



## Full wwPDB EM Validation Report ⓘ

May 28, 2024 – 07:42 pm BST

PDB ID : 8P02  
EMDB ID : EMD-17324  
Title : Cryo-EM structure of Phthaloyl-CoA decarboxylase (Pcd) bound with product, benzoyl-CoA  
Authors : Kayastha, K.; Ermler, U.  
Deposited on : 2023-05-09  
Resolution : 2.30 Å(reported)  
Based on initial model : .

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.dev92  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

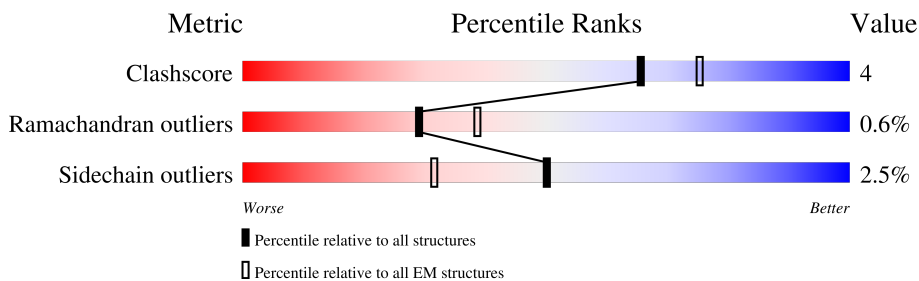
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	514	
1	B	514	
1	C	514	
1	D	514	
1	E	514	
1	F	514	

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
3	BYN	A	602	X	-	-	-
3	BYN	B	602	X	-	-	-
3	BYN	C	602	X	-	-	-
3	BYN	D	602	X	-	-	-
3	BYN	E	602	X	-	-	-
3	BYN	F	602	X	-	-	-

## 2 Entry composition [i](#)

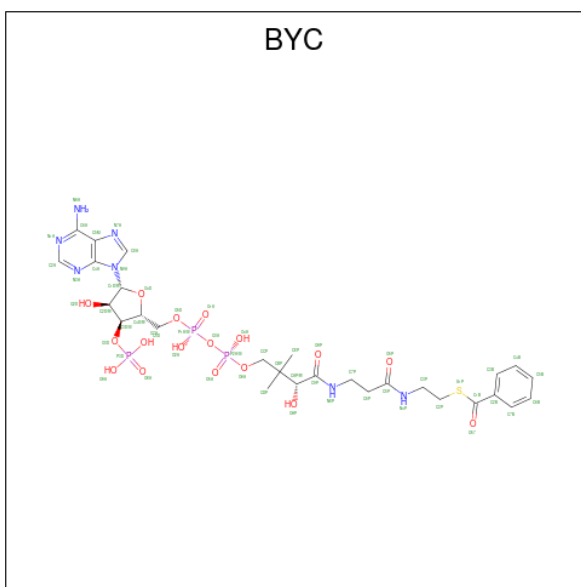
There are 7 unique types of molecules in this entry. The entry contains 24929 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phthaloyl-CoA decarboxylase (Pcd).

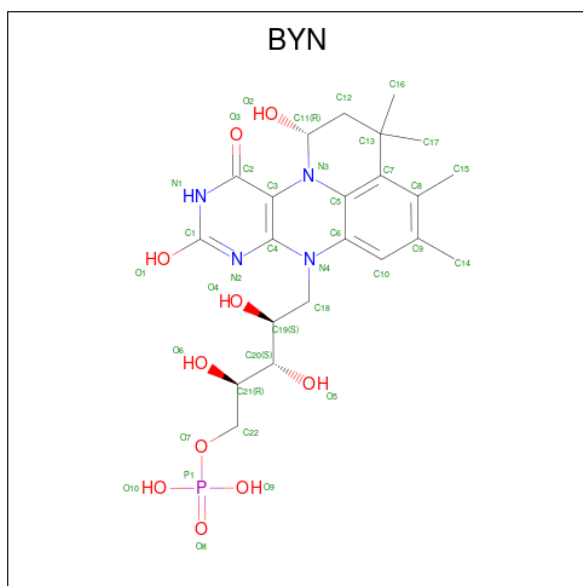
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	514	Total 4049	C 2567	N 699	O 755	S 28	0	0
1	B	514	Total 4049	C 2567	N 699	O 755	S 28	0	0
1	C	514	Total 4049	C 2567	N 699	O 755	S 28	0	0
1	D	514	Total 4049	C 2567	N 699	O 755	S 28	0	0
1	E	514	Total 4049	C 2567	N 699	O 755	S 28	0	0
1	F	514	Total 4049	C 2567	N 699	O 755	S 28	0	0

- Molecule 2 is benzoyl coenzyme A (three-letter code: BYC) (formula:  $C_{28}H_{40}N_7O_{17}P_3S$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
2	A	1	Total 56	C 28	N 7	O 17	P 3	S 1	0
2	B	1	Total 56	C 28	N 7	O 17	P 3	S 1	0
2	C	1	Total 56	C 28	N 7	O 17	P 3	S 1	0
2	D	1	Total 56	C 28	N 7	O 17	P 3	S 1	0
2	E	1	Total 56	C 28	N 7	O 17	P 3	S 1	0
2	F	1	Total 56	C 28	N 7	O 17	P 3	S 1	0

- Molecule 3 is hydroxylated prenyl-FMN (three-letter code: BYN) (formula: C<sub>22</sub>H<sub>31</sub>N<sub>4</sub>O<sub>10</sub>P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	A	1	Total 36	C 22	N 4	O 9	P 1	0
3	B	1	Total 36	C 22	N 4	O 9	P 1	0
3	C	1	Total 36	C 22	N 4	O 9	P 1	0
3	D	1	Total 36	C 22	N 4	O 9	P 1	0
3	E	1	Total 36	C 22	N 4	O 9	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	F	1	36	22	4	9	1	0

- Molecule 4 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	2	Total	Fe	0
			2	2	
4	B	2	Total	Fe	0
			2	2	
4	C	2	Total	Fe	0
			2	2	
4	D	2	Total	Fe	0
			2	2	
4	E	2	Total	Fe	0
			2	2	
4	F	2	Total	Fe	0
			2	2	

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Ca	0
			1	1	
5	B	1	Total	Ca	0
			1	1	
5	C	1	Total	Ca	0
			1	1	
5	D	1	Total	Ca	0
			1	1	
5	E	1	Total	Ca	0
			1	1	
5	F	1	Total	Ca	0
			1	1	

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
6	A	1	Total	K	0
			1	1	

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Mol	Chain	Residues	Atoms	AltConf
6	B	1	Total K 1 1	0
6	C	1	Total K 1 1	0
6	D	1	Total K 1 1	0
6	E	1	Total K 1 1	0
6	F	1	Total K 1 1	0

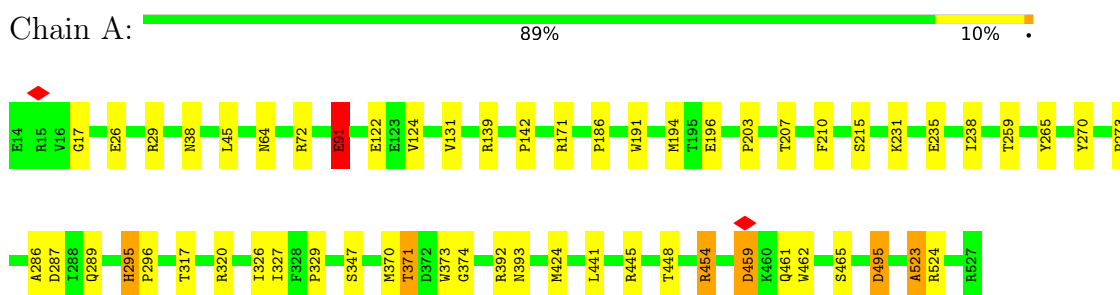
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	AltConf
7	A	10	Total O 10 10	0
7	B	8	Total O 8 8	0
7	C	9	Total O 9 9	0
7	D	11	Total O 11 11	0
7	E	11	Total O 11 11	0
7	F	10	Total O 10 10	0

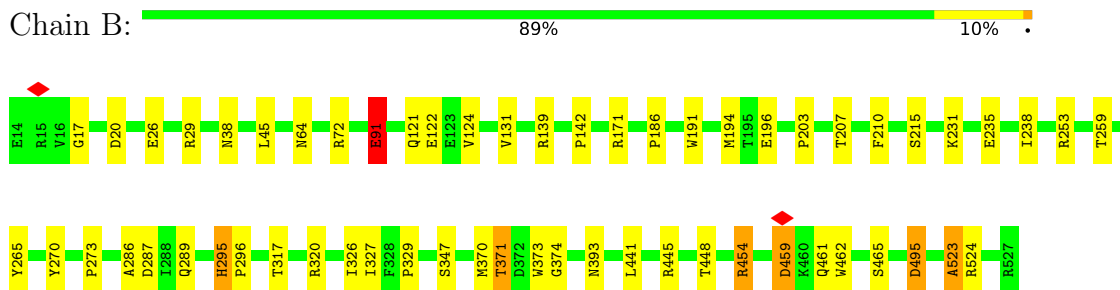
### 3 Residue-property plots [i](#)

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.

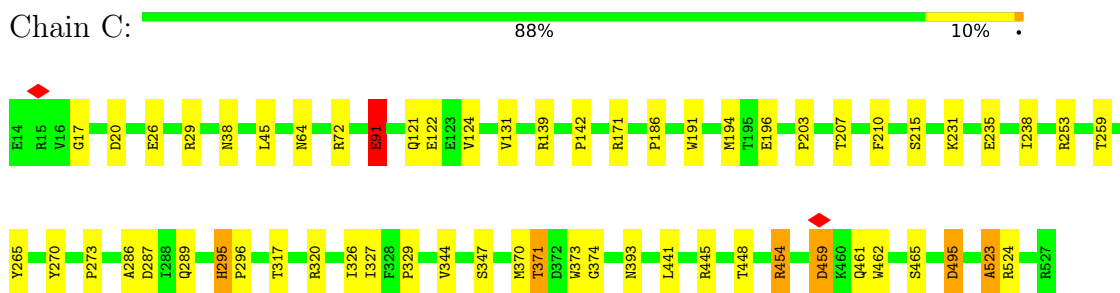
- Molecule 1: Phthaloyl-CoA decarboxylase (Pcd)



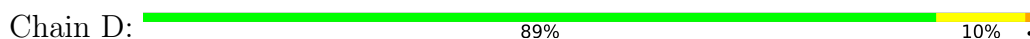
- Molecule 1: Phthaloyl-CoA decarboxylase (Pcd)



- Molecule 1: Phthaloyl-CoA decarboxylase (Pcd)



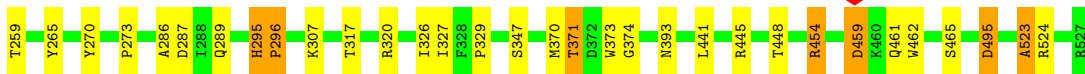
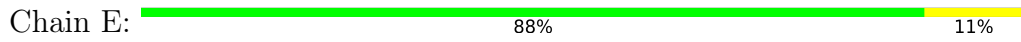
- Molecule 1: Phthaloyl-CoA decarboxylase (Pcd)



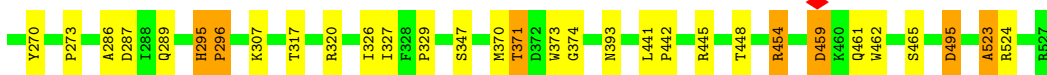
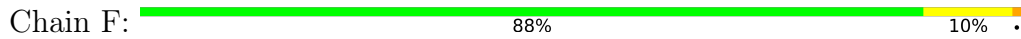




• Molecule 1: Phthaloyl-CoA decarboxylase (Pcd)



• Molecule 1: Phthaloyl-CoA decarboxylase (Pcd)



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, D3	Depositor
Number of particles used	821681	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	52.27	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.038	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00552	Depositor
Map size (Å)	267.84, 267.84, 267.84	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	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: K, BYN, FE, CA, BYC

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	0.51	1/4150 (0.0%)	0.54	1/5632 (0.0%)
1	B	0.51	1/4150 (0.0%)	0.54	1/5632 (0.0%)
1	C	0.51	1/4150 (0.0%)	0.54	1/5632 (0.0%)
1	D	0.51	1/4150 (0.0%)	0.54	1/5632 (0.0%)
1	E	0.51	1/4150 (0.0%)	0.54	1/5632 (0.0%)
1	F	0.51	1/4150 (0.0%)	0.54	1/5632 (0.0%)
All	All	0.51	6/24900 (0.0%)	0.54	6/33792 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	2
1	B	1	2
1	C	1	2
1	D	1	2
1	E	1	2
1	F	1	2
All	All	6	12

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	523	ALA	C-N	15.27	1.69	1.34
1	A	523	ALA	C-N	15.25	1.69	1.34
1	E	523	ALA	C-N	15.25	1.69	1.34
1	F	523	ALA	C-N	15.24	1.69	1.34
1	D	523	ALA	C-N	15.24	1.69	1.34
1	B	523	ALA	C-N	15.24	1.69	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	91	GLU	CA-CB-CG	6.72	128.18	113.40
1	D	91	GLU	CA-CB-CG	6.72	128.18	113.40
1	F	91	GLU	CA-CB-CG	6.71	128.17	113.40
1	B	91	GLU	CA-CB-CG	6.70	128.15	113.40
1	A	91	GLU	CA-CB-CG	6.69	128.13	113.40
1	E	91	GLU	CA-CB-CG	6.69	128.12	113.40

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	371	THR	CB
1	B	371	THR	CB
1	C	371	THR	CB
1	D	371	THR	CB
1	E	371	THR	CB
1	F	371	THR	CB

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	GLY	Peptide
1	A	286	ALA	Peptide
1	B	17	GLY	Peptide
1	B	286	ALA	Peptide
1	C	17	GLY	Peptide
1	C	286	ALA	Peptide
1	D	17	GLY	Peptide
1	D	286	ALA	Peptide
1	E	17	GLY	Peptide
1	E	286	ALA	Peptide
1	F	17	GLY	Peptide
1	F	286	ALA	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4049	0	3950	33	0
1	B	4049	0	3950	34	0
1	C	4049	0	3950	35	0
1	D	4049	0	3950	32	0
1	E	4049	0	3950	36	0
1	F	4049	0	3950	36	0
2	A	56	0	36	2	0
2	B	56	0	36	2	0
2	C	56	0	36	2	0
2	D	56	0	36	2	0
2	E	56	0	36	2	0
2	F	56	0	36	2	0
3	A	36	0	0	1	0
3	B	36	0	0	1	0
3	C	36	0	0	1	0
3	D	36	0	0	1	0
3	E	36	0	0	1	0
3	F	36	0	0	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	2	0	0	0	0
4	F	2	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
7	A	10	0	0	0	0
7	B	8	0	0	0	0
7	C	9	0	0	0	0
7	D	11	0	0	0	0
7	E	11	0	0	0	0
7	F	10	0	0	0	0
All	All	24929	0	23916	201	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 4.

