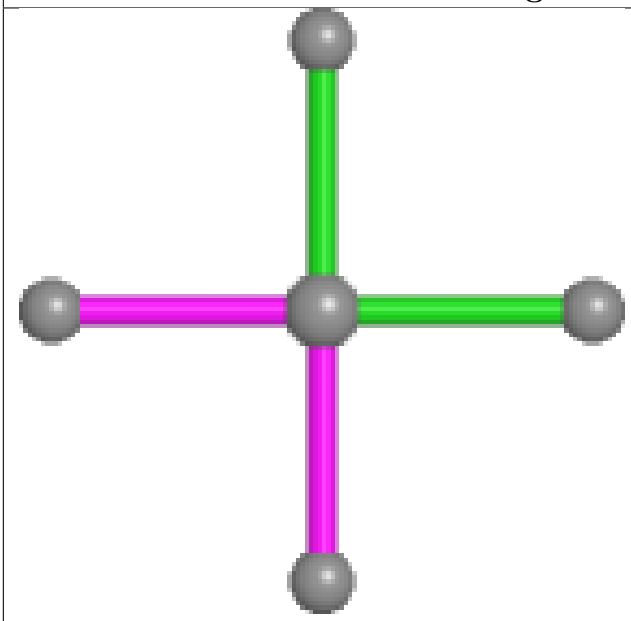


Rings

Ligand PO4 G 801



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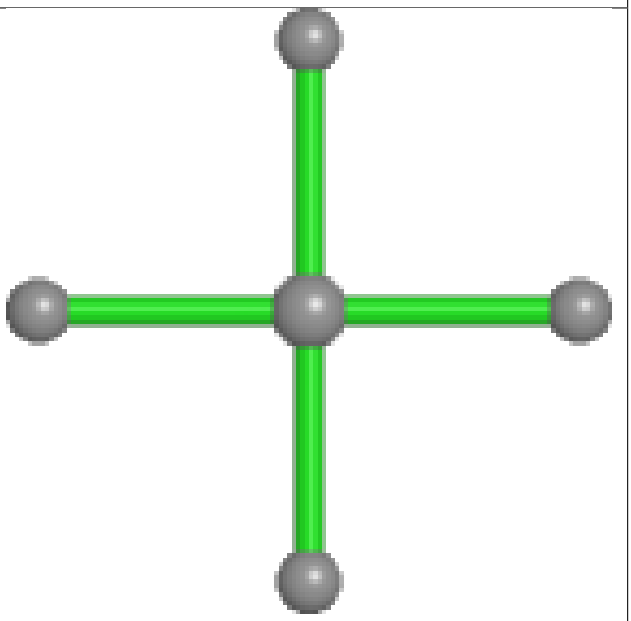

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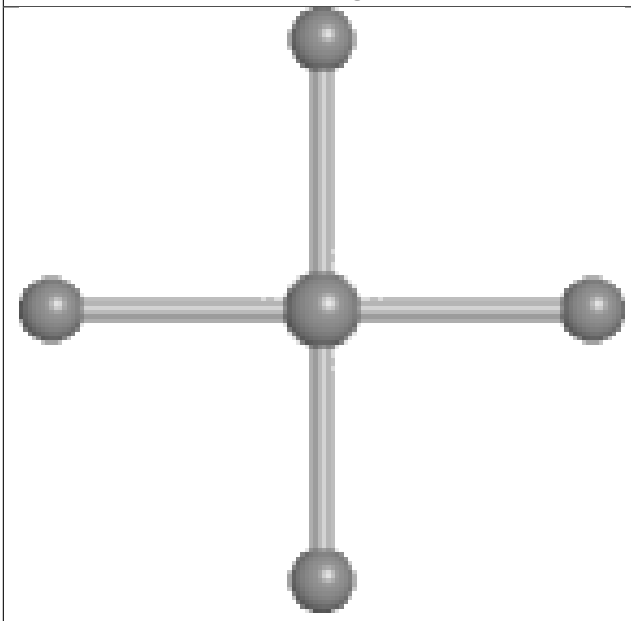
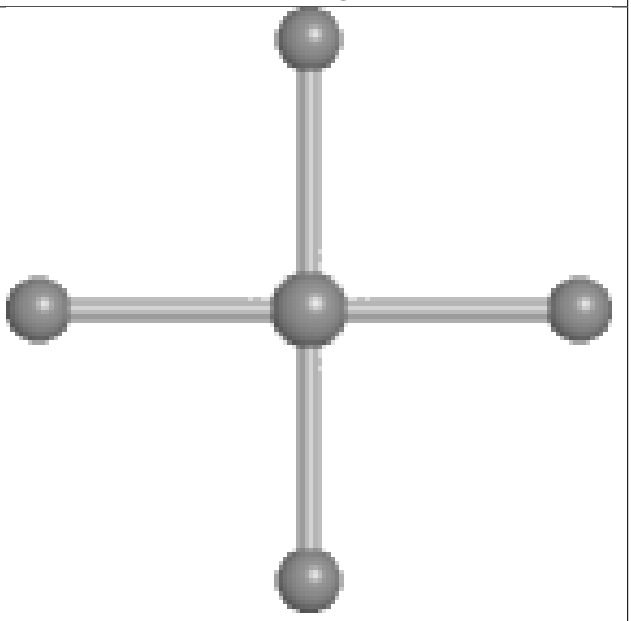
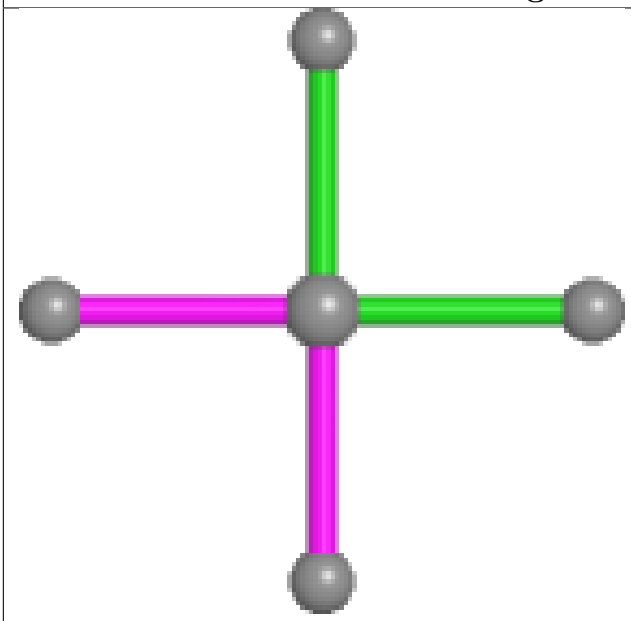