All (201) 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:B:523:ALA:C	1:B:524:ARG:N	1.69	1.45
1:C:523:ALA:C	1:C:524:ARG:N	1.69	1.45
1:E:523:ALA:C	1:E:524:ARG:N	1.69	1.43
1:F:523:ALA:C	1:F:524:ARG:N	1.69	1.43
1:D:523:ALA:C	1:D:524:ARG:N	1.69	1.42
1:A:523:ALA:C	1:A:524:ARG:N	1.69	1.42
1:D:445:ARG:H	1:E:393:ASN:HD21	1.37	0.73
1:A:445:ARG:H	1:F:393:ASN:HD21	1.38	0.71
1:D:393:ASN:HD21	1:E:445:ARG:H	1.37	0.70
1:A:393:ASN:HD21	1:F:445:ARG:H	1.39	0.69
1:B:445:ARG:H	1:C:393:ASN:HD21	1.39	0.69
1:B:393:ASN:HD21	1:C:445:ARG:H	1.39	0.69
1:E:495:ASP:OD2	1:E:495:ASP:N	2.28	0.67
1:F:495:ASP:OD2	1:F:495:ASP:N	2.28	0.67
1:A:495:ASP:OD2	1:A:495:ASP:N	2.28	0.67
1:D:495:ASP:OD2	1:D:495:ASP:N	2.28	0.67
1:C:495:ASP:OD2	1:C:495:ASP:N	2.28	0.66
1:B:495:ASP:OD2	1:B:495:ASP:N	2.28	0.65
1:E:327:ILE:HG23	1:E:329:PRO:HD3	1.84	0.59
1:F:327:ILE:HG23	1:F:329:PRO:HD3	1.84	0.59
1:B:327:ILE:HG23	1:B:329:PRO:HD3	1.84	0.59
1:C:327:ILE:HG23	1:C:329:PRO:HD3	1.84	0.59
1:A:327:ILE:HG23	1:A:329:PRO:HD3	1.84	0.58
1:D:327:ILE:HG23	1:D:329:PRO:HD3	1.84	0.58
1:A:371:THR:HG23	1:A:374:GLY:H	1.68	0.58
1:D:371:THR:HG23	1:D:374:GLY:H	1.68	0.58
1:C:371:THR:HG23	1:C:374:GLY:H	1.68	0.58
1:B:371:THR:HG23	1:B:374:GLY:H	1.68	0.58
1:F:371:THR:HG23	1:F:374:GLY:H	1.68	0.58
1:E:371:THR:HG23	1:E:374:GLY:H	1.68	0.57
1:E:370:MET:O	1:E:371:THR:HG22	2.05	0.56
1:F:370:MET:O	1:F:371:THR:HG22	2.05	0.56
1:B:370:MET:O	1:B:371:THR:HG22	2.05	0.56
1:C:370:MET:O	1:C:371:THR:HG22	2.05	0.56
1:A:203:PRO:HB2	1:A:270:TYR:HB3	1.88	0.56
1:D:203:PRO:HB2	1:D:270:TYR:HB3	1.88	0.56
1:F:203:PRO:HB2	1:F:270:TYR:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:370:MET:O	1:D:371:THR:HG22	2.05	0.56
3:D:602:BYN:O5	3:D:602:BYN:O7	2.23	0.56
3:A:602:BYN:O5	3:A:602:BYN:O7	2.23	0.56
1:E:203:PRO:HB2	1:E:270:TYR:HB3	1.88	0.56
1:A:370:MET:O	1:A:371:THR:HG22	2.05	0.56
3:F:602:BYN:O5	3:F:602:BYN:O7	2.23	0.55
3:E:602:BYN:O5	3:E:602:BYN:O7	2.23	0.55
1:B:91:GLU:OE1	1:B:91:GLU:N	2.40	0.55
1:C:91:GLU:N	1:C:91:GLU:OE1	2.40	0.55
3:C:602:BYN:O5	3:C:602:BYN:O7	2.23	0.55
1:E:196:GLU:OE1	1:E:231:LYS:NZ	2.40	0.55
1:B:196:GLU:OE1	1:B:231:LYS:NZ	2.40	0.55
1:C:196:GLU:OE1	1:C:231:LYS:NZ	2.40	0.55
1:F:91:GLU:OE1	1:F:91:GLU:N	2.40	0.55
1:F:196:GLU:OE1	1:F:231:LYS:NZ	2.40	0.55
1:B:203:PRO:HB2	1:B:270:TYR:HB3	1.88	0.55
3:B:602:BYN:O5	3:B:602:BYN:O7	2.23	0.55
1:C:203:PRO:HB2	1:C:270:TYR:HB3	1.88	0.55
1:D:91:GLU:N	1:D:91:GLU:OE1	2.40	0.55
1:E:91:GLU:N	1:E:91:GLU:OE1	2.40	0.55
1:A:91:GLU:N	1:A:91:GLU:OE1	2.40	0.55
1:A:196:GLU:OE1	1:A:231:LYS:NZ	2.40	0.55
1:D:196:GLU:OE1	1:D:231:LYS:NZ	2.40	0.55
1:D:207:THR:HG21	1:D:259:THR:HG22	1.92	0.52
1:A:207:THR:HG21	1:A:259:THR:HG22	1.92	0.52
1:F:122:GLU:OE2	1:F:320:ARG:N	2.44	0.51
1:E:122:GLU:OE2	1:E:320:ARG:N	2.44	0.51
1:A:122:GLU:OE2	1:A:320:ARG:N	2.44	0.51
1:B:122:GLU:OE2	1:B:320:ARG:N	2.44	0.51
1:D:122:GLU:OE2	1:D:320:ARG:N	2.44	0.51
1:C:122:GLU:OE2	1:C:320:ARG:N	2.44	0.51
1:F:207:THR:HG21	1:F:259:THR:HG22	1.92	0.51
1:E:207:THR:HG21	1:E:259:THR:HG22	1.92	0.51
1:A:171:ARG:HD2	1:A:295:HIS:HE1	1.76	0.51
1:C:171:ARG:HD2	1:C:295:HIS:HE1	1.76	0.51
1:E:210:PHE:HB2	1:E:265:TYR:HB2	1.93	0.51
1:D:171:ARG:HD2	1:D:295:HIS:HE1	1.76	0.51
1:E:26:GLU:OE2	1:E:29:ARG:NH1	2.45	0.51
1:B:171:ARG:HD2	1:B:295:HIS:HE1	1.76	0.50
1:B:207:THR:HG21	1:B:259:THR:HG22	1.92	0.50
1:F:26:GLU:OE2	1:F:29:ARG:NH1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:210:PHE:HB2	1:F:265:TYR:HB2	1.93	0.50
1:C:207:THR:HG21	1:C:259:THR:HG22	1.92	0.50
1:A:210:PHE:HB2	1:A:265:TYR:HB2	1.93	0.50
1:D:210:PHE:HB2	1:D:265:TYR:HB2	1.93	0.50
1:E:171:ARG:HD2	1:E:295:HIS:HE1	1.76	0.50
1:A:371:THR:HG23	1:A:374:GLY:N	2.26	0.50
1:D:371:THR:HG23	1:D:374:GLY:N	2.26	0.50
1:F:171:ARG:HD2	1:F:295:HIS:HE1	1.76	0.50
1:A:26:GLU:OE2	1:A:29:ARG:NH1	2.44	0.49
1:B:210:PHE:HB2	1:B:265:TYR:HB2	1.93	0.49
1:C:210:PHE:HB2	1:C:265:TYR:HB2	1.93	0.49
1:D:26:GLU:OE2	1:D:29:ARG:NH1	2.45	0.49
1:B:26:GLU:OE2	1:B:29:ARG:NH1	2.45	0.49
1:C:26:GLU:OE2	1:C:29:ARG:NH1	2.45	0.49
1:C:371:THR:HG23	1:C:374:GLY:N	2.26	0.49
1:E:371:THR:HG23	1:E:374:GLY:N	2.26	0.49
1:B:371:THR:HG23	1:B:374:GLY:N	2.26	0.49
1:F:371:THR:HG23	1:F:374:GLY:N	2.26	0.49
1:B:289:GLN:NE2	2:B:601:BYC:O4A	2.46	0.49
1:C:289:GLN:NE2	2:C:601:BYC:O4A	2.46	0.49
1:F:235:GLU:HA	1:F:238:ILE:HD12	1.95	0.48
1:E:235:GLU:HA	1:E:238:ILE:HD12	1.95	0.48
1:C:235:GLU:HA	1:C:238:ILE:HD12	1.95	0.48
1:B:235:GLU:HA	1:B:238:ILE:HD12	1.95	0.48
1:D:289:GLN:NE2	2:D:601:BYC:O4A	2.46	0.48
1:F:289:GLN:NE2	2:F:601:BYC:O4A	2.46	0.48
1:A:289:GLN:NE2	2:A:601:BYC:O4A	2.46	0.47
1:E:289:GLN:NE2	2:E:601:BYC:O4A	2.46	0.47
1:A:373:TRP:CH2	2:A:601:BYC:H7B	2.50	0.47
1:F:373:TRP:CH2	2:F:601:BYC:H7B	2.50	0.47
1:A:38:ASN:O	1:A:64:ASN:ND2	2.48	0.47
1:D:38:ASN:O	1:D:64:ASN:ND2	2.47	0.47
1:D:373:TRP:CH2	2:D:601:BYC:H7B	2.49	0.47
1:E:373:TRP:CH2	2:E:601:BYC:H7B	2.49	0.47
1:E:139:ARG:HH21	1:E:142:PRO:HA	1.79	0.47
1:F:139:ARG:HH21	1:F:142:PRO:HA	1.79	0.47
1:A:235:GLU:HA	1:A:238:ILE:HD12	1.95	0.47
1:B:38:ASN:O	1:B:64:ASN:ND2	2.48	0.47
1:C:38:ASN:O	1:C:64:ASN:ND2	2.48	0.47
1:D:235:GLU:HA	1:D:238:ILE:HD12	1.95	0.47
1:E:38:ASN:O	1:E:64:ASN:ND2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:ARG:HH21	1:A:142:PRO:HA	1.79	0.46
1:B:139:ARG:HH21	1:B:142:PRO:HA	1.79	0.46
1:C:139:ARG:HH21	1:C:142:PRO:HA	1.79	0.46
1:F:38:ASN:O	1:F:64:ASN:ND2	2.48	0.46
1:A:459:ASP:OD1	1:A:459:ASP:N	2.49	0.46
1:D:139:ARG:HH21	1:D:142:PRO:HA	1.79	0.46
1:D:459:ASP:OD1	1:D:459:ASP:N	2.49	0.46
1:F:459:ASP:OD1	1:F:459:ASP:N	2.49	0.46
1:B:373:TRP:CH2	2:B:601:BYC:H7B	2.50	0.46
1:C:373:TRP:CH2	2:C:601:BYC:H7B	2.50	0.46
1:E:459:ASP:OD1	1:E:459:ASP:N	2.49	0.46
1:B:454:ARG:HB2	1:B:462:TRP:CE2	2.52	0.45
1:C:454:ARG:HB2	1:C:462:TRP:CE2	2.52	0.45
1:E:171:ARG:HD2	1:E:295:HIS:CE1	2.52	0.45
1:F:171:ARG:HD2	1:F:295:HIS:CE1	2.52	0.45
1:B:459:ASP:N	1:B:459:ASP:OD1	2.49	0.45
1:D:124:VAL:HG13	1:D:317:THR:HG22	1.98	0.45
1:E:454:ARG:HB2	1:E:462:TRP:CE2	2.52	0.45
1:F:454:ARG:HB2	1:F:462:TRP:CE2	2.52	0.45
1:A:124:VAL:HG13	1:A:317:THR:HG22	1.98	0.45
1:C:459:ASP:OD1	1:C:459:ASP:N	2.49	0.45
1:F:124:VAL:HG13	1:F:317:THR:HG22	1.98	0.45
1:C:124:VAL:HG13	1:C:317:THR:HG22	1.98	0.45
1:E:124:VAL:HG13	1:E:317:THR:HG22	1.98	0.45
1:C:171:ARG:HD2	1:C:295:HIS:CE1	2.51	0.45
1:B:171:ARG:HD2	1:B:295:HIS:CE1	2.52	0.45
1:B:124:VAL:HG13	1:B:317:THR:HG22	1.98	0.45
1:D:171:ARG:HD2	1:D:295:HIS:CE1	2.52	0.45
1:A:171:ARG:HD2	1:A:295:HIS:CE1	2.51	0.44
1:A:454:ARG:HB2	1:A:462:TRP:CE2	2.52	0.44
1:D:454:ARG:HB2	1:D:462:TRP:CE2	2.52	0.44
1:C:194:MET:HG3	1:C:273:PRO:HB3	2.01	0.43
1:B:194:MET:HG3	1:B:273:PRO:HB3	2.01	0.43
1:B:289:GLN:H	1:B:461:GLN:HE21	1.67	0.42
1:F:213:PRO:HA	1:F:214:PRO:HD3	1.95	0.42
1:C:289:GLN:H	1:C:461:GLN:HE21	1.67	0.42
1:D:194:MET:HG3	1:D:273:PRO:HB3	2.01	0.42
1:E:194:MET:HG3	1:E:273:PRO:HB3	2.01	0.42
1:A:194:MET:HG3	1:A:273:PRO:HB3	2.01	0.42
1:E:213:PRO:HA	1:E:214:PRO:HD3	1.94	0.42
1:F:194:MET:HG3	1:F:273:PRO:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:ARG:HH21	1:E:326:ILE:HD11	1.84	0.42
1:B:45:LEU:HD13	1:B:142:PRO:HG3	2.02	0.42
1:C:45:LEU:HD13	1:C:142:PRO:HG3	2.02	0.42
1:E:289:GLN:H	1:E:461:GLN:HE21	1.67	0.42
1:F:289:GLN:H	1:F:461:GLN:HE21	1.67	0.42
1:F:72:ARG:HH21	1:F:326:ILE:HD11	1.85	0.42
1:F:295:HIS:HA	1:F:296:PRO:HD3	1.94	0.42
1:A:289:GLN:H	1:A:461:GLN:HE21	1.66	0.42
1:D:289:GLN:H	1:D:461:GLN:HE21	1.67	0.42
1:A:72:ARG:HH21	1:A:326:ILE:HD11	1.84	0.42
1:E:45:LEU:HD13	1:E:142:PRO:HG3	2.02	0.42
1:B:121:GLN:OE1	1:B:253:ARG:NE	2.46	0.42
1:C:344:VAL:H	1:C:344:VAL:HG12	1.66	0.41
1:D:72:ARG:HH21	1:D:326:ILE:HD11	1.84	0.41
1:D:445:ARG:H	1:E:393:ASN:ND2	2.11	0.41
1:E:295:HIS:HA	1:E:296:PRO:HD3	1.94	0.41
1:F:45:LEU:HD13	1:F:142:PRO:HG3	2.02	0.41
1:C:121:GLN:OE1	1:C:253:ARG:NE	2.46	0.41
1:B:72:ARG:HH21	1:B:326:ILE:HD11	1.85	0.41
1:A:186:PRO:HA	1:A:191:TRP:CD2	2.55	0.41
1:C:72:ARG:HH21	1:C:326:ILE:HD11	1.85	0.41
1:D:186:PRO:HA	1:D:191:TRP:CD2	2.55	0.41
1:E:186:PRO:HA	1:E:191:TRP:CD2	2.55	0.41
1:F:186:PRO:HA	1:F:191:TRP:CD2	2.55	0.41
1:B:20:ASP:N	1:B:20:ASP:OD1	2.54	0.41
1:B:393:ASN:ND2	1:C:445:ARG:H	2.14	0.41
1:B:445:ARG:H	1:C:393:ASN:ND2	2.14	0.41
1:C:20:ASP:N	1:C:20:ASP:OD1	2.54	0.41
1:D:158:GLY:HA3	1:D:159:PRO:HD3	1.88	0.41
1:E:307:LYS:HE2	1:E:307:LYS:HB3	1.96	0.41
1:F:20:ASP:N	1:F:20:ASP:OD1	2.54	0.41
1:A:45:LEU:HD13	1:A:142:PRO:HG3	2.02	0.41
1:A:445:ARG:H	1:F:393:ASN:ND2	2.12	0.41
1:D:45:LEU:HD13	1:D:142:PRO:HG3	2.02	0.41
1:E:20:ASP:OD1	1:E:20:ASP:N	2.54	0.41
1:B:186:PRO:HA	1:B:191:TRP:CD2	2.55	0.40
1:C:186:PRO:HA	1:C:191:TRP:CD2	2.55	0.40
1:A:392:ARG:NH1	1:F:442:PRO:O	2.54	0.40
1:F:307:LYS:HE2	1:F:307:LYS:HB3	1.96	0.40
1:A:424:MET:HE2	1:A:424:MET:HB2	1.93	0.40
1:E:109:LYS:HA	1:E:110:PRO:HD3	1.96	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	512/514 (100%)	490 (96%)	19 (4%)	3 (1%)	25	31
1	B	512/514 (100%)	490 (96%)	19 (4%)	3 (1%)	25	31
1	C	512/514 (100%)	490 (96%)	19 (4%)	3 (1%)	25	31
1	D	512/514 (100%)	490 (96%)	19 (4%)	3 (1%)	25	31
1	E	512/514 (100%)	490 (96%)	19 (4%)	3 (1%)	25	31
1	F	512/514 (100%)	490 (96%)	19 (4%)	3 (1%)	25	31
All	All	3072/3084 (100%)	2940 (96%)	114 (4%)	18 (1%)	29	31

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	287	ASP
1	B	287	ASP
1	C	287	ASP
1	D	287	ASP
1	E	287	ASP
1	F	287	ASP
1	A	295	HIS
1	B	295	HIS
1	C	295	HIS
1	D	295	HIS
1	E	295	HIS
1	F	295	HIS
1	A	296	PRO
1	B	296	PRO
1	C	296	PRO
1	D	296	PRO
1	E	296	PRO

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Mol	Chain	Res	Type
1	F	296	PRO

### 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	432/432 (100%)	421 (98%)	11 (2%)	47	65
1	B	432/432 (100%)	421 (98%)	11 (2%)	47	65
1	C	432/432 (100%)	421 (98%)	11 (2%)	47	65
1	D	432/432 (100%)	421 (98%)	11 (2%)	47	65
1	E	432/432 (100%)	421 (98%)	11 (2%)	47	65
1	F	432/432 (100%)	421 (98%)	11 (2%)	47	65
All	All	2592/2592 (100%)	2526 (98%)	66 (2%)	50	65

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91	GLU
1	A	131	VAL
1	A	215	SER
1	A	347	SER
1	A	371	THR
1	A	441	LEU
1	A	448	THR
1	A	454	ARG
1	A	459	ASP
1	A	465	SER
1	A	495	ASP
1	B	91	GLU
1	B	131	VAL
1	B	215	SER
1	B	347	SER
1	B	371	THR
1	B	441	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	448	THR
1	B	454	ARG
1	B	459	ASP
1	B	465	SER
1	B	495	ASP
1	C	91	GLU
1	C	131	VAL
1	C	215	SER
1	C	347	SER
1	C	371	THR
1	C	441	LEU
1	C	448	THR
1	C	454	ARG
1	C	459	ASP
1	C	465	SER
1	C	495	ASP
1	D	91	GLU
1	D	131	VAL
1	D	215	SER
1	D	347	SER
1	D	371	THR
1	D	441	LEU
1	D	448	THR
1	D	454	ARG
1	D	459	ASP
1	D	465	SER
1	D	495	ASP
1	E	91	GLU
1	E	131	VAL
1	E	215	SER
1	E	347	SER
1	E	371	THR
1	E	441	LEU
1	E	448	THR
1	E	454	ARG
1	E	459	ASP
1	E	465	SER
1	E	495	ASP
1	F	91	GLU
1	F	131	VAL
1	F	215	SER
1	F	347	SER

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Mol	Chain	Res	Type
1	F	371	THR
1	F	441	LEU
1	F	448	THR
1	F	454	ARG
1	F	459	ASP
1	F	465	SER
1	F	495	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	393	ASN
1	A	461	GLN
1	B	393	ASN
1	B	461	GLN
1	C	393	ASN
1	C	461	GLN
1	D	393	ASN
1	D	461	GLN
1	E	393	ASN
1	E	461	GLN
1	F	393	ASN
1	F	461	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 24 are monoatomic - leaving 12 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
3	BYN	F	602	4,6	36,39,40	2.90	12 (33%)	50,62,64	2.33	16 (32%)
3	BYN	D	602	4,6	36,39,40	2.91	12 (33%)	50,62,64	2.34	15 (30%)
3	BYN	C	602	4,6	36,39,40	2.90	12 (33%)	50,62,64	2.33	15 (30%)
2	BYC	E	601	-	51,59,59	4.07	22 (43%)	64,87,87	1.85	13 (20%)
2	BYC	D	601	-	51,59,59	4.08	21 (41%)	64,87,87	1.86	13 (20%)
3	BYN	A	602	4,6	36,39,40	2.91	12 (33%)	50,62,64	2.33	15 (30%)
2	BYC	F	601	-	51,59,59	4.07	21 (41%)	64,87,87	1.86	13 (20%)
2	BYC	B	601	-	51,59,59	4.07	22 (43%)	64,87,87	1.85	13 (20%)
3	BYN	B	602	4,6	36,39,40	2.91	12 (33%)	50,62,64	2.33	16 (32%)
3	BYN	E	602	4,6	36,39,40	2.90	12 (33%)	50,62,64	2.33	15 (30%)
2	BYC	C	601	-	51,59,59	4.07	21 (41%)	64,87,87	1.85	13 (20%)
2	BYC	A	601	-	51,59,59	4.07	22 (43%)	64,87,87	1.86	13 (20%)

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	BYN	F	602	4,6	1/1/5/6	6/18/30/33	0/4/4/4
3	BYN	D	602	4,6	1/1/5/6	6/18/30/33	0/4/4/4
3	BYN	C	602	4,6	1/1/5/6	6/18/30/33	0/4/4/4
2	BYC	E	601	-	-	25/51/71/71	0/4/4/4
2	BYC	D	601	-	-	25/51/71/71	0/4/4/4
3	BYN	A	602	4,6	1/1/5/6	6/18/30/33	0/4/4/4
3	BYN	B	602	4,6	1/1/5/6	6/18/30/33	0/4/4/4
3	BYN	E	602	4,6	1/1/5/6	6/18/30/33	0/4/4/4
2	BYC	B	601	-	-	25/51/71/71	0/4/4/4
2	BYC	F	601	-	-	25/51/71/71	0/4/4/4
2	BYC	C	601	-	-	25/51/71/71	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BYC	A	601	-	-	25/51/71/71	0/4/4/4