Torsions

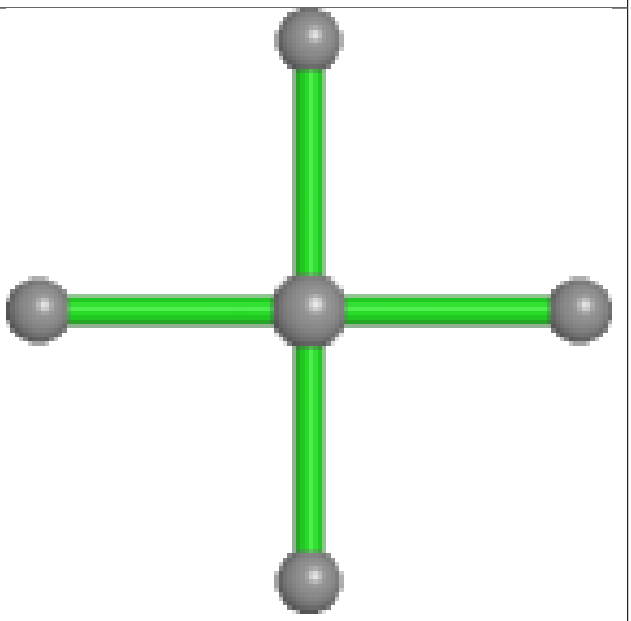


Rings

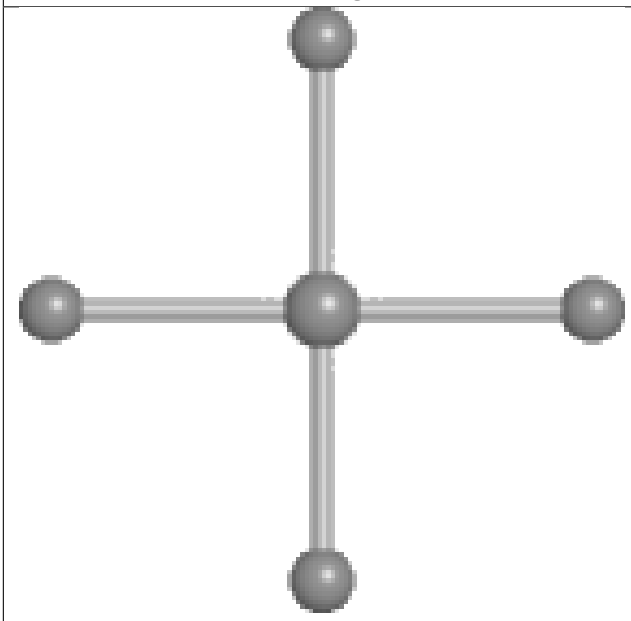
Ligand PO4 B 801



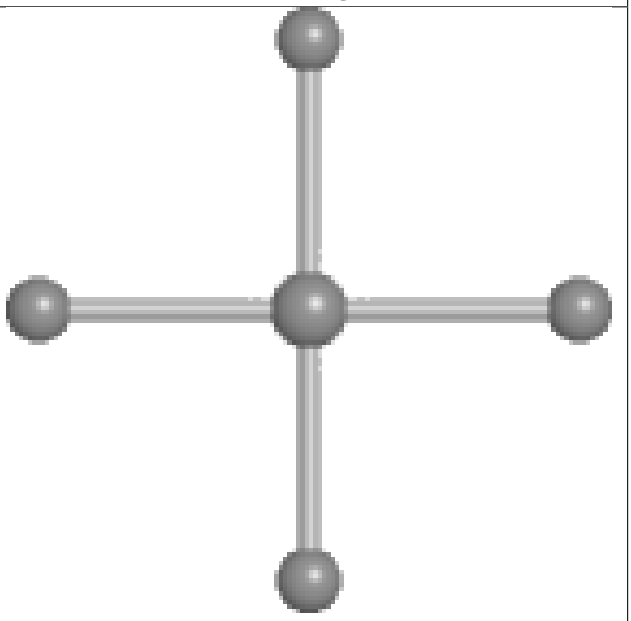
Bond lengths



Bond angles

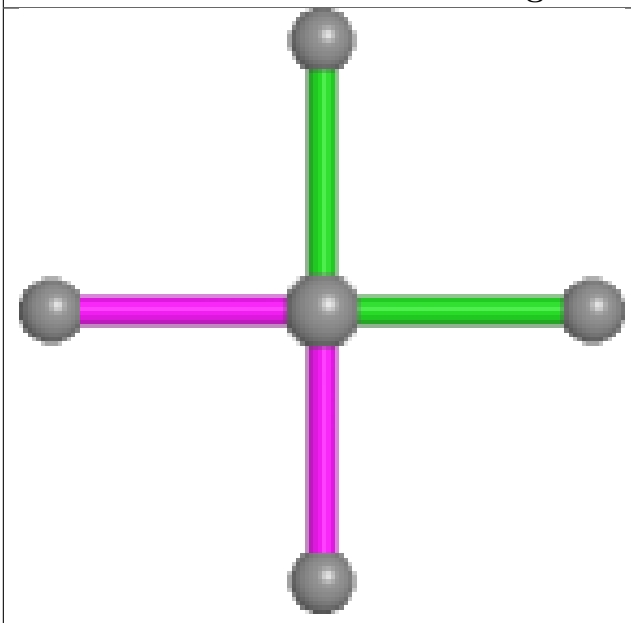


Torsions

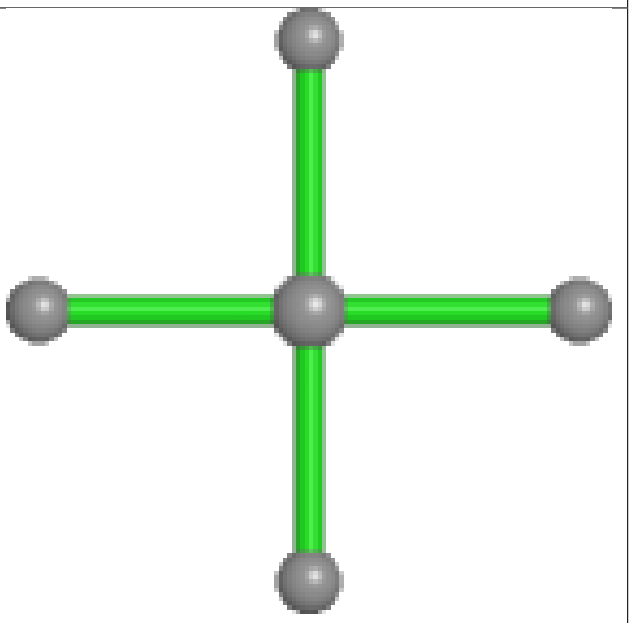


Rings

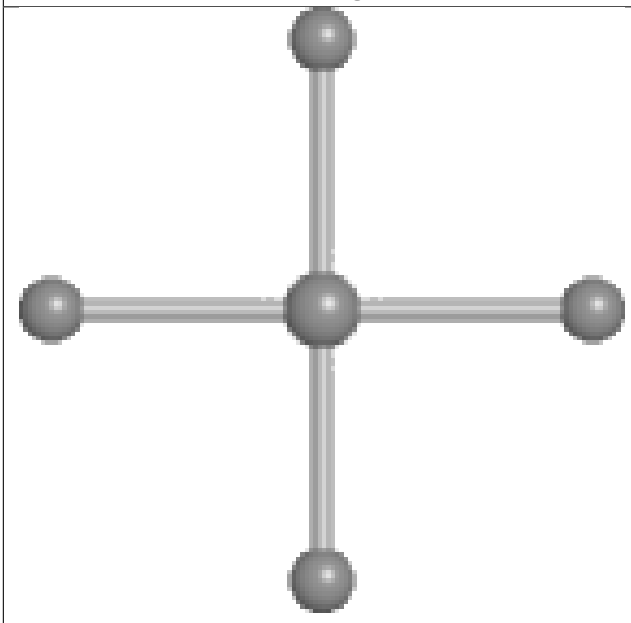
Ligand PO4 A 801



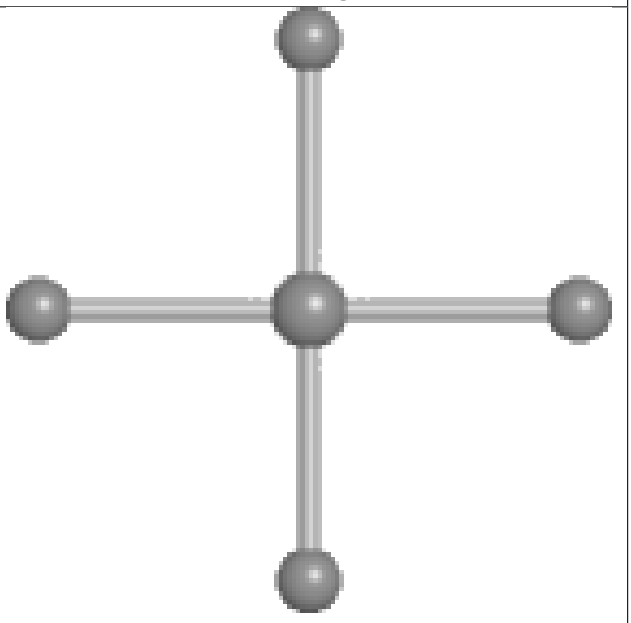
Bond lengths



Bond angles

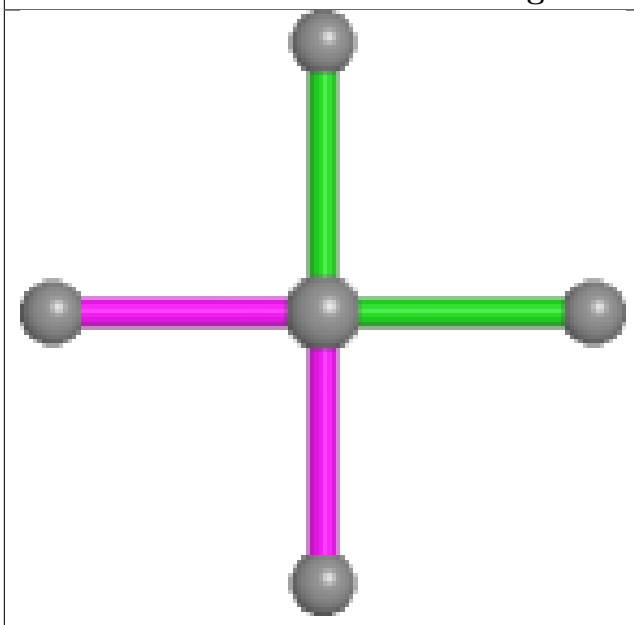


Torsions

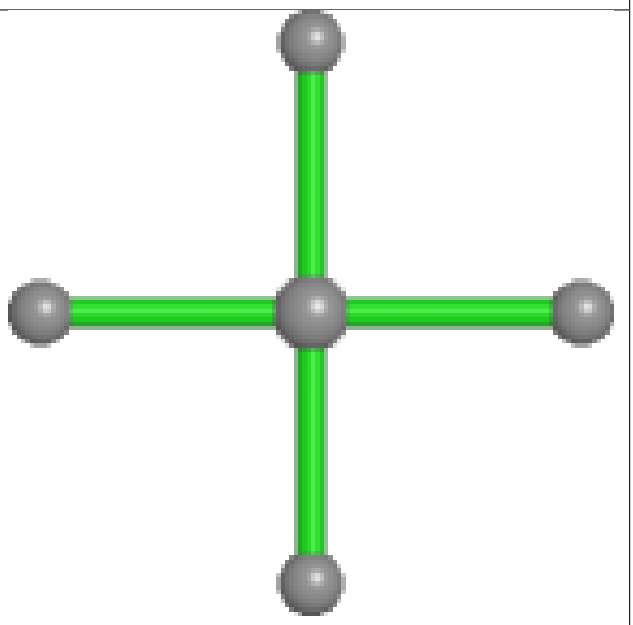