All (201) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	601	BYC	O4D-C1D	15.88	1.63	1.41
2	A	601	BYC	O4D-C1D	15.85	1.63	1.41
2	D	601	BYC	O4D-C1D	15.85	1.63	1.41
2	B	601	BYC	O4D-C1D	15.82	1.63	1.41
2	E	601	BYC	O4D-C1D	15.81	1.63	1.41
2	C	601	BYC	O4D-C1D	15.80	1.63	1.41
2	D	601	BYC	C2D-C1D	-15.66	1.30	1.53
2	B	601	BYC	C2D-C1D	-15.64	1.30	1.53
2	C	601	BYC	C2D-C1D	-15.62	1.30	1.53
2	E	601	BYC	C2D-C1D	-15.59	1.30	1.53
2	A	601	BYC	C2D-C1D	-15.59	1.30	1.53
2	F	601	BYC	C2D-C1D	-15.58	1.30	1.53
3	B	602	BYN	C5-C6	8.96	1.52	1.40
3	A	602	BYN	C5-C6	8.95	1.52	1.40
3	D	602	BYN	C5-C6	8.94	1.52	1.40
3	E	602	BYN	C5-C6	8.93	1.52	1.40
3	C	602	BYN	C5-C6	8.91	1.52	1.40
3	F	602	BYN	C5-C6	8.88	1.52	1.40
3	D	602	BYN	O3-C2	8.44	1.39	1.23
3	B	602	BYN	O3-C2	8.43	1.39	1.23
3	A	602	BYN	O3-C2	8.42	1.39	1.23
3	E	602	BYN	O3-C2	8.42	1.39	1.23
3	F	602	BYN	O3-C2	8.42	1.39	1.23
3	C	602	BYN	O3-C2	8.41	1.39	1.23
2	D	601	BYC	C5P-N4P	7.34	1.50	1.33
2	C	601	BYC	C5P-N4P	7.34	1.50	1.33
2	E	601	BYC	C5P-N4P	7.32	1.50	1.33
2	F	601	BYC	C5P-N4P	7.31	1.50	1.33
2	B	601	BYC	C5P-N4P	7.31	1.50	1.33
2	A	601	BYC	C5P-N4P	7.30	1.50	1.33
2	C	601	BYC	O57-C1B	7.06	1.36	1.21
2	C	601	BYC	O4D-C4D	-7.05	1.29	1.45
2	D	601	BYC	O57-C1B	7.04	1.36	1.21
2	E	601	BYC	O57-C1B	7.04	1.36	1.21
2	F	601	BYC	O57-C1B	7.04	1.36	1.21
2	F	601	BYC	O4D-C4D	-7.04	1.29	1.45
2	B	601	BYC	O4D-C4D	-7.03	1.29	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	BYC	O4D-C4D	-7.03	1.29	1.45
2	E	601	BYC	O4D-C4D	-7.02	1.29	1.45
2	A	601	BYC	O4D-C4D	-7.02	1.29	1.45
2	B	601	BYC	O57-C1B	7.00	1.36	1.21
2	A	601	BYC	O57-C1B	6.99	1.36	1.21
2	A	601	BYC	C9P-N8P	5.83	1.46	1.33
2	D	601	BYC	C9P-N8P	5.83	1.46	1.33
2	C	601	BYC	C9P-N8P	5.81	1.46	1.33
2	E	601	BYC	C9P-N8P	5.81	1.46	1.33
2	B	601	BYC	C9P-N8P	5.80	1.46	1.33
2	F	601	BYC	C9P-N8P	5.79	1.46	1.33
3	B	602	BYN	C4-N4	5.70	1.49	1.37
3	A	602	BYN	C4-N4	5.69	1.49	1.37
3	D	602	BYN	C4-N4	5.69	1.49	1.37
3	C	602	BYN	C4-N4	5.66	1.49	1.37
3	F	602	BYN	C4-N4	5.66	1.49	1.37
3	E	602	BYN	C4-N4	5.65	1.49	1.37
3	D	602	BYN	C6-N4	5.32	1.50	1.41
3	A	602	BYN	C6-N4	5.31	1.50	1.41
3	E	602	BYN	C6-N4	5.30	1.50	1.41
3	F	602	BYN	C6-N4	5.30	1.50	1.41
3	C	602	BYN	C6-N4	5.28	1.50	1.41
3	B	602	BYN	C6-N4	5.24	1.50	1.41
2	F	601	BYC	O9P-C9P	-4.40	1.14	1.23
2	E	601	BYC	O9P-C9P	-4.39	1.14	1.23
2	C	601	BYC	O9P-C9P	-4.39	1.14	1.23
2	A	601	BYC	O9P-C9P	-4.38	1.14	1.23
2	D	601	BYC	O9P-C9P	-4.38	1.14	1.23
2	B	601	BYC	O9P-C9P	-4.37	1.14	1.23
3	B	602	BYN	C7-C8	4.30	1.56	1.40
3	C	602	BYN	C7-C8	4.30	1.55	1.40
3	E	602	BYN	C7-C8	4.29	1.55	1.40
3	A	602	BYN	C7-C8	4.29	1.55	1.40
3	D	602	BYN	C7-C8	4.29	1.55	1.40
3	F	602	BYN	C7-C8	4.27	1.55	1.40
2	E	601	BYC	C6A-N6A	3.89	1.48	1.34
2	F	601	BYC	C6A-N6A	3.89	1.48	1.34
2	B	601	BYC	C6A-N6A	3.88	1.48	1.34
2	A	601	BYC	C6A-N6A	3.88	1.48	1.34
2	D	601	BYC	C6A-N6A	3.88	1.48	1.34
2	C	601	BYC	C6A-N6A	3.87	1.48	1.34
2	E	601	BYC	P3D-O3D	3.81	1.66	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	601	BYC	P3D-O3D	3.79	1.66	1.59
2	D	601	BYC	P3D-O3D	3.78	1.66	1.59
2	A	601	BYC	P3D-O3D	3.77	1.66	1.59
2	C	601	BYC	P3D-O3D	3.77	1.66	1.59
2	B	601	BYC	C2B-C1B	3.76	1.56	1.49
2	A	601	BYC	C2B-C1B	3.75	1.56	1.49
2	B	601	BYC	P3D-O3D	3.74	1.66	1.59
2	E	601	BYC	C2B-C1B	3.74	1.56	1.49
2	C	601	BYC	C2B-C1B	3.72	1.56	1.49
2	D	601	BYC	C2B-C1B	3.71	1.56	1.49
2	F	601	BYC	C2B-C1B	3.70	1.56	1.49
2	E	601	BYC	CDP-CBP	3.39	1.61	1.53
2	B	601	BYC	CDP-CBP	3.38	1.61	1.53
2	D	601	BYC	CDP-CBP	3.37	1.61	1.53
2	C	601	BYC	CDP-CBP	3.36	1.61	1.53
2	A	601	BYC	CDP-CBP	3.35	1.61	1.53
2	F	601	BYC	CDP-CBP	3.35	1.61	1.53
3	E	602	BYN	C4-N2	3.06	1.41	1.34
3	C	602	BYN	C4-N2	3.05	1.41	1.34
3	B	602	BYN	C4-N2	3.05	1.41	1.34
3	D	602	BYN	C4-N2	3.04	1.41	1.34
3	F	602	BYN	C4-N2	3.04	1.41	1.34
3	A	602	BYN	C4-N2	3.02	1.41	1.34
3	B	602	BYN	P1-O10	-2.67	1.44	1.54
3	E	602	BYN	P1-O10	-2.67	1.44	1.54
3	D	602	BYN	P1-O10	-2.67	1.44	1.54
3	A	602	BYN	P1-O10	-2.65	1.44	1.54
3	F	602	BYN	P1-O10	-2.65	1.44	1.54
3	C	602	BYN	P1-O10	-2.65	1.44	1.54
2	D	601	BYC	O3D-C3D	-2.63	1.34	1.44
2	E	601	BYC	O3D-C3D	-2.62	1.34	1.44
2	A	601	BYC	O3D-C3D	-2.61	1.34	1.44
2	B	601	BYC	O3D-C3D	-2.61	1.34	1.44
2	F	601	BYC	O3D-C3D	-2.61	1.34	1.44
2	C	601	BYC	O3D-C3D	-2.61	1.34	1.44
3	F	602	BYN	P1-O9	-2.58	1.44	1.54
3	B	602	BYN	P1-O9	-2.57	1.44	1.54
3	A	602	BYN	P1-O9	-2.57	1.44	1.54
3	C	602	BYN	P1-O9	-2.56	1.45	1.54
3	D	602	BYN	P1-O9	-2.55	1.45	1.54
3	E	602	BYN	P1-O9	-2.55	1.45	1.54
2	E	601	BYC	P2A-O6A	2.44	1.69	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	BYC	P2A-O6A	2.43	1.69	1.59
2	A	601	BYC	P2A-O6A	2.43	1.69	1.59
2	B	601	BYC	P2A-O6A	2.42	1.69	1.59
3	C	602	BYN	C3-C2	2.42	1.49	1.43
2	A	601	BYC	P1A-O5D	2.42	1.69	1.59
3	D	602	BYN	C3-C2	2.42	1.49	1.43
2	E	601	BYC	C3P-N4P	2.41	1.51	1.46
2	F	601	BYC	C3P-N4P	2.41	1.51	1.46
2	B	601	BYC	C3P-N4P	2.41	1.51	1.46
2	C	601	BYC	P2A-O6A	2.41	1.69	1.59
2	F	601	BYC	P2A-O6A	2.41	1.69	1.59
3	E	602	BYN	C3-C2	2.40	1.49	1.43
3	F	602	BYN	C3-C2	2.40	1.49	1.43
2	A	601	BYC	O5P-C5P	-2.40	1.18	1.23
2	F	601	BYC	P1A-O5D	2.40	1.69	1.59
3	B	602	BYN	C3-C2	2.40	1.49	1.43
2	D	601	BYC	P1A-O5D	2.40	1.69	1.59
2	A	601	BYC	C3P-N4P	2.40	1.51	1.46
2	E	601	BYC	P1A-O5D	2.40	1.69	1.59
3	A	602	BYN	C3-C2	2.40	1.49	1.43
2	C	601	BYC	C3P-N4P	2.40	1.51	1.46
2	C	601	BYC	O5P-C5P	-2.39	1.18	1.23
2	B	601	BYC	P1A-O5D	2.39	1.69	1.59
2	C	601	BYC	P1A-O5D	2.39	1.69	1.59
2	B	601	BYC	O5P-C5P	-2.37	1.18	1.23
2	B	601	BYC	C5D-C4D	2.37	1.59	1.51
2	E	601	BYC	O5P-C5P	-2.37	1.18	1.23
2	F	601	BYC	O5P-C5P	-2.37	1.18	1.23
3	C	602	BYN	O4-C19	-2.37	1.38	1.43
2	D	601	BYC	O5P-C5P	-2.36	1.18	1.23
2	D	601	BYC	C3P-N4P	2.36	1.51	1.46
2	E	601	BYC	C5D-C4D	2.36	1.58	1.51
2	F	601	BYC	C5D-C4D	2.36	1.58	1.51
3	B	602	BYN	O4-C19	-2.35	1.38	1.43
3	E	602	BYN	O4-C19	-2.35	1.38	1.43
3	A	602	BYN	O4-C19	-2.35	1.38	1.43
2	A	601	BYC	C5D-C4D	2.34	1.58	1.51
2	D	601	BYC	C5D-C4D	2.34	1.58	1.51
2	C	601	BYC	C5D-C4D	2.34	1.58	1.51
3	F	602	BYN	O4-C19	-2.33	1.38	1.43
2	A	601	BYC	O2D-C2D	2.31	1.48	1.43
3	D	602	BYN	O4-C19	-2.31	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	601	BYC	O2D-C2D	2.30	1.48	1.43
2	B	601	BYC	C7B-C2B	-2.30	1.35	1.39
2	B	601	BYC	O2D-C2D	2.30	1.48	1.43
2	C	601	BYC	O2D-C2D	2.29	1.48	1.43
2	E	601	BYC	O2D-C2D	2.29	1.48	1.43
2	D	601	BYC	O2D-C2D	2.28	1.48	1.43
2	A	601	BYC	C7B-C2B	-2.27	1.35	1.39
2	C	601	BYC	C7B-C2B	-2.27	1.35	1.39
2	F	601	BYC	C7B-C2B	-2.25	1.35	1.39
2	D	601	BYC	C7B-C2B	-2.24	1.35	1.39
2	E	601	BYC	C7B-C2B	-2.23	1.35	1.39
2	A	601	BYC	P1A-O2A	-2.18	1.45	1.55
2	D	601	BYC	P1A-O2A	-2.18	1.45	1.55
3	D	602	BYN	C1-N1	2.17	1.41	1.36
3	E	602	BYN	C1-N1	2.17	1.41	1.36
2	F	601	BYC	P1A-O2A	-2.16	1.45	1.55
2	B	601	BYC	P1A-O2A	-2.16	1.45	1.55
2	E	601	BYC	P1A-O2A	-2.16	1.45	1.55
2	C	601	BYC	P1A-O2A	-2.16	1.45	1.55
3	C	602	BYN	C1-N1	2.16	1.41	1.36
3	A	602	BYN	C1-N1	2.14	1.41	1.36
3	B	602	BYN	C1-N1	2.12	1.41	1.36
3	F	602	BYN	C1-N1	2.12	1.41	1.36
3	F	602	BYN	O6-C21	-2.05	1.39	1.43
3	B	602	BYN	O6-C21	-2.04	1.39	1.43
2	F	601	BYC	P3D-O9A	-2.04	1.47	1.54
2	E	601	BYC	P3D-O9A	-2.03	1.47	1.54
3	A	602	BYN	O6-C21	-2.03	1.39	1.43
2	A	601	BYC	C1B-S1P	2.03	1.80	1.76
3	C	602	BYN	O6-C21	-2.03	1.39	1.43
2	A	601	BYC	P3D-O9A	-2.03	1.47	1.54
3	E	602	BYN	O6-C21	-2.02	1.39	1.43
2	C	601	BYC	P3D-O9A	-2.02	1.47	1.54
3	D	602	BYN	O6-C21	-2.02	1.39	1.43
2	B	601	BYC	C1B-S1P	2.02	1.80	1.76
2	B	601	BYC	P3D-O9A	-2.01	1.47	1.54
2	D	601	BYC	P3D-O9A	-2.01	1.47	1.54
2	E	601	BYC	C1B-S1P	2.01	1.80	1.76

All (170) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	601	BYC	O57-C1B-S1P	-6.56	107.63	122.58
2	D	601	BYC	O57-C1B-S1P	-6.55	107.65	122.58
2	B	601	BYC	O57-C1B-S1P	-6.55	107.67	122.58
2	E	601	BYC	O57-C1B-S1P	-6.55	107.67	122.58
2	C	601	BYC	O57-C1B-S1P	-6.55	107.67	122.58
2	A	601	BYC	O57-C1B-S1P	-6.54	107.69	122.58
3	D	602	BYN	C13-C7-C5	-6.13	114.78	121.48
3	F	602	BYN	C13-C7-C5	-6.12	114.80	121.48
3	B	602	BYN	C13-C7-C5	-6.10	114.82	121.48
3	A	602	BYN	C13-C7-C5	-6.09	114.82	121.48
3	E	602	BYN	C13-C7-C5	-6.09	114.83	121.48
3	C	602	BYN	C13-C7-C5	-6.08	114.84	121.48
3	D	602	BYN	C6-N4-C4	-6.01	111.40	120.77
3	A	602	BYN	C6-N4-C4	-5.98	111.45	120.77
3	B	602	BYN	C6-N4-C4	-5.98	111.45	120.77
3	E	602	BYN	C6-N4-C4	-5.98	111.46	120.77
3	F	602	BYN	C6-N4-C4	-5.97	111.47	120.77
3	C	602	BYN	C6-N4-C4	-5.97	111.47	120.77
3	D	602	BYN	C3-C2-N1	5.58	120.82	110.99
3	E	602	BYN	C3-C2-N1	5.57	120.81	110.99
3	F	602	BYN	C3-C2-N1	5.57	120.81	110.99
3	B	602	BYN	C3-C2-N1	5.57	120.80	110.99
3	A	602	BYN	C3-C2-N1	5.56	120.80	110.99
3	C	602	BYN	C3-C2-N1	5.56	120.79	110.99
2	C	601	BYC	O57-C1B-C2B	-5.30	109.00	122.13
2	E	601	BYC	O57-C1B-C2B	-5.30	109.00	122.13
2	B	601	BYC	O57-C1B-C2B	-5.29	109.01	122.13
2	D	601	BYC	O57-C1B-C2B	-5.29	109.02	122.13
2	F	601	BYC	O57-C1B-C2B	-5.29	109.03	122.13
2	A	601	BYC	O57-C1B-C2B	-5.28	109.04	122.13
2	A	601	BYC	N3A-C2A-N1A	-5.10	120.71	128.68
2	F	601	BYC	N3A-C2A-N1A	-5.09	120.73	128.68
2	E	601	BYC	N3A-C2A-N1A	-5.07	120.75	128.68
2	B	601	BYC	N3A-C2A-N1A	-5.07	120.75	128.68
2	D	601	BYC	N3A-C2A-N1A	-5.07	120.75	128.68
2	C	601	BYC	N3A-C2A-N1A	-5.05	120.79	128.68
3	E	602	BYN	C1-N2-C4	4.59	122.22	113.47
3	D	602	BYN	C1-N2-C4	4.58	122.20	113.47
3	C	602	BYN	C1-N2-C4	4.57	122.18	113.47
3	A	602	BYN	C1-N2-C4	4.57	122.17	113.47
3	F	602	BYN	C1-N2-C4	4.56	122.16	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	BYN	C1-N2-C4	4.56	122.16	113.47
2	C	601	BYC	C3P-N4P-C5P	-4.14	115.15	122.84
2	A	601	BYC	C3P-N4P-C5P	-4.14	115.15	122.84
2	E	601	BYC	C3P-N4P-C5P	-4.13	115.17	122.84
2	D	601	BYC	C3P-N4P-C5P	-4.12	115.19	122.84
2	B	601	BYC	C3P-N4P-C5P	-4.12	115.19	122.84
2	F	601	BYC	C3P-N4P-C5P	-4.11	115.20	122.84
3	E	602	BYN	C16-C13-C7	4.11	124.69	112.13
3	B	602	BYN	C16-C13-C7	4.10	124.68	112.13
3	C	602	BYN	C16-C13-C7	4.10	124.68	112.13
3	A	602	BYN	C16-C13-C7	4.10	124.66	112.13
3	F	602	BYN	C16-C13-C7	4.09	124.65	112.13
3	D	602	BYN	C16-C13-C7	4.09	124.64	112.13
2	E	601	BYC	C2P-S1P-C1B	4.00	104.83	99.80
2	D	601	BYC	C2P-S1P-C1B	4.00	104.82	99.80
2	F	601	BYC	C2P-S1P-C1B	4.00	104.82	99.80
3	F	602	BYN	C15-C8-C9	-4.00	112.36	119.71
3	A	602	BYN	C15-C8-C9	-4.00	112.36	119.71
3	D	602	BYN	C15-C8-C9	-4.00	112.36	119.71
2	C	601	BYC	C2P-S1P-C1B	3.99	104.81	99.80
3	C	602	BYN	C15-C8-C9	-3.99	112.37	119.71
3	E	602	BYN	C15-C8-C9	-3.98	112.38	119.71
3	B	602	BYN	C15-C8-C9	-3.98	112.39	119.71
2	A	601	BYC	C2P-S1P-C1B	3.97	104.78	99.80
2	B	601	BYC	C2P-S1P-C1B	3.96	104.77	99.80
2	D	601	BYC	C6P-C5P-N4P	3.84	122.89	116.42
2	F	601	BYC	C6P-C5P-N4P	3.84	122.88	116.42
2	B	601	BYC	C6P-C5P-N4P	3.83	122.87	116.42
2	E	601	BYC	C6P-C5P-N4P	3.83	122.87	116.42
2	C	601	BYC	C6P-C5P-N4P	3.83	122.87	116.42
2	A	601	BYC	C6P-C5P-N4P	3.82	122.86	116.42
3	B	602	BYN	O9-P1-O7	3.54	116.14	106.73
3	C	602	BYN	O9-P1-O7	3.53	116.12	106.73
3	A	602	BYN	O9-P1-O7	3.53	116.12	106.73
3	F	602	BYN	O9-P1-O7	3.52	116.09	106.73
3	E	602	BYN	O9-P1-O7	3.51	116.07	106.73
3	D	602	BYN	O9-P1-O7	3.51	116.07	106.73
3	E	602	BYN	O3-C2-N1	-3.23	113.92	120.12
3	F	602	BYN	O3-C2-N1	-3.23	113.92	120.12
3	A	602	BYN	O3-C2-N1	-3.23	113.93	120.12
3	B	602	BYN	O3-C2-N1	-3.21	113.96	120.12
3	D	602	BYN	O3-C2-N1	-3.21	113.97	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	602	BYN	O3-C2-N1	-3.21	113.97	120.12
3	F	602	BYN	C16-C13-C12	-3.13	96.65	109.20
3	D	602	BYN	C16-C13-C12	-3.13	96.66	109.20
3	A	602	BYN	C16-C13-C12	-3.12	96.67	109.20
3	C	602	BYN	C16-C13-C12	-3.12	96.67	109.20
3	E	602	BYN	C16-C13-C12	-3.12	96.68	109.20
3	B	602	BYN	C16-C13-C12	-3.12	96.69	109.20
3	D	602	BYN	C10-C6-N4	-3.10	117.65	121.84
3	F	602	BYN	C10-C6-N4	-3.09	117.66	121.84
3	A	602	BYN	C10-C6-N4	-3.08	117.67	121.84
3	C	602	BYN	C10-C6-N4	-3.07	117.69	121.84
3	E	602	BYN	C10-C6-N4	-3.07	117.69	121.84
2	D	601	BYC	C3D-C2D-C1D	3.07	106.68	99.89
3	B	602	BYN	C10-C6-N4	-3.06	117.69	121.84
2	F	601	BYC	C3D-C2D-C1D	3.05	106.66	99.89
2	B	601	BYC	C3D-C2D-C1D	3.05	106.65	99.89
2	E	601	BYC	C3D-C2D-C1D	3.05	106.65	99.89
2	A	601	BYC	C3D-C2D-C1D	3.05	106.65	99.89
2	C	601	BYC	C3D-C2D-C1D	3.05	106.65	99.89
3	A	602	BYN	C5-C6-N4	2.89	122.60	118.92
3	F	602	BYN	C5-C6-N4	2.89	122.60	118.92
3	D	602	BYN	C5-C6-N4	2.89	122.59	118.92
3	C	602	BYN	C5-C6-N4	2.88	122.59	118.92
3	B	602	BYN	C5-C6-N4	2.88	122.58	118.92
3	E	602	BYN	C5-C6-N4	2.85	122.55	118.92
2	F	601	BYC	O5P-C5P-N4P	-2.78	117.76	123.01
2	B	601	BYC	O5P-C5P-N4P	-2.77	117.78	123.01
2	D	601	BYC	O5P-C5P-N4P	-2.77	117.78	123.01
2	E	601	BYC	O5P-C5P-N4P	-2.76	117.80	123.01
2	C	601	BYC	O5P-C5P-N4P	-2.76	117.81	123.01
2	A	601	BYC	O5P-C5P-N4P	-2.72	117.88	123.01
3	B	602	BYN	C21-C20-C19	-2.63	107.89	113.36
3	F	602	BYN	C21-C20-C19	-2.62	107.91	113.36
3	E	602	BYN	C21-C20-C19	-2.62	107.91	113.36
3	C	602	BYN	C21-C20-C19	-2.61	107.93	113.36
3	D	602	BYN	C21-C20-C19	-2.61	107.93	113.36
3	A	602	BYN	C21-C20-C19	-2.60	107.95	113.36
2	B	601	BYC	C7P-C6P-C5P	2.54	116.58	112.36
2	C	601	BYC	P2A-O3A-P1A	-2.53	124.13	132.83
2	A	601	BYC	C7P-C6P-C5P	2.53	116.57	112.36
2	F	601	BYC	C7P-C6P-C5P	2.53	116.57	112.36
2	B	601	BYC	P2A-O3A-P1A	-2.53	124.16	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	BYC	P2A-O3A-P1A	-2.52	124.16	132.83
2	C	601	BYC	C7P-C6P-C5P	2.52	116.56	112.36
2	A	601	BYC	P2A-O3A-P1A	-2.51	124.20	132.83
2	D	601	BYC	C7P-C6P-C5P	2.51	116.54	112.36
2	E	601	BYC	C7P-C6P-C5P	2.51	116.54	112.36
2	F	601	BYC	P2A-O3A-P1A	-2.51	124.22	132.83
3	D	602	BYN	O10-P1-O7	2.51	113.40	106.73
2	E	601	BYC	P2A-O3A-P1A	-2.50	124.24	132.83
3	E	602	BYN	O10-P1-O7	2.49	113.36	106.73
3	B	602	BYN	O10-P1-O7	2.49	113.35	106.73
3	A	602	BYN	O10-P1-O7	2.49	113.35	106.73
3	C	602	BYN	O10-P1-O7	2.48	113.33	106.73
3	F	602	BYN	O10-P1-O7	2.47	113.31	106.73
2	E	601	BYC	C4A-C5M-N7A	-2.43	106.87	109.40
2	D	601	BYC	C4A-C5M-N7A	-2.41	106.89	109.40
2	A	601	BYC	C4A-C5M-N7A	-2.40	106.90	109.40
2	F	601	BYC	C4A-C5M-N7A	-2.40	106.90	109.40
2	C	601	BYC	C4A-C5M-N7A	-2.38	106.92	109.40
2	B	601	BYC	C4A-C5M-N7A	-2.38	106.92	109.40
3	B	602	BYN	C14-C9-C10	-2.36	115.13	119.49
3	A	602	BYN	C14-C9-C10	-2.35	115.15	119.49
3	E	602	BYN	C14-C9-C10	-2.34	115.16	119.49
3	C	602	BYN	C14-C9-C10	-2.33	115.18	119.49
3	D	602	BYN	C14-C9-C10	-2.33	115.19	119.49
3	F	602	BYN	C14-C9-C10	-2.31	115.22	119.49
3	A	602	BYN	C6-C5-N3	-2.26	115.97	118.92
3	D	602	BYN	C6-C5-N3	-2.26	115.98	118.92
3	C	602	BYN	C6-C5-N3	-2.26	115.98	118.92
3	F	602	BYN	C6-C5-N3	-2.26	115.98	118.92
3	E	602	BYN	C6-C5-N3	-2.25	115.99	118.92
3	B	602	BYN	C6-C5-N3	-2.24	116.00	118.92
2	D	601	BYC	CAP-C9P-N8P	2.20	120.97	116.58
2	F	601	BYC	CAP-C9P-N8P	2.20	120.96	116.58
2	C	601	BYC	CAP-C9P-N8P	2.20	120.96	116.58
2	A	601	BYC	CAP-C9P-N8P	2.19	120.94	116.58
2	B	601	BYC	CAP-C9P-N8P	2.19	120.93	116.58
2	E	601	BYC	CAP-C9P-N8P	2.18	120.91	116.58
2	A	601	BYC	C2A-N1A-C6A	2.07	122.29	118.75
2	E	601	BYC	C2A-N1A-C6A	2.06	122.28	118.75
2	D	601	BYC	C2A-N1A-C6A	2.05	122.26	118.75
2	F	601	BYC	C2A-N1A-C6A	2.05	122.26	118.75
2	B	601	BYC	C2A-N1A-C6A	2.05	122.25	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	602	BYN	C22-C21-C20	-2.03	108.29	112.20
2	C	601	BYC	C2A-N1A-C6A	2.01	122.19	118.75
3	B	602	BYN	C22-C21-C20	-2.00	108.34	112.20

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	602	BYN	C20
3	B	602	BYN	C20
3	C	602	BYN	C20
3	D	602	BYN	C20
3	E	602	BYN	C20
3	F	602	BYN	C20

All (186) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	BYC	O57-C1B-S1P-C2P
2	A	601	BYC	P1A-O3A-P2A-O6A
2	A	601	BYC	N8P-C9P-CAP-OAP
2	A	601	BYC	C9P-CAP-CBP-CCP
2	A	601	BYC	C9P-CAP-CBP-CDP
2	A	601	BYC	C9P-CAP-CBP-CEP
2	A	601	BYC	OAP-CAP-CBP-CCP
2	A	601	BYC	OAP-CAP-CBP-CDP
2	A	601	BYC	OAP-CAP-CBP-CEP
2	B	601	BYC	O57-C1B-S1P-C2P
2	B	601	BYC	P1A-O3A-P2A-O6A
2	B	601	BYC	N8P-C9P-CAP-OAP
2	B	601	BYC	C9P-CAP-CBP-CCP
2	B	601	BYC	C9P-CAP-CBP-CDP
2	B	601	BYC	C9P-CAP-CBP-CEP
2	B	601	BYC	OAP-CAP-CBP-CCP
2	B	601	BYC	OAP-CAP-CBP-CDP
2	B	601	BYC	OAP-CAP-CBP-CEP
2	C	601	BYC	O57-C1B-S1P-C2P
2	C	601	BYC	P1A-O3A-P2A-O6A
2	C	601	BYC	N8P-C9P-CAP-OAP
2	C	601	BYC	C9P-CAP-CBP-CCP
2	C	601	BYC	C9P-CAP-CBP-CDP
2	C	601	BYC	C9P-CAP-CBP-CEP
2	C	601	BYC	OAP-CAP-CBP-CCP

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Mol	Chain	Res	Type	Atoms
2	C	601	BYC	OAP-CAP-CBP-CDP
2	C	601	BYC	OAP-CAP-CBP-CEP
2	D	601	BYC	O57-C1B-S1P-C2P
2	D	601	BYC	P1A-O3A-P2A-O6A
2	D	601	BYC	N8P-C9P-CAP-OAP
2	D	601	BYC	C9P-CAP-CBP-CCP
2	D	601	BYC	C9P-CAP-CBP-CDP
2	D	601	BYC	C9P-CAP-CBP-CEP
2	D	601	BYC	OAP-CAP-CBP-CCP
2	D	601	BYC	OAP-CAP-CBP-CDP
2	D	601	BYC	OAP-CAP-CBP-CEP
2	E	601	BYC	O57-C1B-S1P-C2P
2	E	601	BYC	P1A-O3A-P2A-O6A
2	E	601	BYC	N8P-C9P-CAP-OAP
2	E	601	BYC	C9P-CAP-CBP-CCP
2	E	601	BYC	C9P-CAP-CBP-CDP
2	E	601	BYC	C9P-CAP-CBP-CEP
2	E	601	BYC	OAP-CAP-CBP-CCP
2	E	601	BYC	OAP-CAP-CBP-CDP
2	E	601	BYC	OAP-CAP-CBP-CEP
2	F	601	BYC	O57-C1B-S1P-C2P
2	F	601	BYC	P1A-O3A-P2A-O6A
2	F	601	BYC	N8P-C9P-CAP-OAP
2	F	601	BYC	C9P-CAP-CBP-CCP
2	F	601	BYC	C9P-CAP-CBP-CDP
2	F	601	BYC	C9P-CAP-CBP-CEP
2	F	601	BYC	OAP-CAP-CBP-CCP
2	F	601	BYC	OAP-CAP-CBP-CDP
2	F	601	BYC	OAP-CAP-CBP-CEP
3	A	602	BYN	C19-C18-N4-C4
3	A	602	BYN	N4-C18-C19-O4
3	A	602	BYN	C18-C19-C20-C21
3	A	602	BYN	C18-C19-C20-O5
3	B	602	BYN	C19-C18-N4-C4
3	B	602	BYN	N4-C18-C19-O4
3	B	602	BYN	C18-C19-C20-C21
3	B	602	BYN	C18-C19-C20-O5
3	C	602	BYN	C19-C18-N4-C4
3	C	602	BYN	N4-C18-C19-O4
3	C	602	BYN	C18-C19-C20-C21
3	C	602	BYN	C18-C19-C20-O5
3	D	602	BYN	C19-C18-N4-C4

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Mol	Chain	Res	Type	Atoms
3	D	602	BYN	N4-C18-C19-O4
3	D	602	BYN	C18-C19-C20-C21
3	D	602	BYN	C18-C19-C20-O5
3	E	602	BYN	C19-C18-N4-C4
3	E	602	BYN	N4-C18-C19-O4
3	E	602	BYN	C18-C19-C20-C21
3	E	602	BYN	C18-C19-C20-O5
3	F	602	BYN	C19-C18-N4-C4
3	F	602	BYN	N4-C18-C19-O4
3	F	602	BYN	C18-C19-C20-C21
3	F	602	BYN	C18-C19-C20-O5
2	A	601	BYC	C3D-C4D-C5D-O5D
2	B	601	BYC	C3D-C4D-C5D-O5D
2	C	601	BYC	C3D-C4D-C5D-O5D
2	D	601	BYC	C3D-C4D-C5D-O5D
2	E	601	BYC	C3D-C4D-C5D-O5D
2	F	601	BYC	C3D-C4D-C5D-O5D
3	A	602	BYN	O4-C19-C20-O5
3	B	602	BYN	O4-C19-C20-O5
3	C	602	BYN	O4-C19-C20-O5
3	D	602	BYN	O4-C19-C20-O5
3	E	602	BYN	O4-C19-C20-O5
3	F	602	BYN	O4-C19-C20-O5
2	A	601	BYC	O4D-C4D-C5D-O5D
2	B	601	BYC	O4D-C4D-C5D-O5D
2	C	601	BYC	O4D-C4D-C5D-O5D
2	D	601	BYC	O4D-C4D-C5D-O5D
2	E	601	BYC	O4D-C4D-C5D-O5D
2	F	601	BYC	O4D-C4D-C5D-O5D
3	F	602	BYN	O4-C19-C20-C21
3	A	602	BYN	O4-C19-C20-C21
3	B	602	BYN	O4-C19-C20-C21
3	C	602	BYN	O4-C19-C20-C21
3	D	602	BYN	O4-C19-C20-C21
3	E	602	BYN	O4-C19-C20-C21
2	A	601	BYC	O9P-C9P-CAP-OAP
2	B	601	BYC	O9P-C9P-CAP-OAP
2	C	601	BYC	O9P-C9P-CAP-OAP
2	D	601	BYC	O9P-C9P-CAP-OAP
2	E	601	BYC	O9P-C9P-CAP-OAP
2	F	601	BYC	O9P-C9P-CAP-OAP
2	A	601	BYC	O9P-C9P-CAP-CBP