Rings

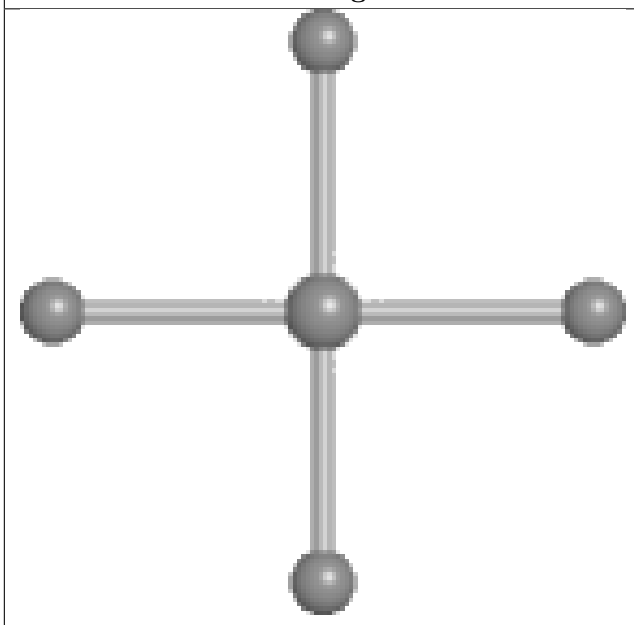
Ligand PO4 D 801



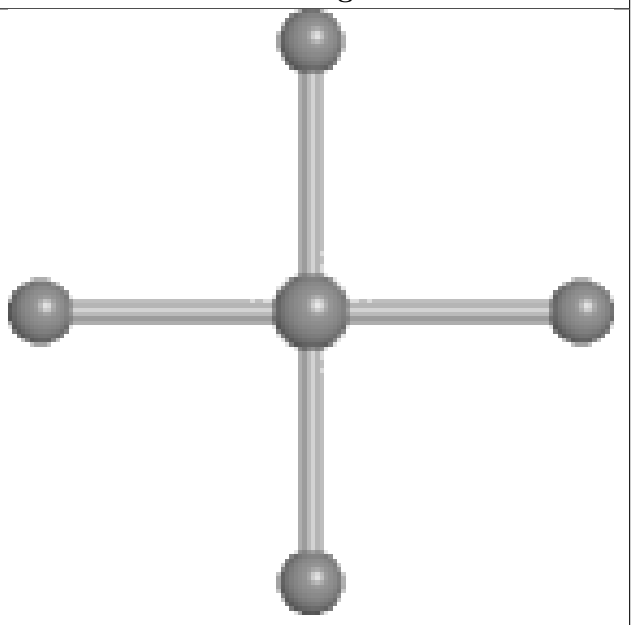
Bond lengths



Bond angles

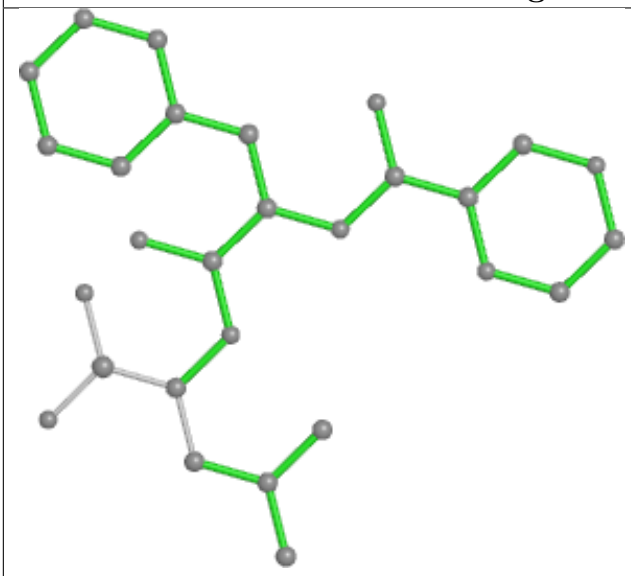


Torsions

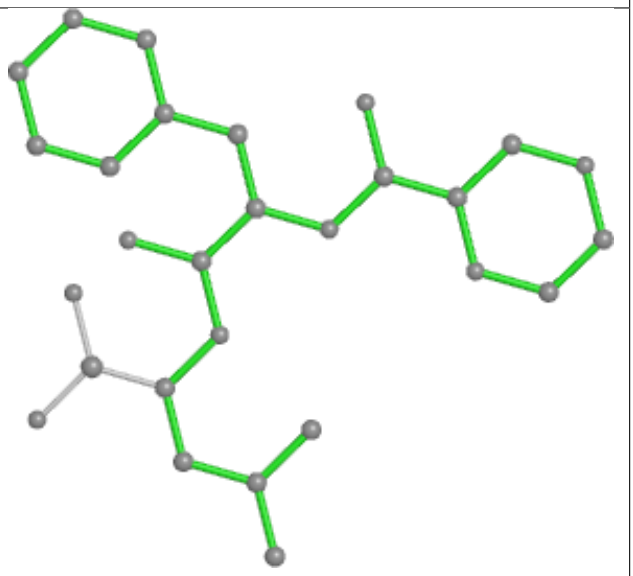


Rings

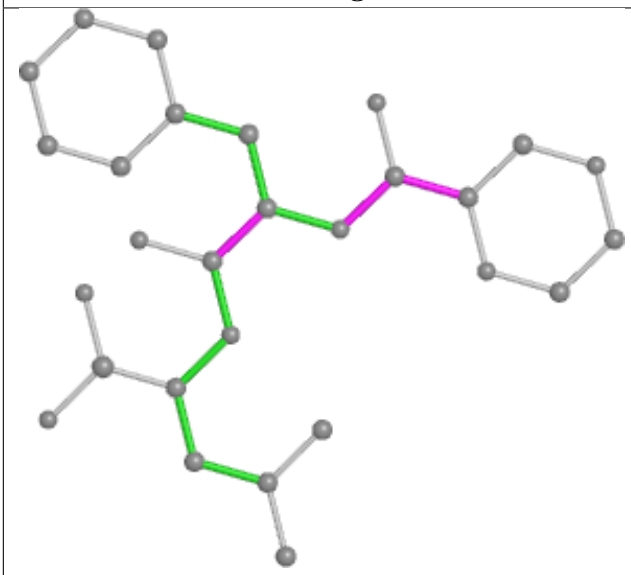
Ligand BO2 E 802



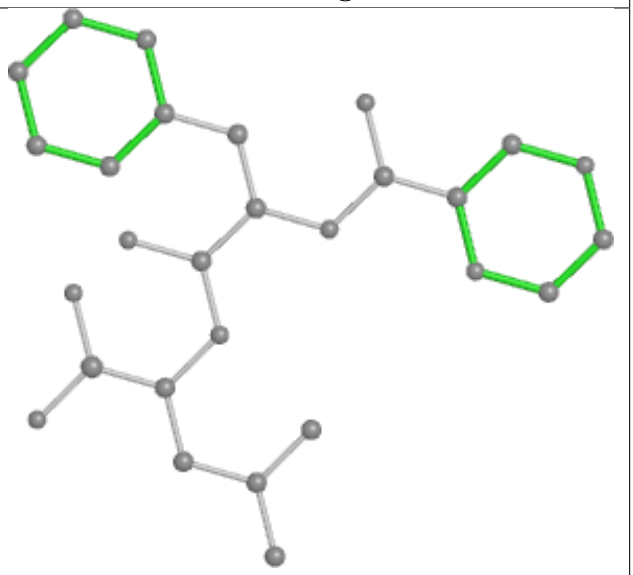
Bond lengths



Bond angles

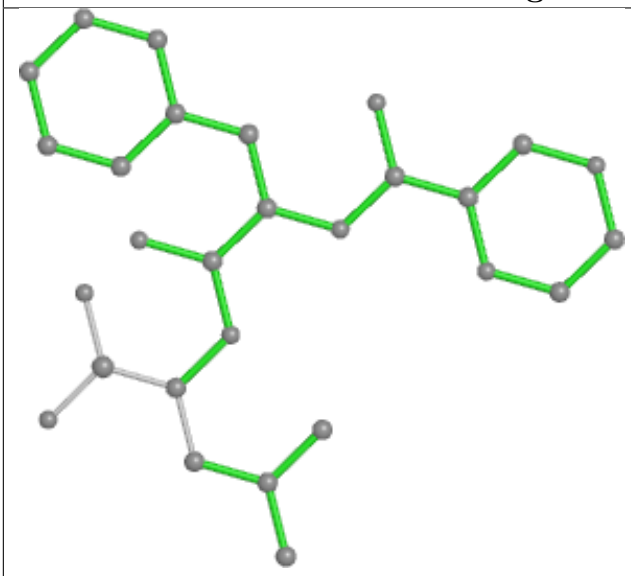


Torsions

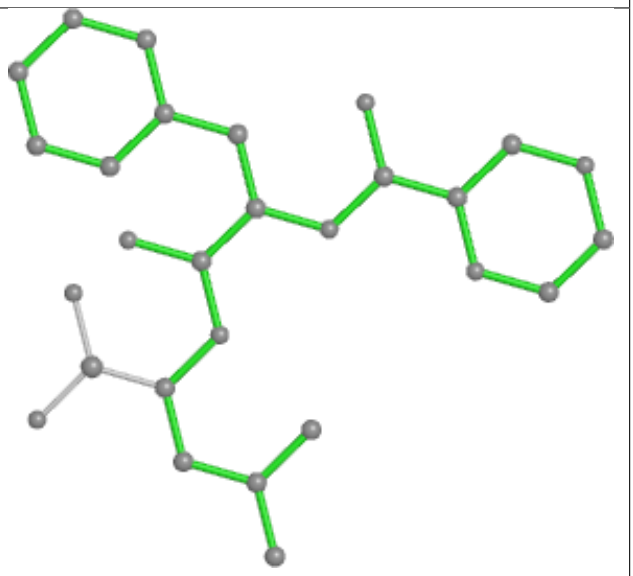


Rings

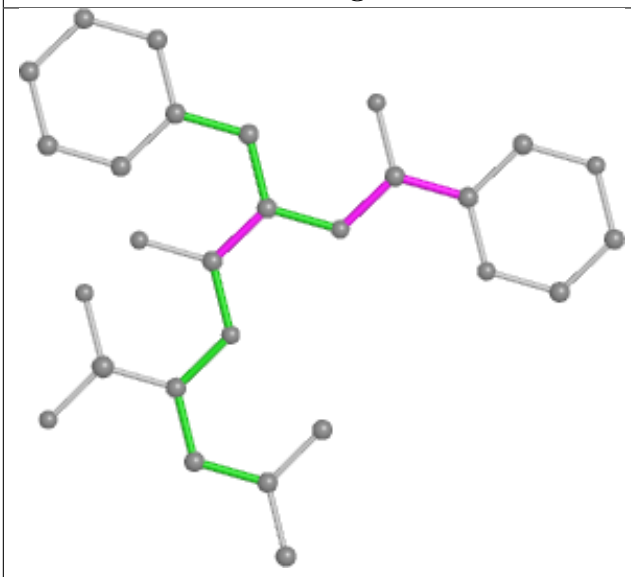