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Mol	Chain	Res	Type	Atoms
2	B	601	BYC	O9P-C9P-CAP-CBP
2	C	601	BYC	O9P-C9P-CAP-CBP
2	D	601	BYC	O9P-C9P-CAP-CBP
2	E	601	BYC	O9P-C9P-CAP-CBP
2	F	601	BYC	O9P-C9P-CAP-CBP
2	A	601	BYC	CCP-O6A-P2A-O3A
2	B	601	BYC	CCP-O6A-P2A-O3A
2	C	601	BYC	CCP-O6A-P2A-O3A
2	D	601	BYC	CCP-O6A-P2A-O3A
2	E	601	BYC	CCP-O6A-P2A-O3A
2	F	601	BYC	CCP-O6A-P2A-O3A
2	A	601	BYC	CCP-O6A-P2A-O4A
2	B	601	BYC	CCP-O6A-P2A-O4A
2	C	601	BYC	CCP-O6A-P2A-O4A
2	D	601	BYC	CCP-O6A-P2A-O4A
2	E	601	BYC	CCP-O6A-P2A-O4A
2	F	601	BYC	CCP-O6A-P2A-O4A
2	A	601	BYC	O5P-C5P-C6P-C7P
2	B	601	BYC	O5P-C5P-C6P-C7P
2	C	601	BYC	O5P-C5P-C6P-C7P
2	D	601	BYC	O5P-C5P-C6P-C7P
2	E	601	BYC	O5P-C5P-C6P-C7P
2	F	601	BYC	O5P-C5P-C6P-C7P
2	A	601	BYC	C5P-C6P-C7P-N8P
2	B	601	BYC	C5P-C6P-C7P-N8P
2	C	601	BYC	C5P-C6P-C7P-N8P
2	D	601	BYC	C5P-C6P-C7P-N8P
2	E	601	BYC	C5P-C6P-C7P-N8P
2	F	601	BYC	C5P-C6P-C7P-N8P
2	A	601	BYC	N4P-C5P-C6P-C7P
2	B	601	BYC	N4P-C5P-C6P-C7P
2	C	601	BYC	N4P-C5P-C6P-C7P
2	D	601	BYC	N4P-C5P-C6P-C7P
2	E	601	BYC	N4P-C5P-C6P-C7P
2	F	601	BYC	N4P-C5P-C6P-C7P
2	A	601	BYC	N8P-C9P-CAP-CBP
2	B	601	BYC	N8P-C9P-CAP-CBP
2	C	601	BYC	N8P-C9P-CAP-CBP
2	D	601	BYC	N8P-C9P-CAP-CBP
2	E	601	BYC	N8P-C9P-CAP-CBP
2	F	601	BYC	N8P-C9P-CAP-CBP
2	A	601	BYC	P2A-O3A-P1A-O1A

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Mol	Chain	Res	Type	Atoms
2	B	601	BYC	P2A-O3A-P1A-O1A
2	C	601	BYC	P2A-O3A-P1A-O1A
2	D	601	BYC	P2A-O3A-P1A-O1A
2	E	601	BYC	P2A-O3A-P1A-O1A
2	F	601	BYC	P2A-O3A-P1A-O1A
2	A	601	BYC	C3D-O3D-P3D-O8A
2	B	601	BYC	C3D-O3D-P3D-O8A
2	C	601	BYC	C3D-O3D-P3D-O8A
2	D	601	BYC	C3D-O3D-P3D-O8A
2	E	601	BYC	C3D-O3D-P3D-O8A
2	F	601	BYC	C3D-O3D-P3D-O8A
2	A	601	BYC	C3D-O3D-P3D-O7A
2	A	601	BYC	C3D-O3D-P3D-O9A
2	B	601	BYC	C3D-O3D-P3D-O7A
2	B	601	BYC	C3D-O3D-P3D-O9A
2	C	601	BYC	C3D-O3D-P3D-O7A
2	C	601	BYC	C3D-O3D-P3D-O9A
2	D	601	BYC	C3D-O3D-P3D-O7A
2	D	601	BYC	C3D-O3D-P3D-O9A
2	E	601	BYC	C3D-O3D-P3D-O7A
2	E	601	BYC	C3D-O3D-P3D-O9A
2	F	601	BYC	C3D-O3D-P3D-O7A
2	F	601	BYC	C3D-O3D-P3D-O9A
2	A	601	BYC	P2A-O3A-P1A-O2A
2	B	601	BYC	P2A-O3A-P1A-O2A
2	C	601	BYC	P2A-O3A-P1A-O2A
2	D	601	BYC	P2A-O3A-P1A-O2A
2	E	601	BYC	P2A-O3A-P1A-O2A
2	F	601	BYC	P2A-O3A-P1A-O2A
2	A	601	BYC	S1P-C1B-C2B-C3B
2	B	601	BYC	S1P-C1B-C2B-C3B
2	C	601	BYC	S1P-C1B-C2B-C3B
2	D	601	BYC	S1P-C1B-C2B-C3B
2	E	601	BYC	S1P-C1B-C2B-C3B
2	F	601	BYC	S1P-C1B-C2B-C3B

There are no ring outliers.

12 monomers are involved in 18 short contacts:

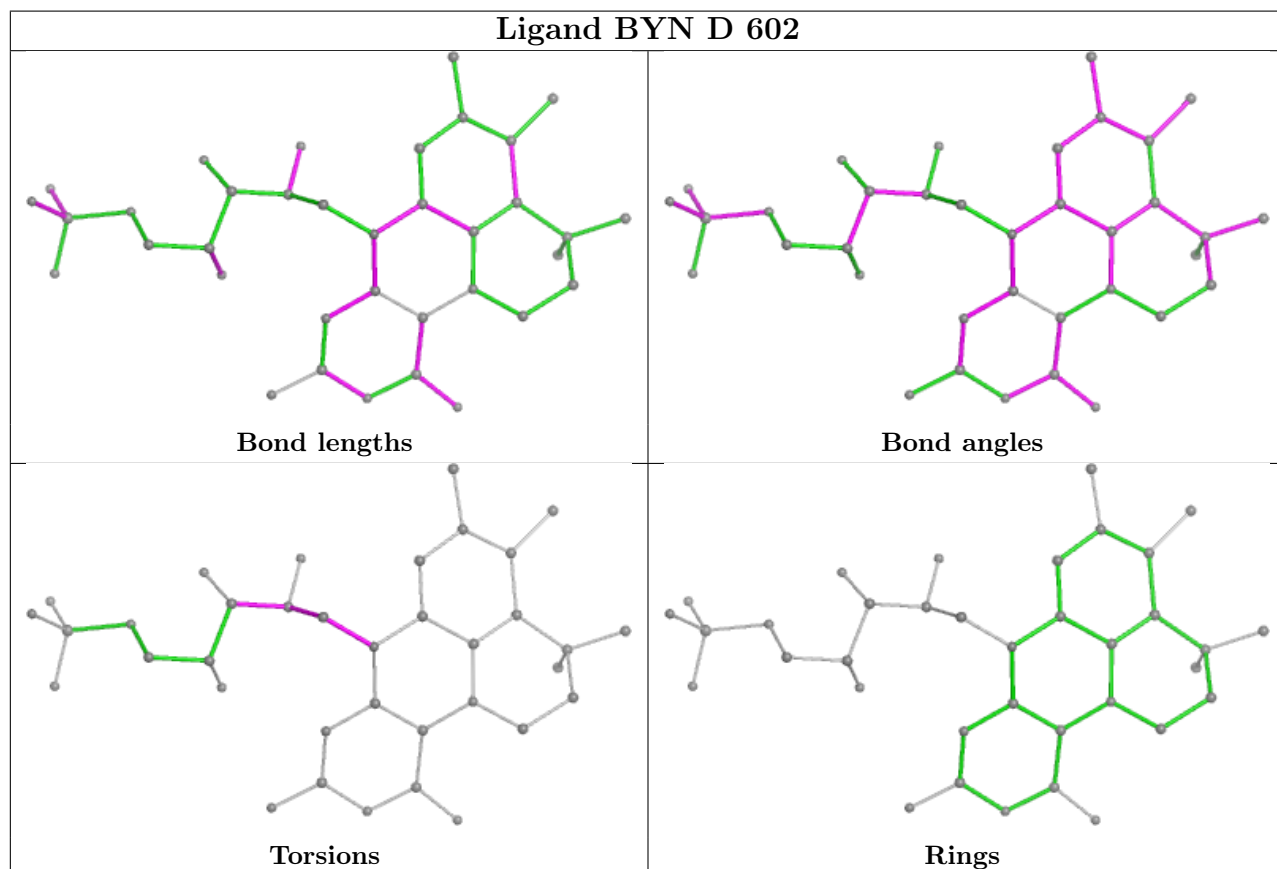
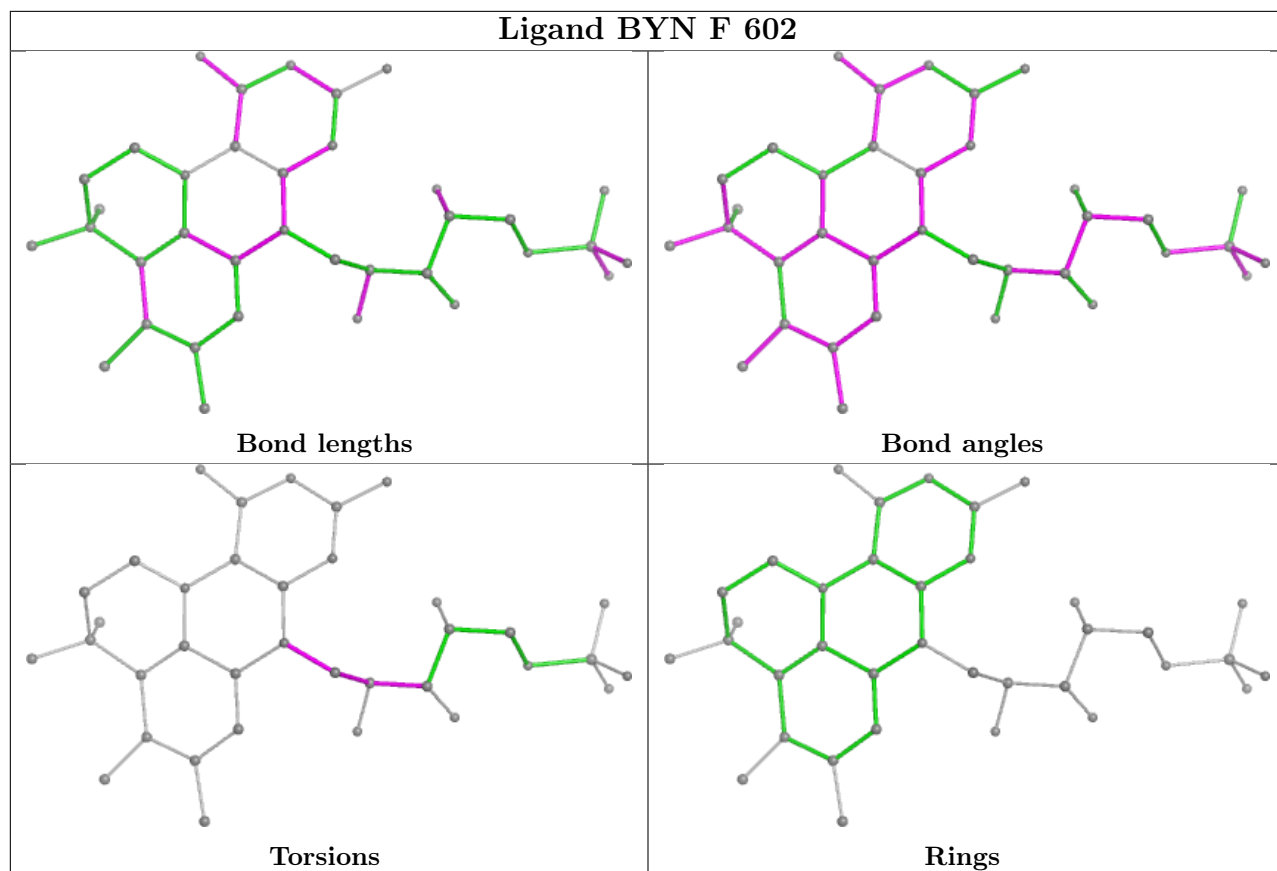
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	602	BYN	1	0
3	D	602	BYN	1	0

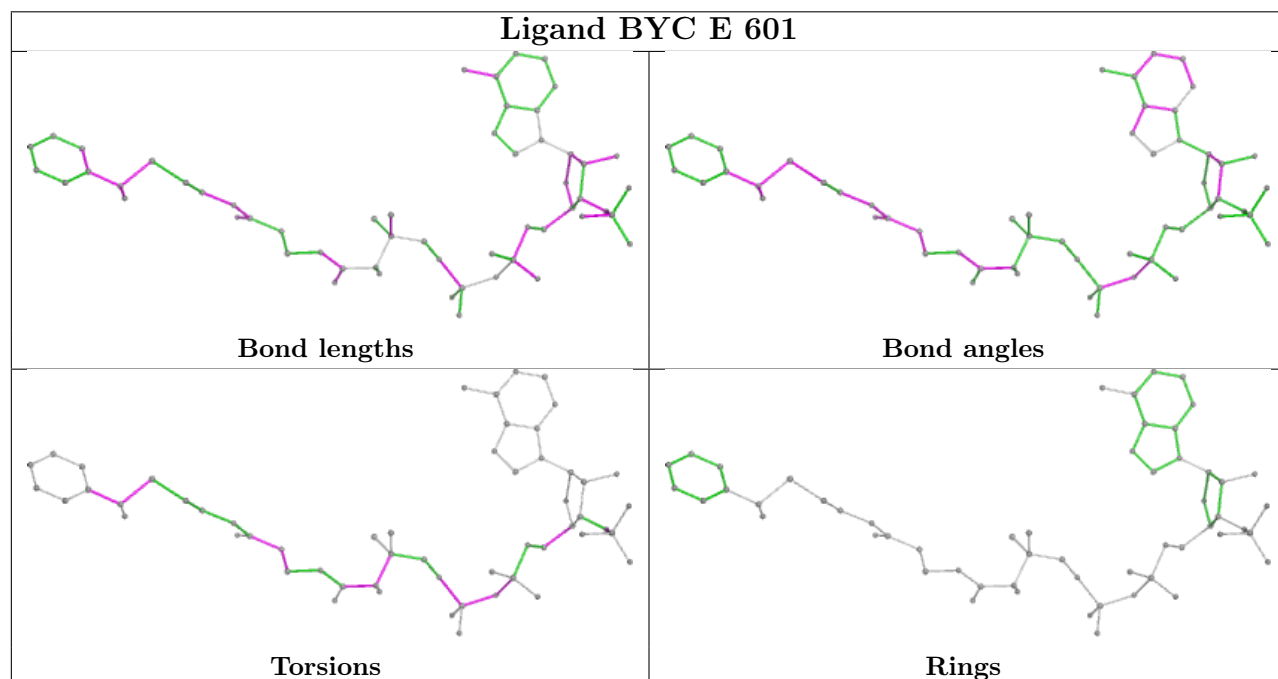
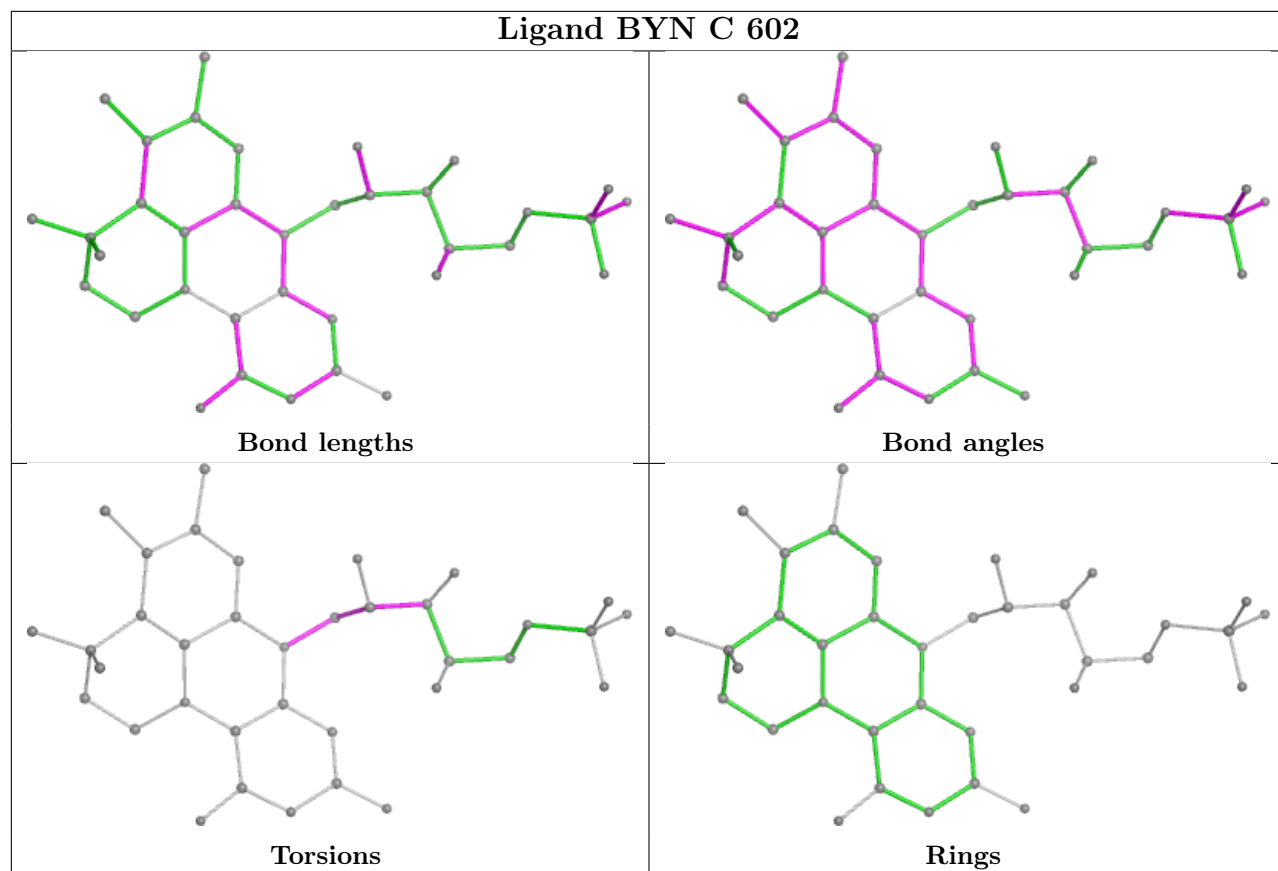
*Continued on next page...*

*Continued from previous page...*

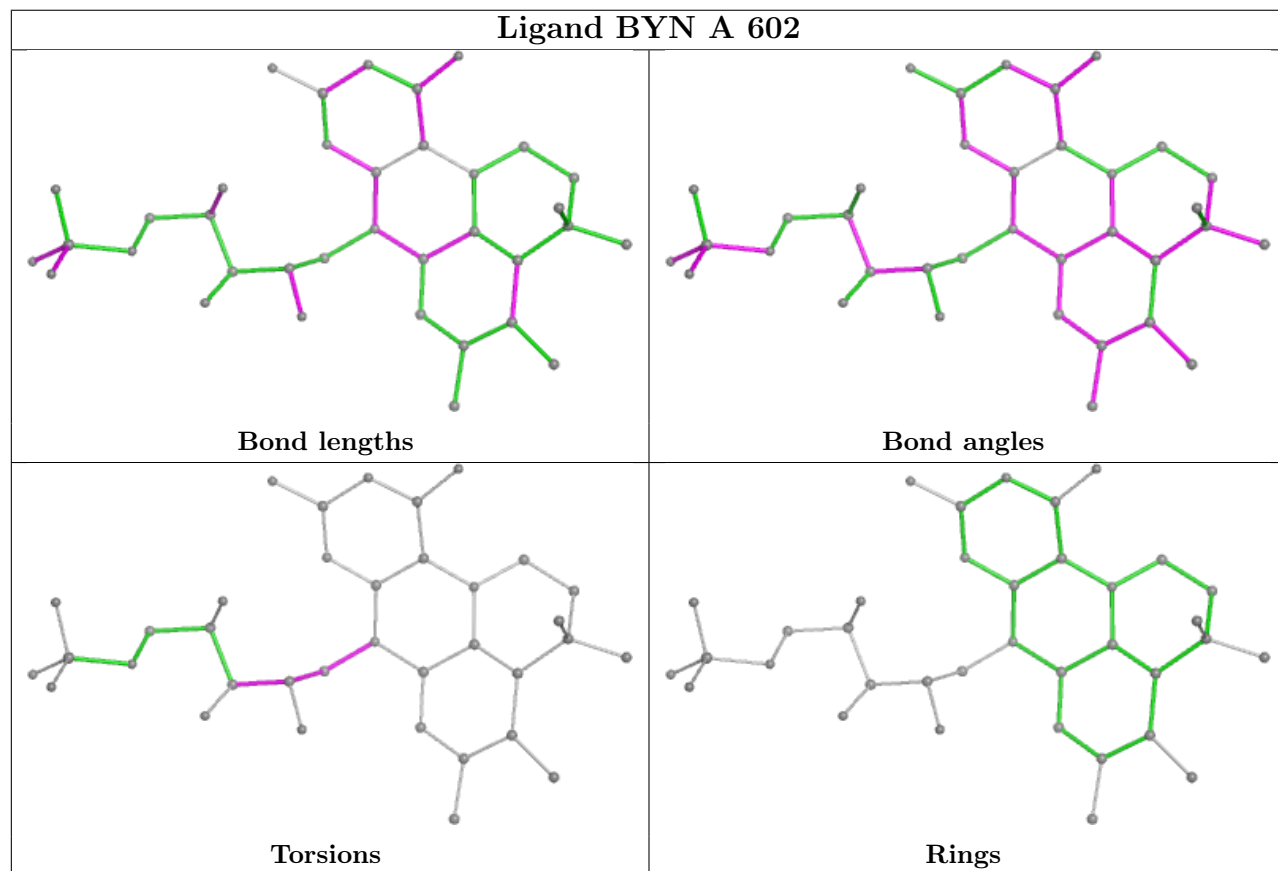
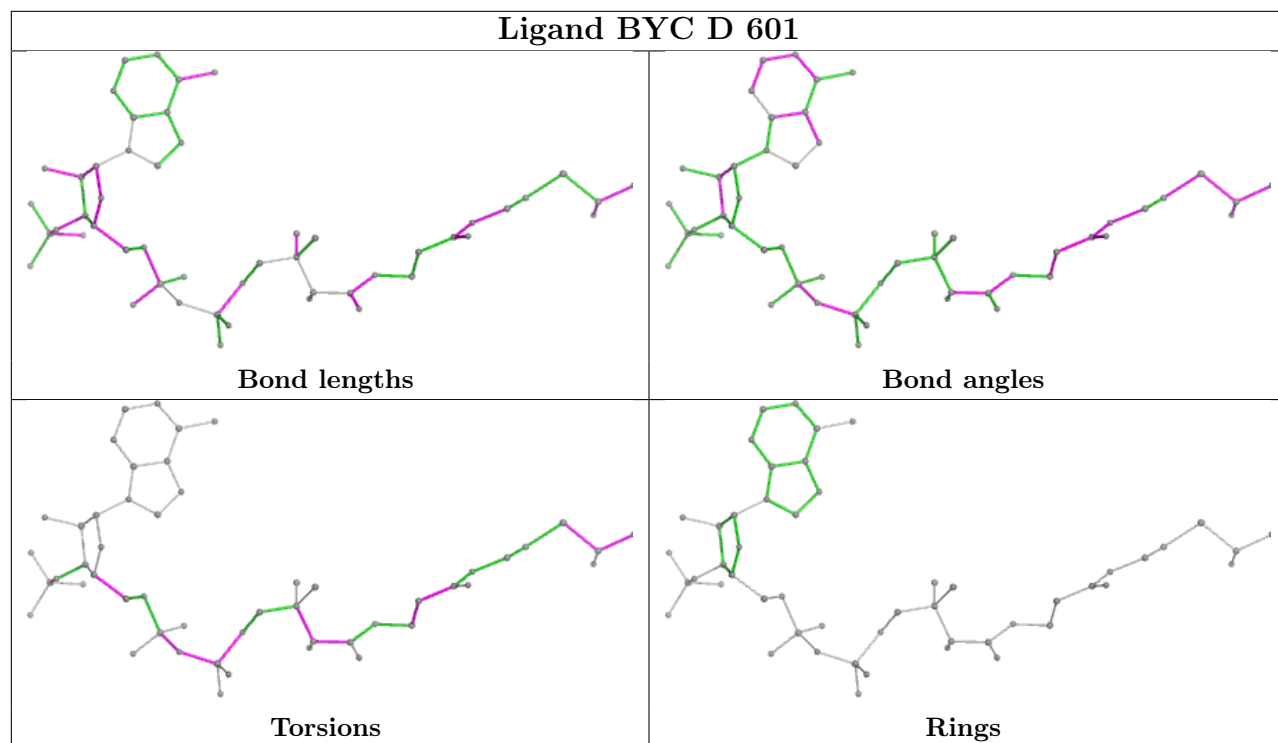
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	602	BYN	1	0
2	E	601	BYC	2	0
2	D	601	BYC	2	0
3	A	602	BYN	1	0
2	F	601	BYC	2	0
2	B	601	BYC	2	0
3	B	602	BYN	1	0
3	E	602	BYN	1	0
2	C	601	BYC	2	0
2	A	601	BYC	2	0

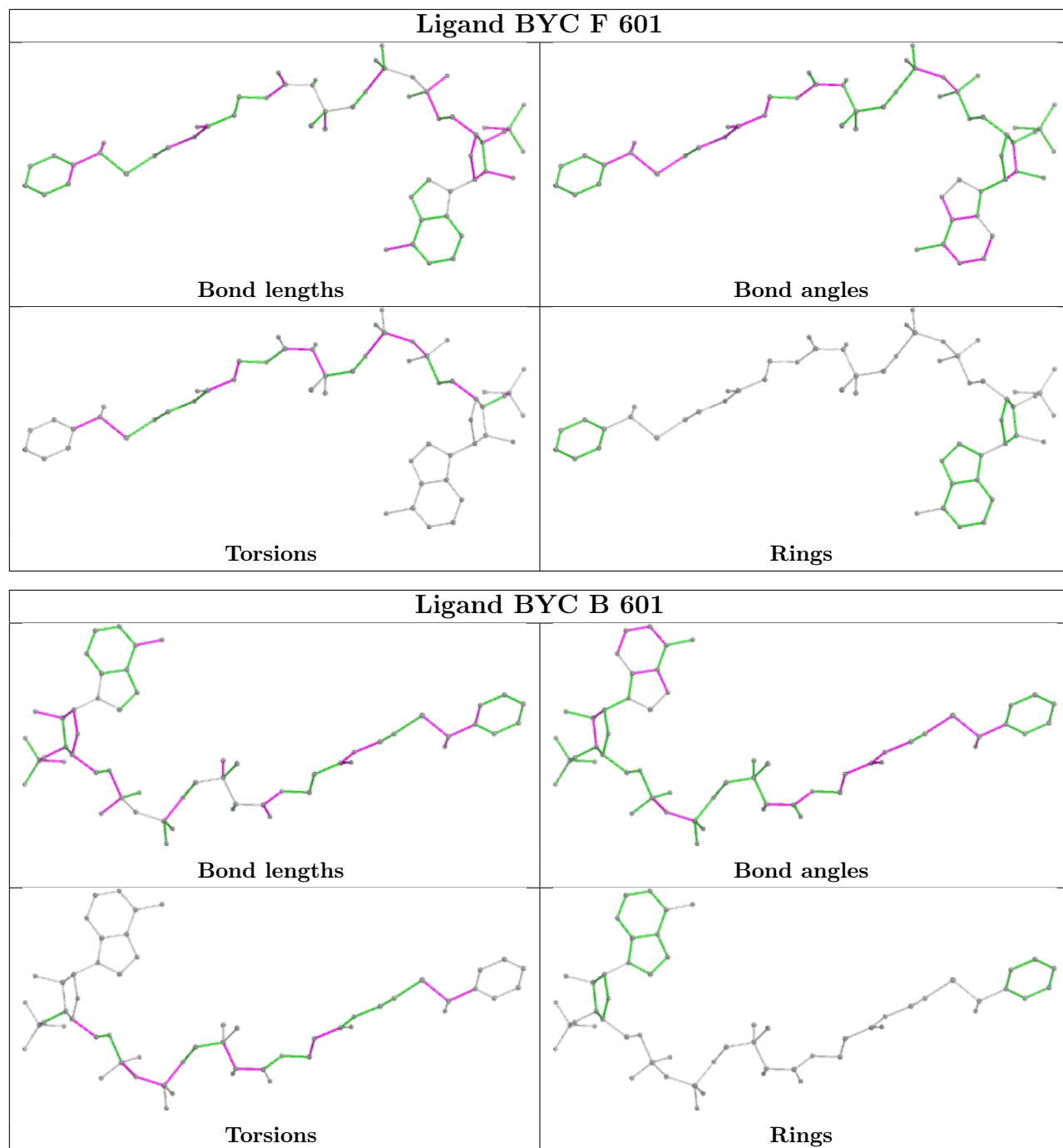
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