Ligand BO2 C 802



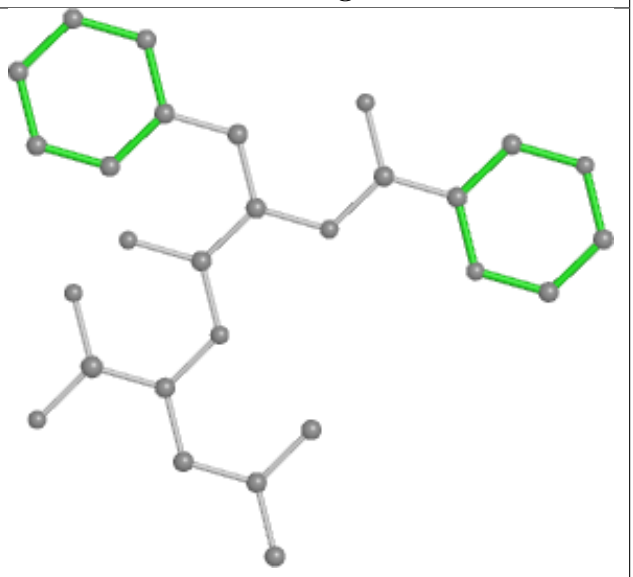
Bond lengths



Bond angles

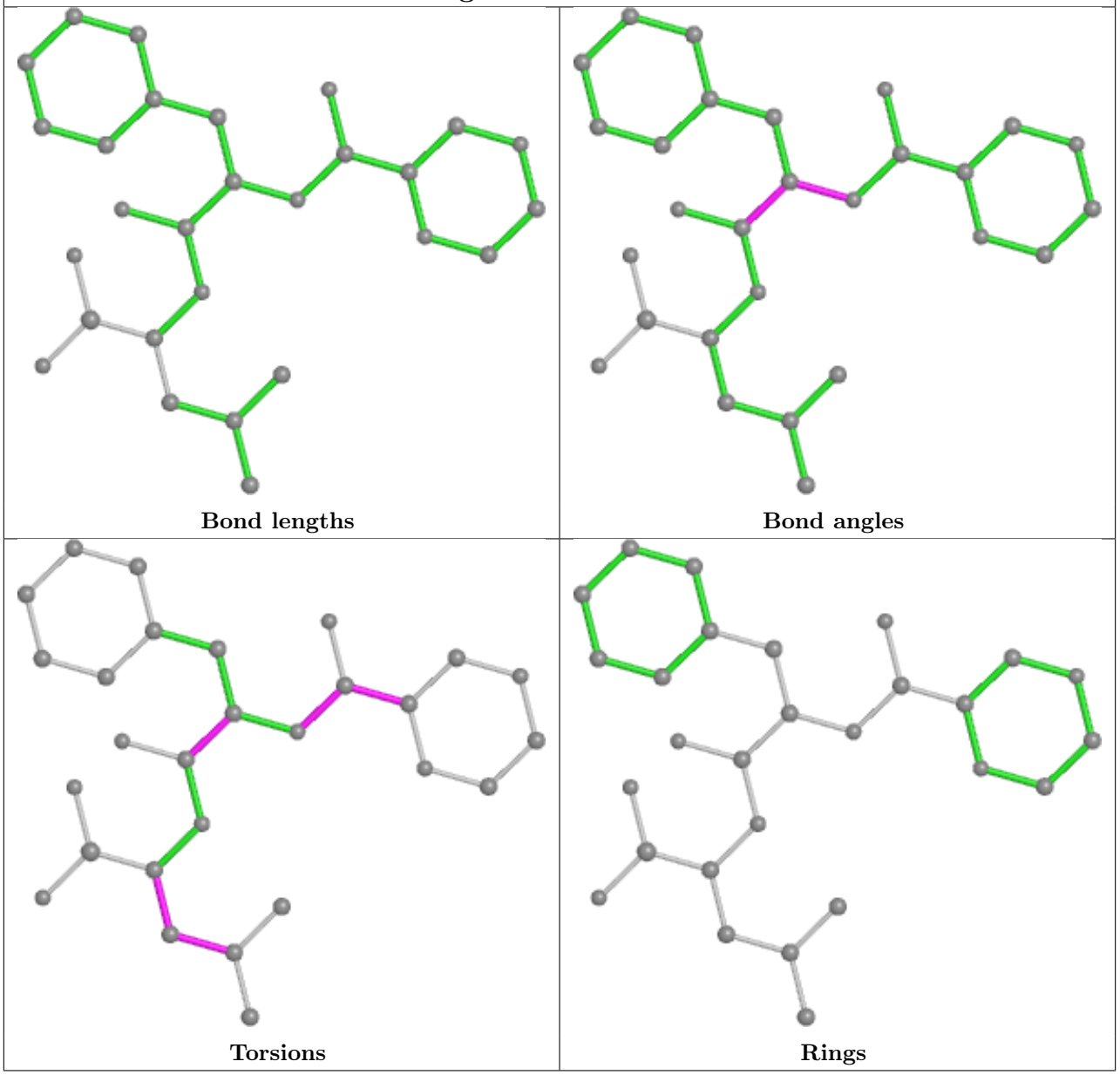


Torsions



Rings

Ligand BO2 D 802



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.

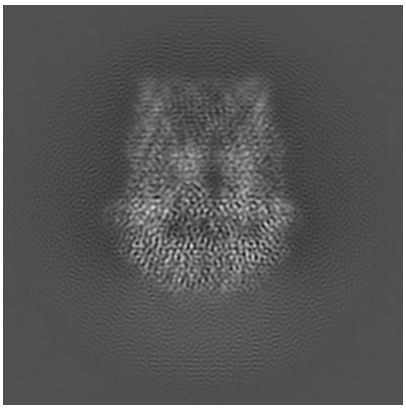
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-36976. These allow visual inspection of the internal detail of the map and identification of artifacts.

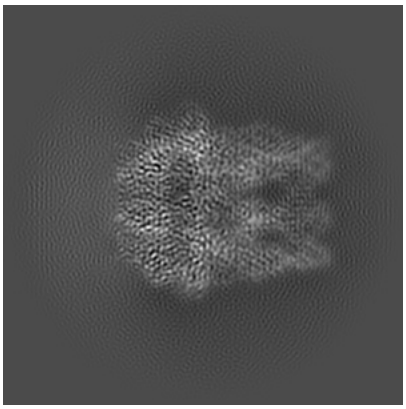
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

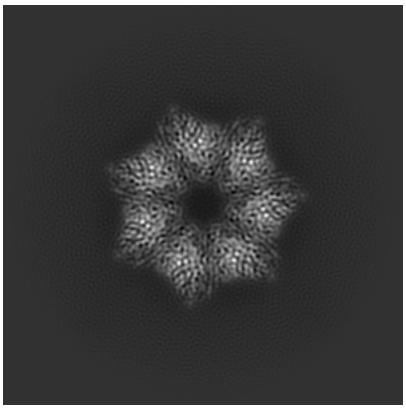
6.1.1 Primary map



X

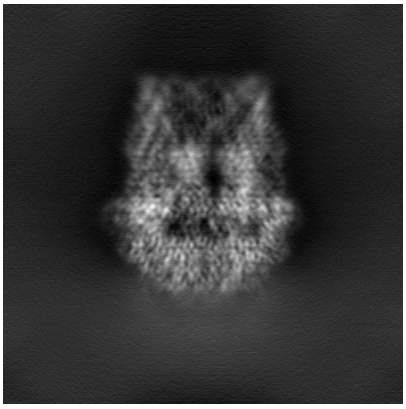


Y

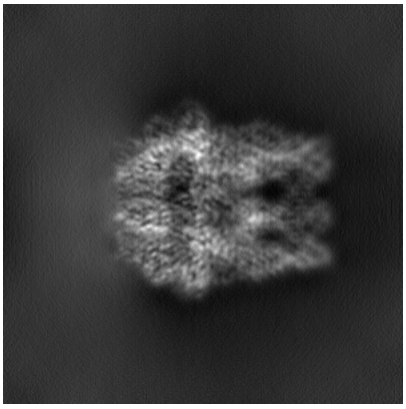


Z

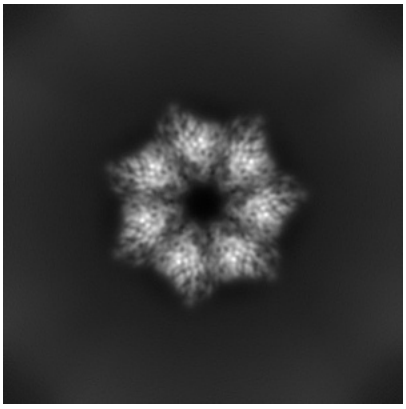
6.1.2 Raw map



X



Y

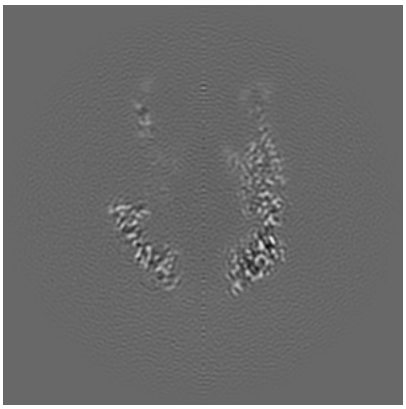


Z

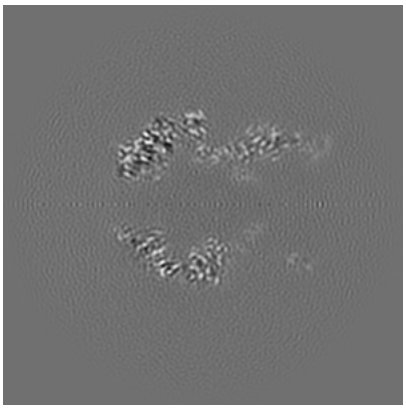
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

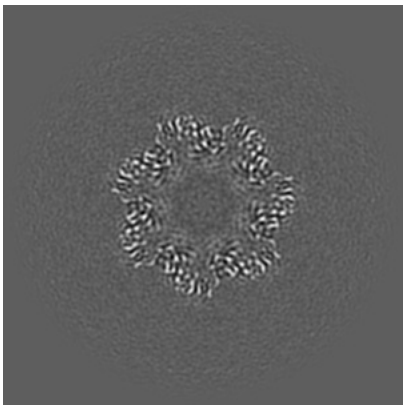
6.2.1 Primary map



X Index: 168

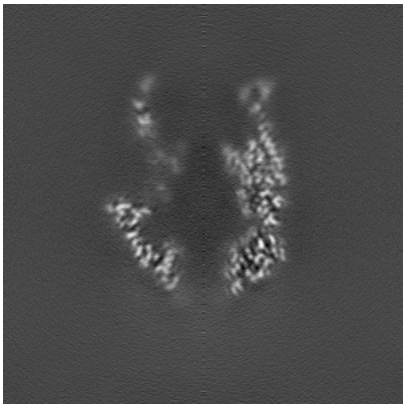


Y Index: 168

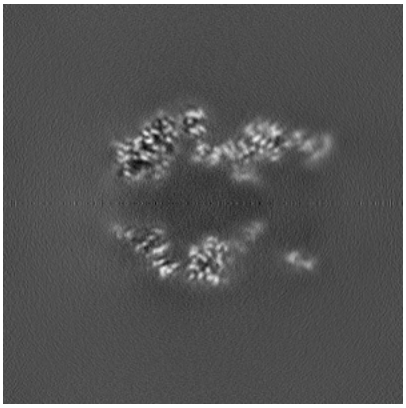


Z Index: 168

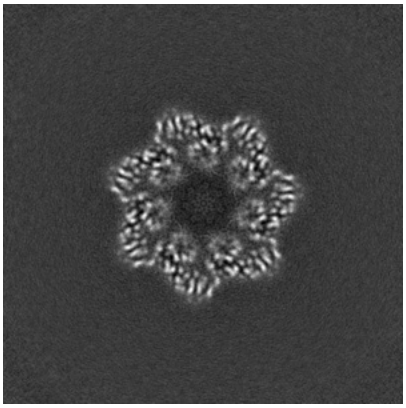
6.2.2 Raw map



X Index: 168



Y Index: 168

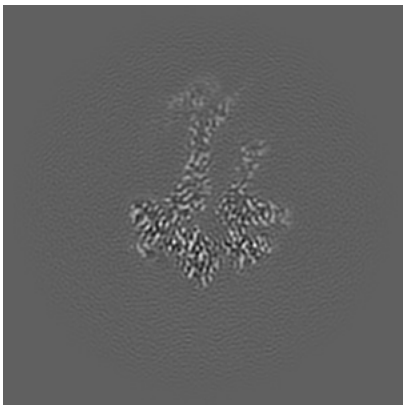


Z Index: 168

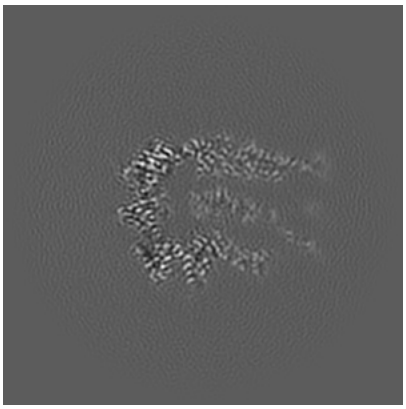
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

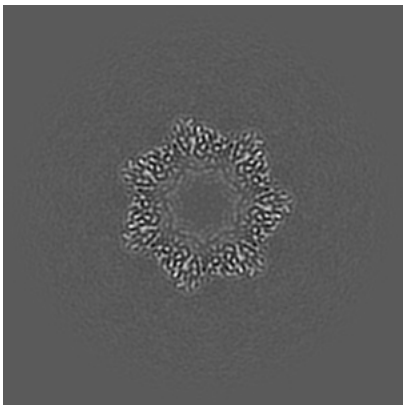
6.3.1 Primary map



X Index: 215

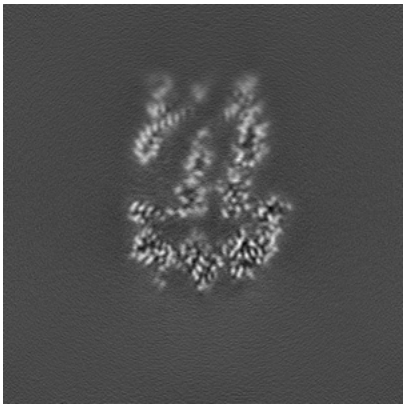


Y Index: 204

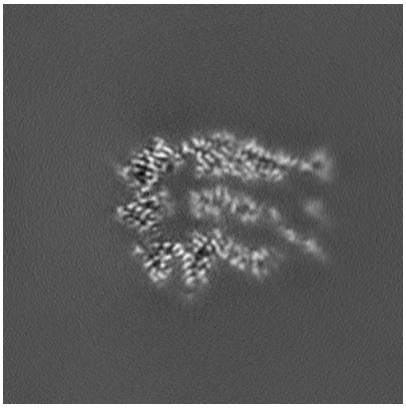


Z Index: 134

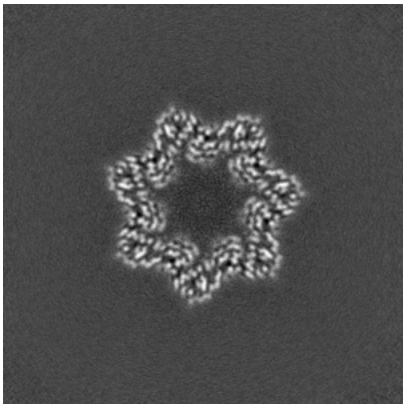
6.3.2 Raw map



X Index: 205



Y Index: 204

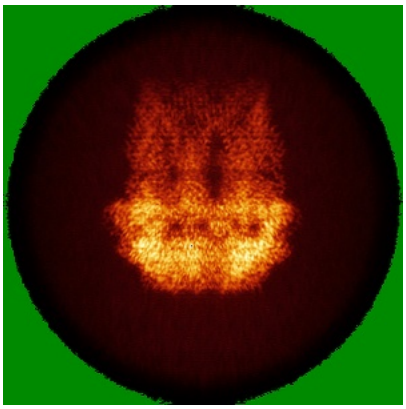


Z Index: 165

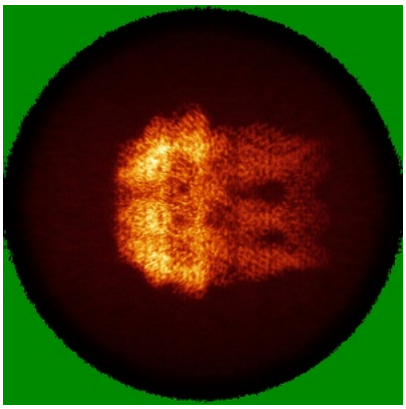
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

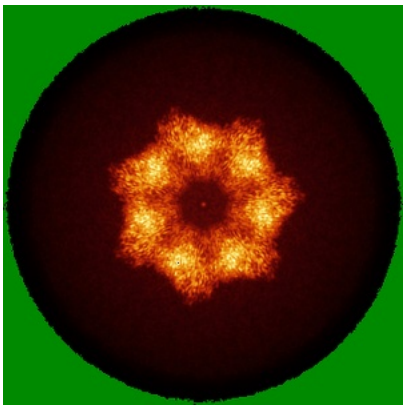
6.4.1 Primary map



X

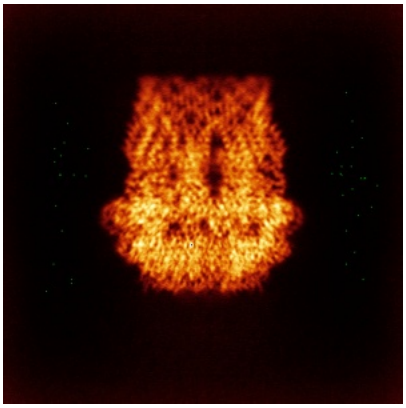


Y

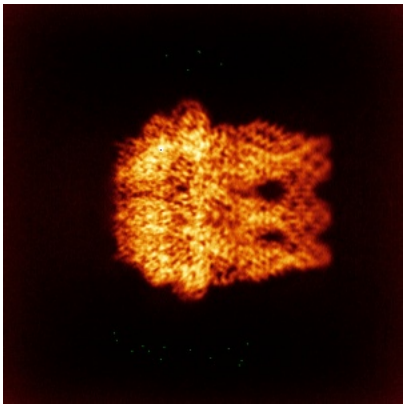


Z

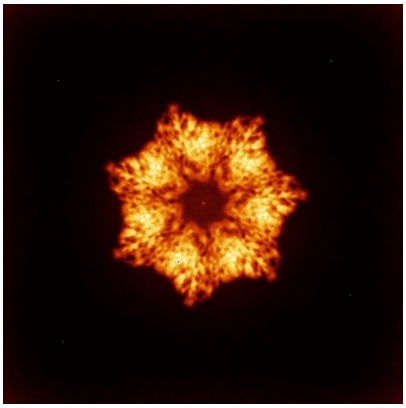
6.4.2 Raw map



X



Y

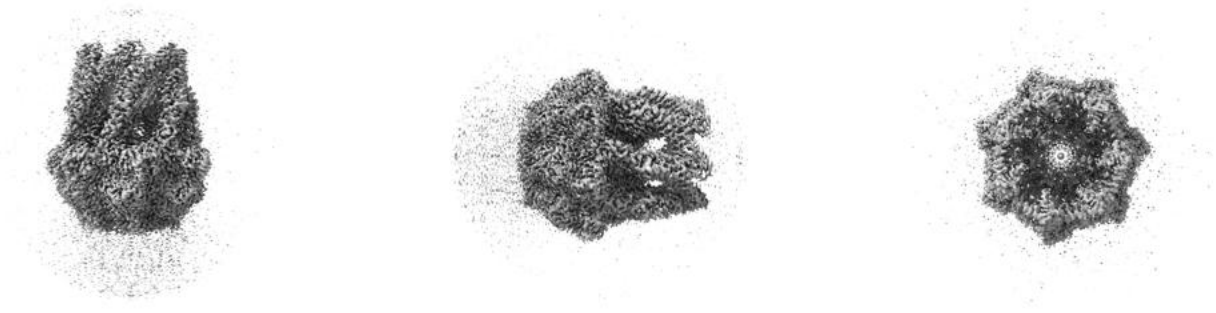


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.1. 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

X Y Z

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.

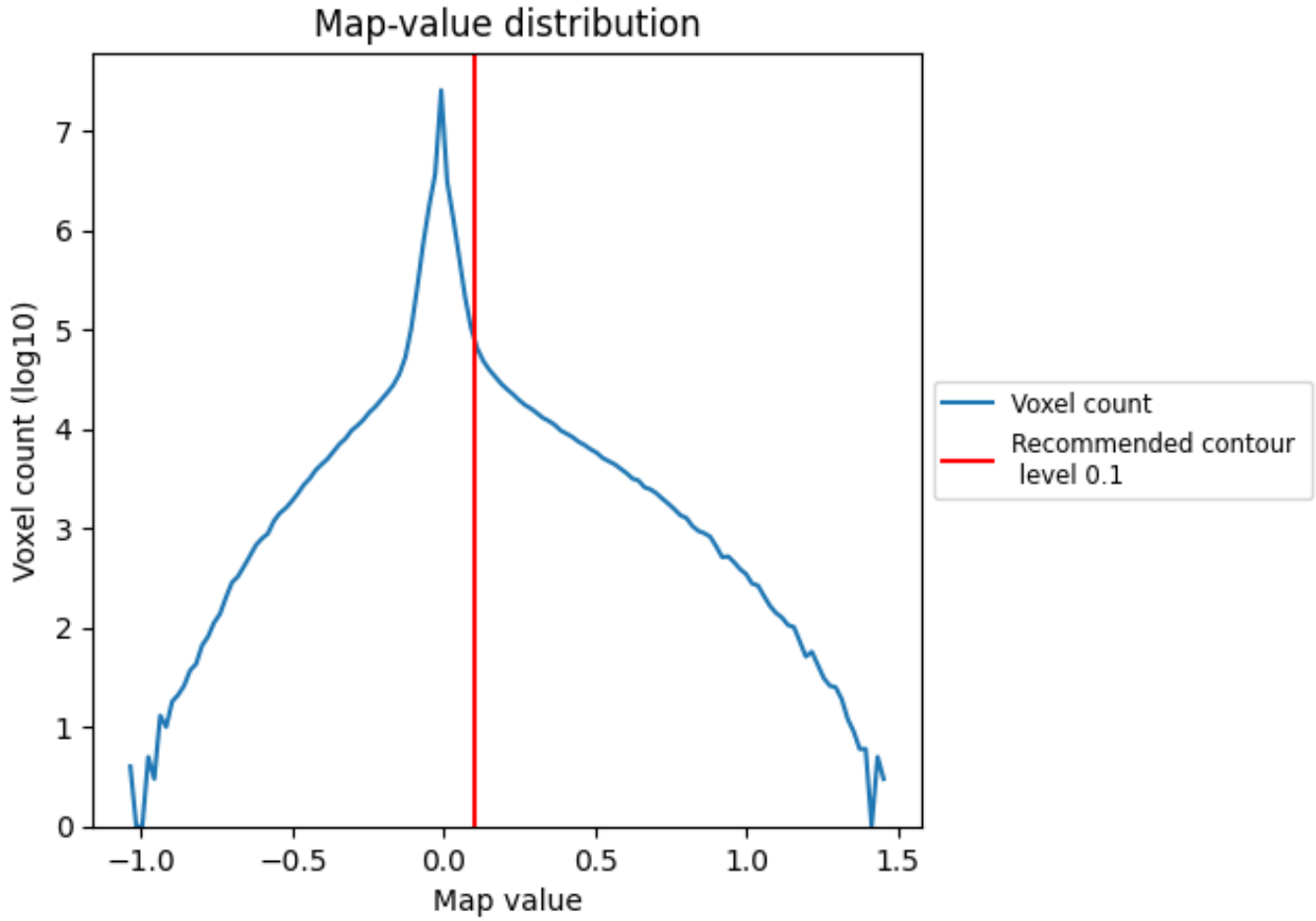
6.6 Mask visualisation (i)

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

7 Map analysis

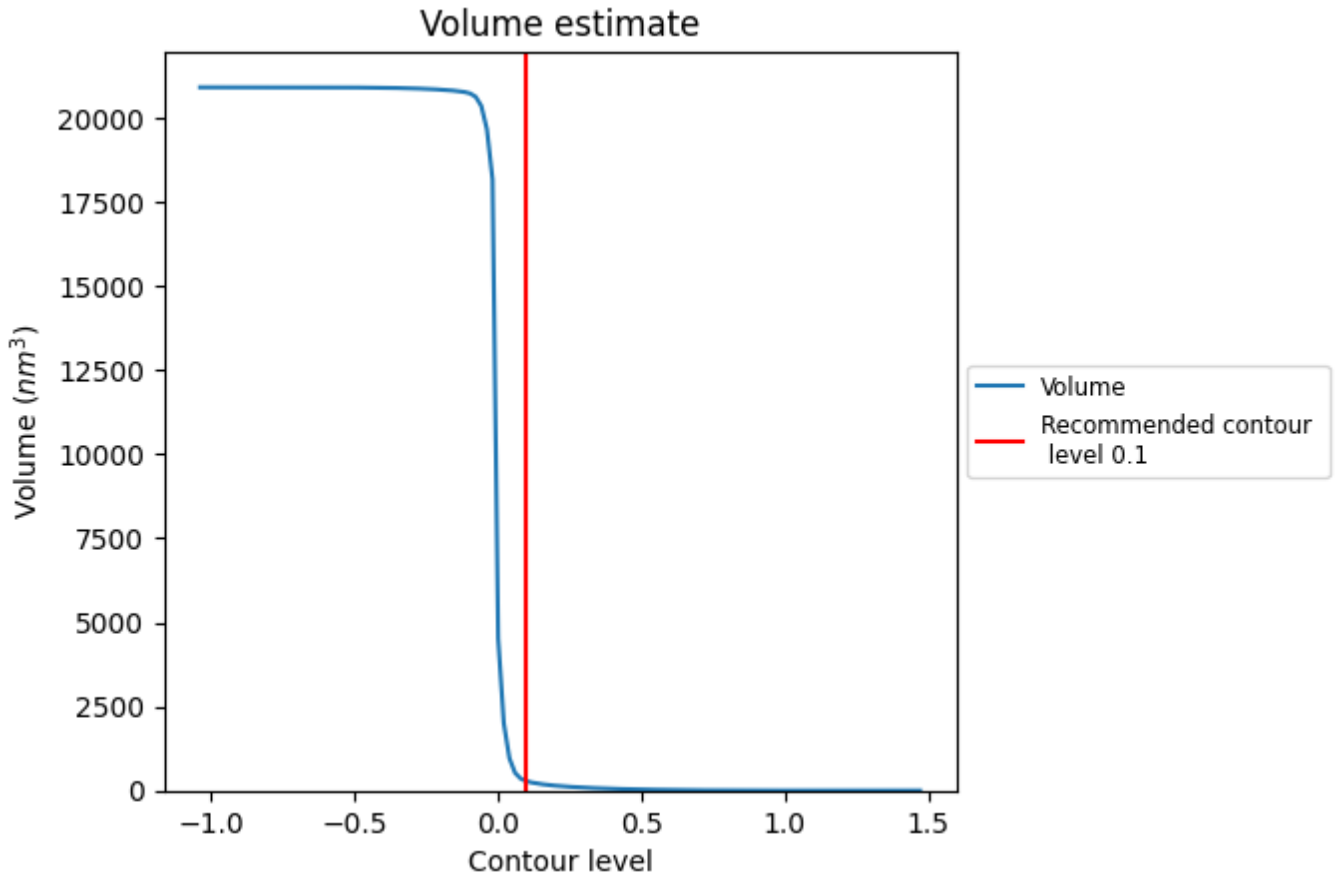
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

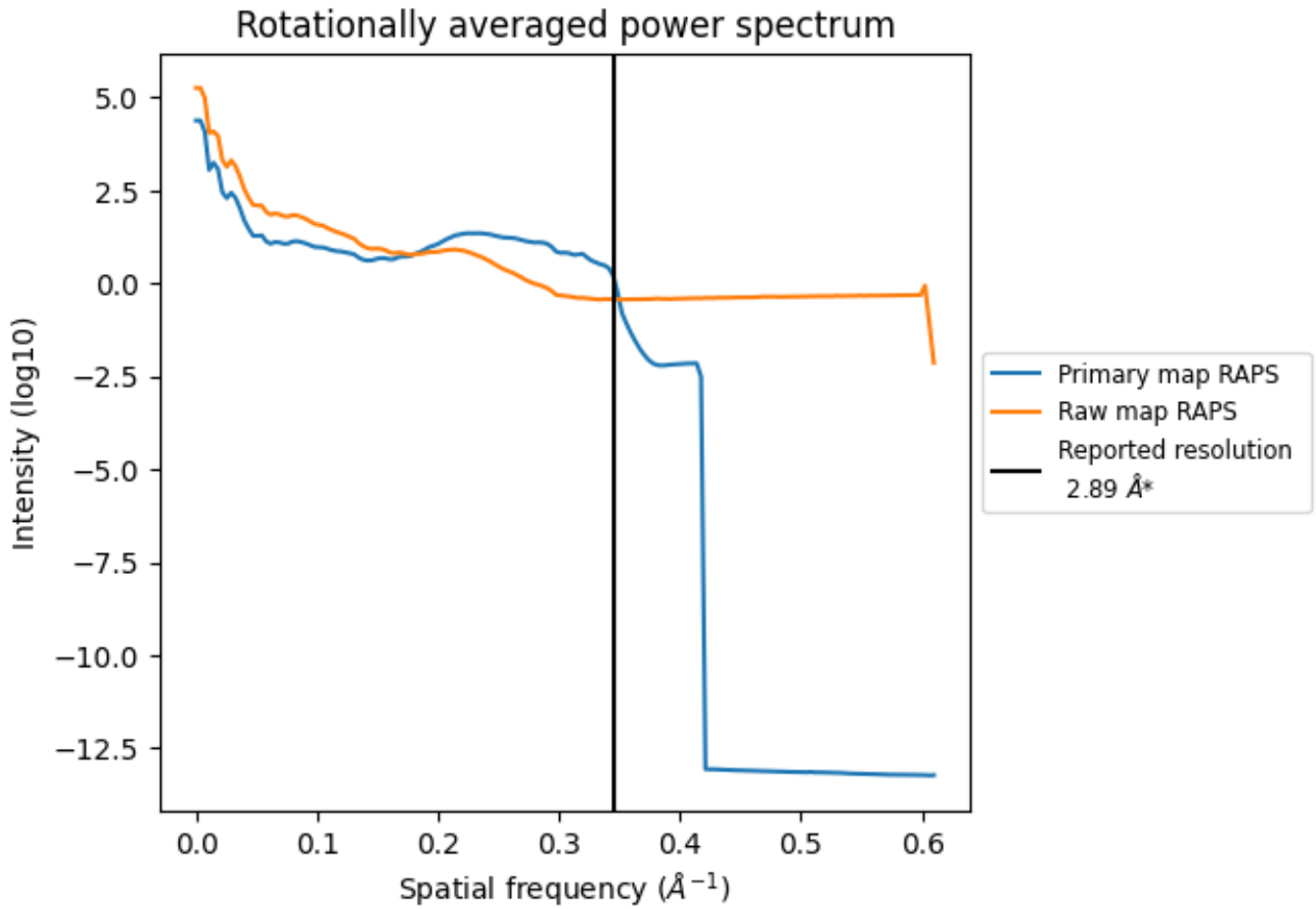
7.2 Volume estimate (i)



The volume at the recommended contour level is 283 nm^3; this corresponds to an approximate mass of 256 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)

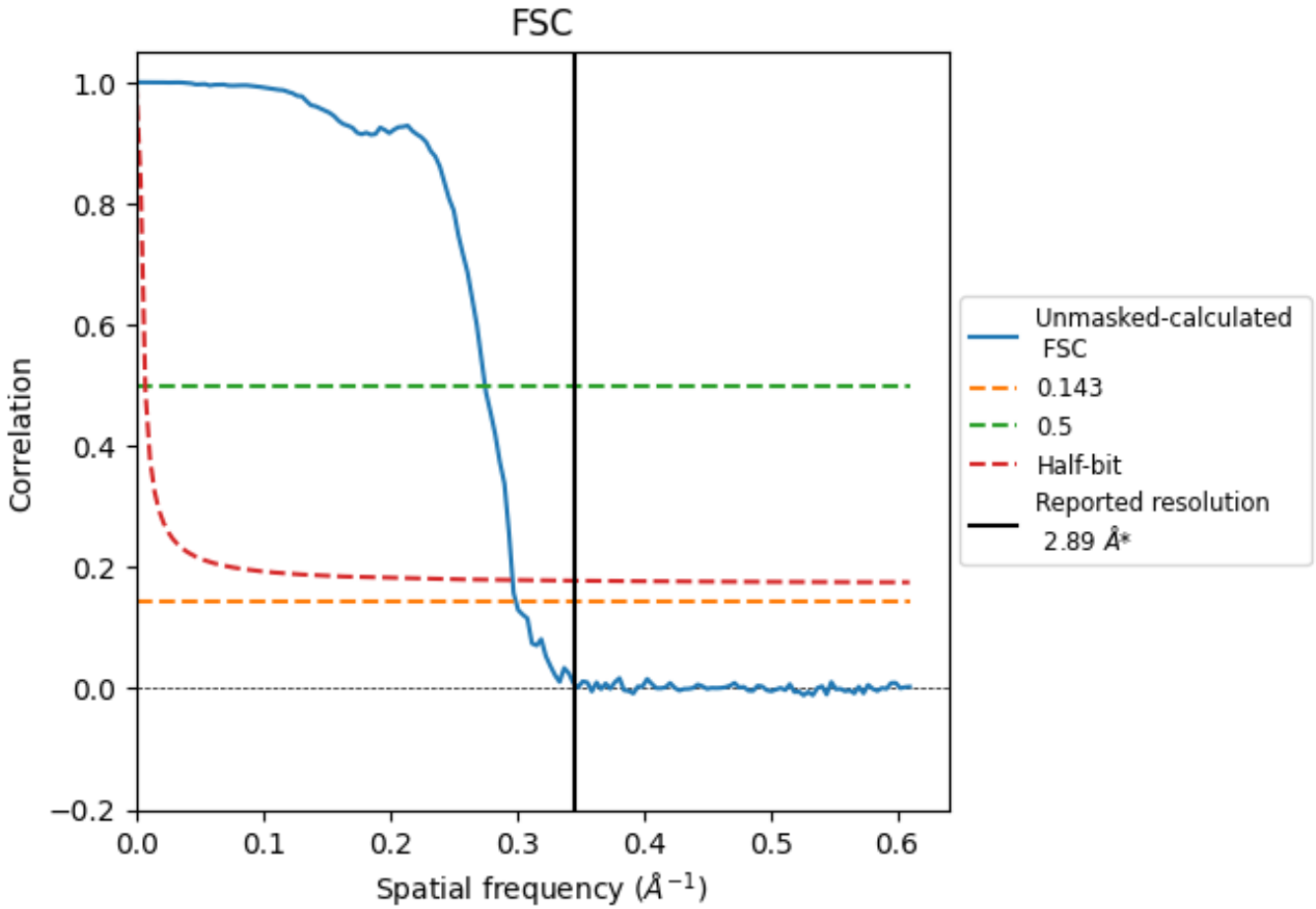


*Reported resolution corresponds to spatial frequency of 0.346 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.346 Å^{-1}

8.2 Resolution estimates (i)

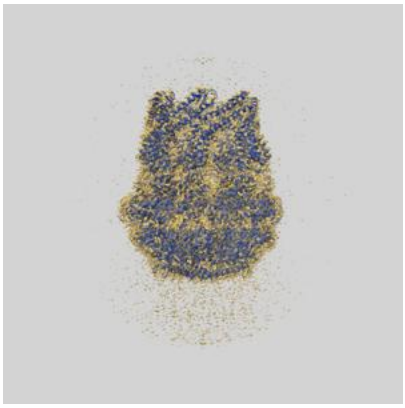
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.89	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.34	3.64	3.37

*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 3.34 differs from the reported value 2.89 by more than 10 %

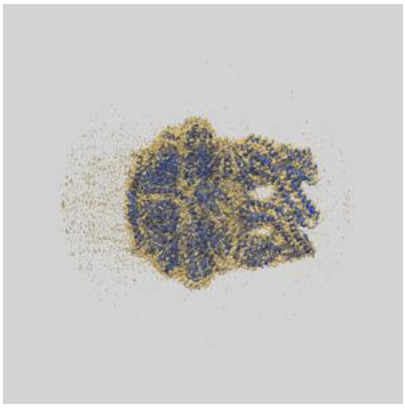
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-36976 and PDB model 8K96. Per-residue inclusion information can be found in section 3 on page 9.

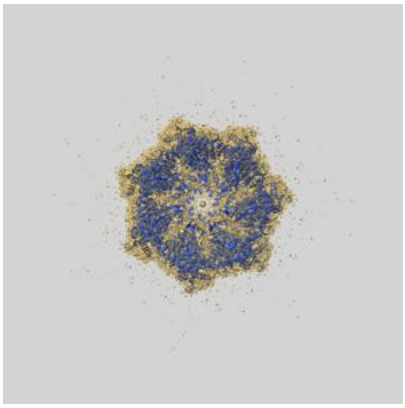
9.1 Map-model overlay



X



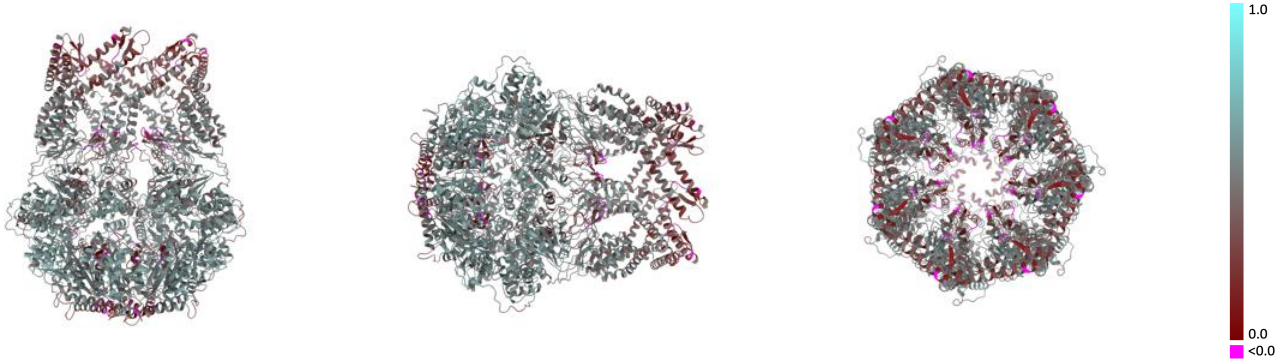
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 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.

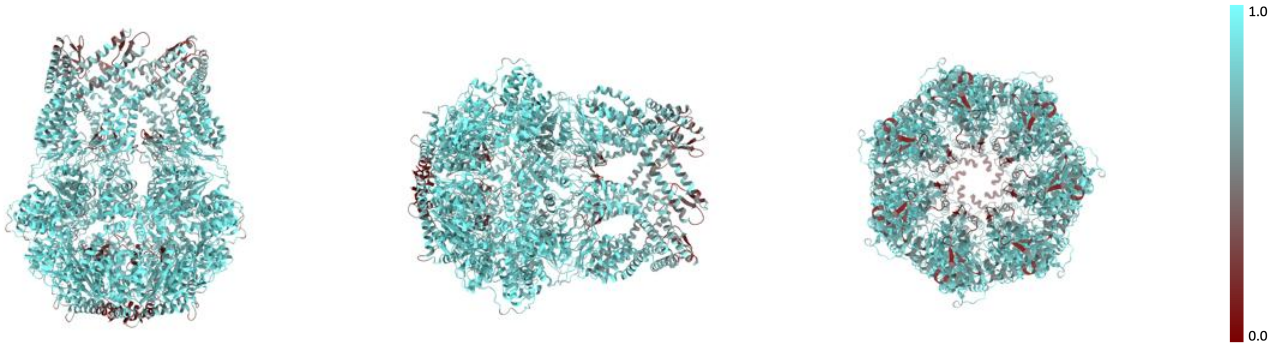
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

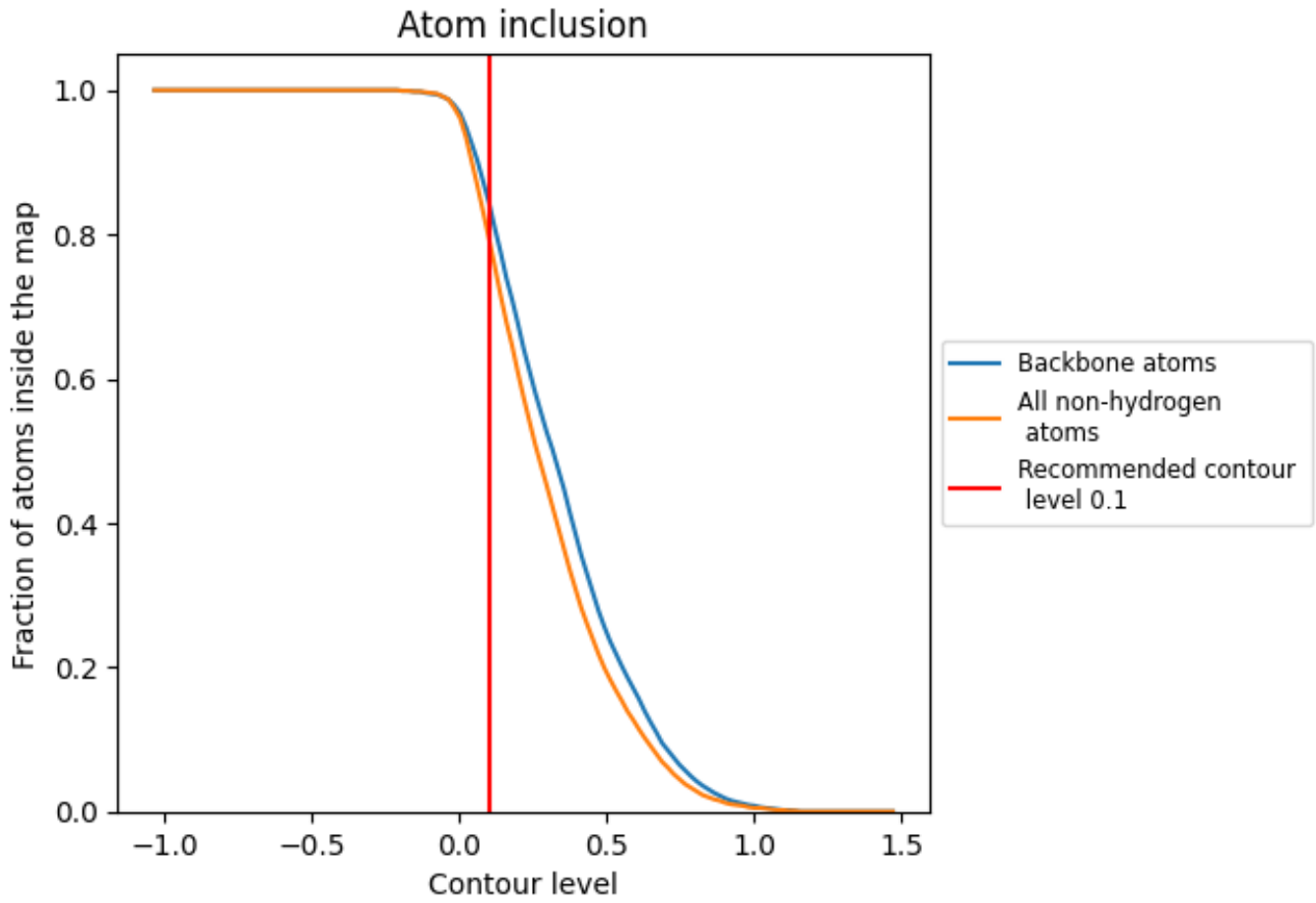
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 80% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7960	0.4580
A	0.7960	0.4580
B	0.7940	0.4570
C	0.7940	0.4580
D	0.7950	0.4590
E	0.7970	0.4580
F	0.7960	0.4590
G	0.7960	0.4580