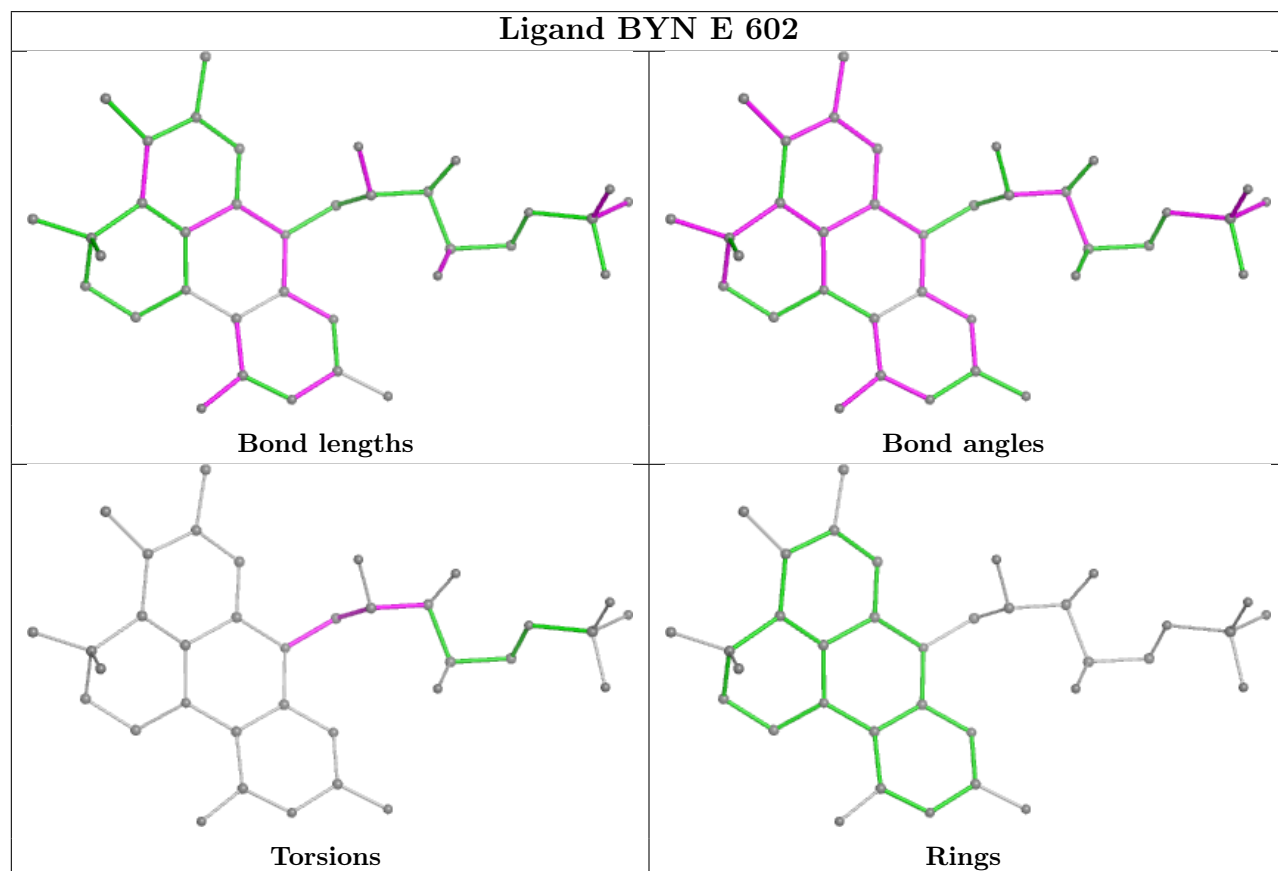
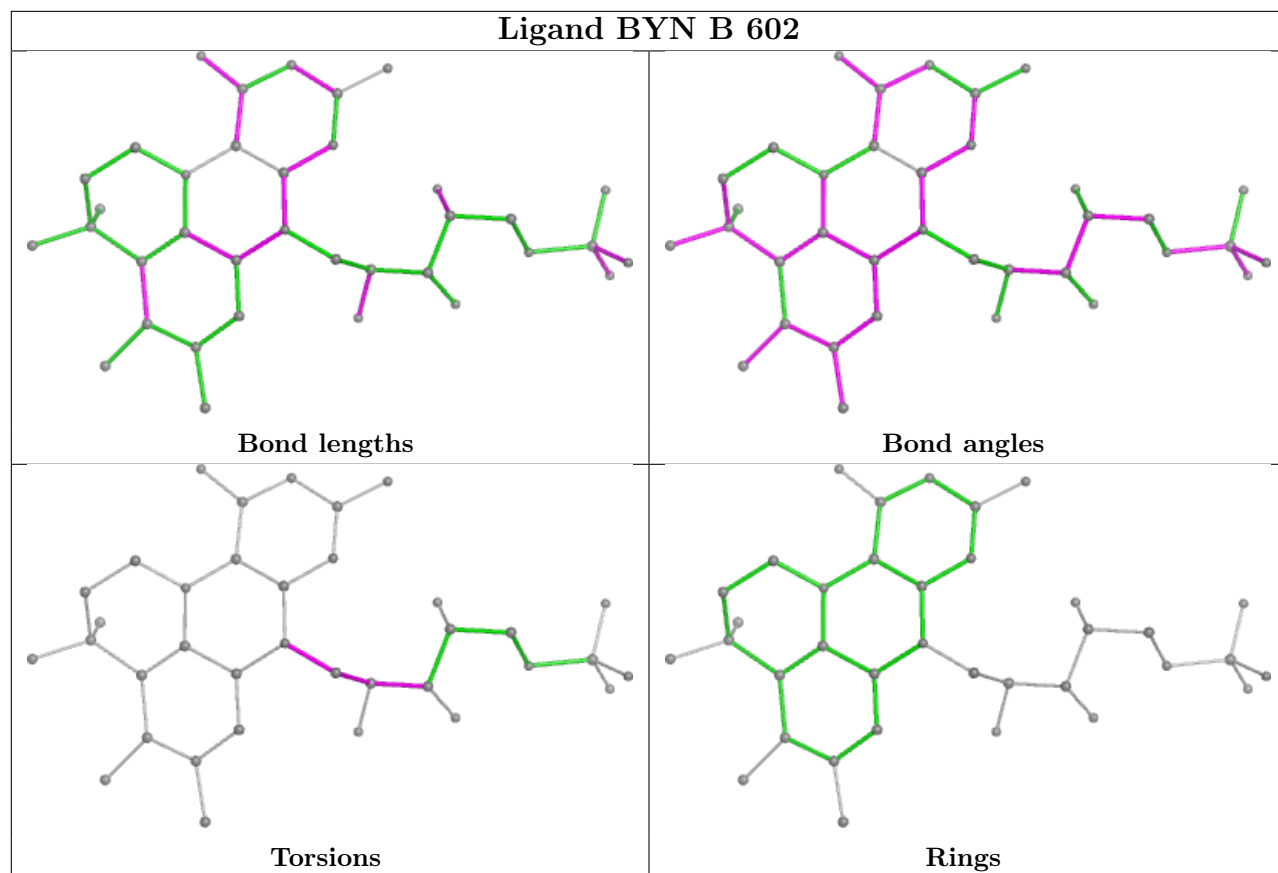


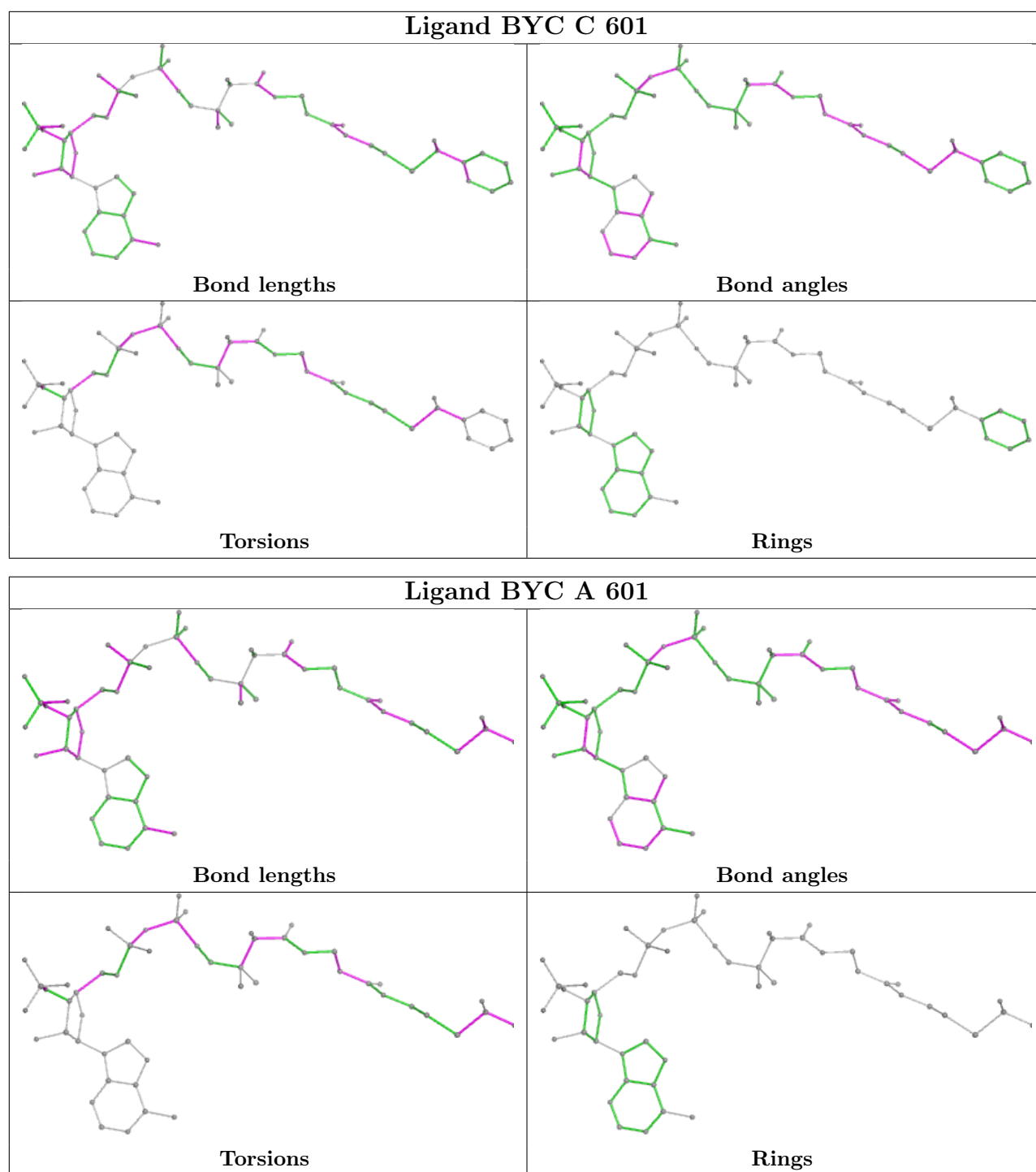












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	B	1
1	C	1
1	D	1
1	E	1
1	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	523:ALA	C	524:ARG	N	1.69
1	B	523:ALA	C	524:ARG	N	1.69
1	C	523:ALA	C	524:ARG	N	1.69
1	D	523:ALA	C	524:ARG	N	1.69
1	E	523:ALA	C	524:ARG	N	1.69
1	F	523:ALA	C	524:ARG	N	1.69

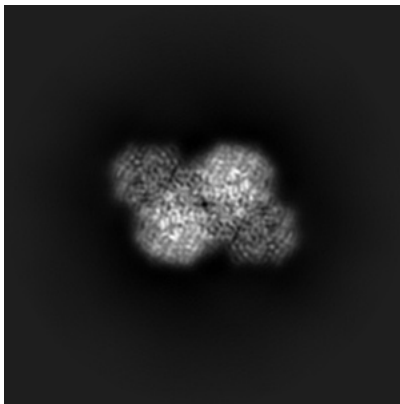
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17324. These allow visual inspection of the internal detail of the map and identification of artifacts.

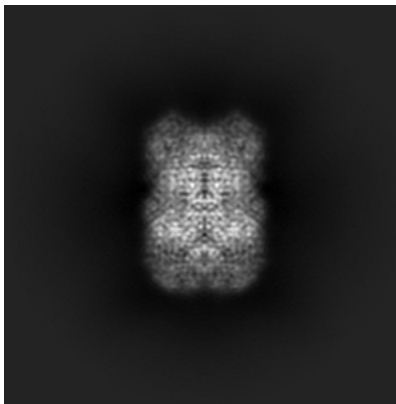
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

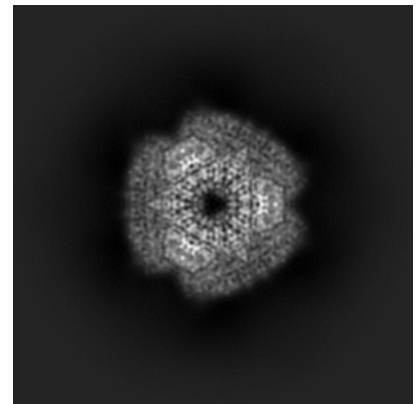
#### 6.1.1 Primary map



X

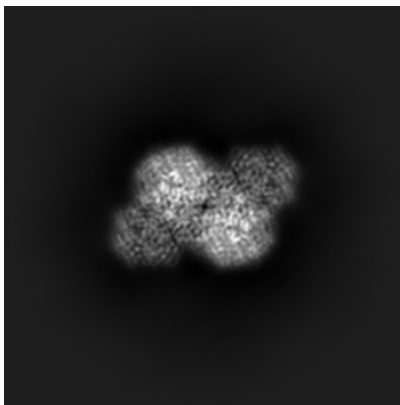


Y

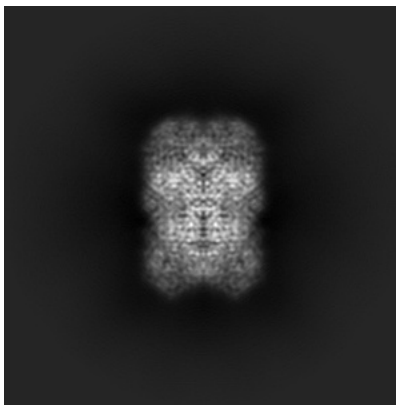


Z

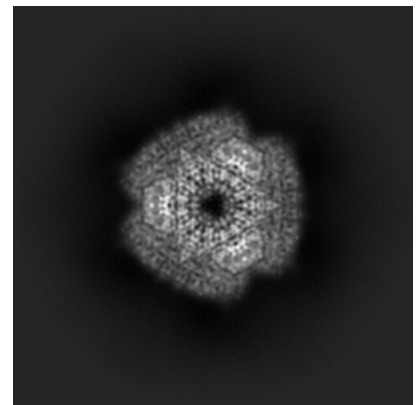
#### 6.1.2 Raw map



X



Y

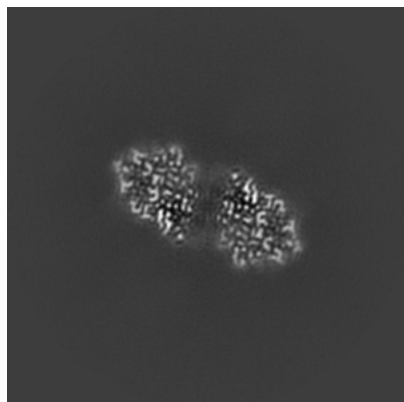


Z

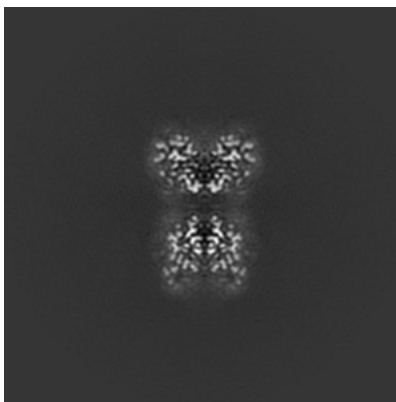
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

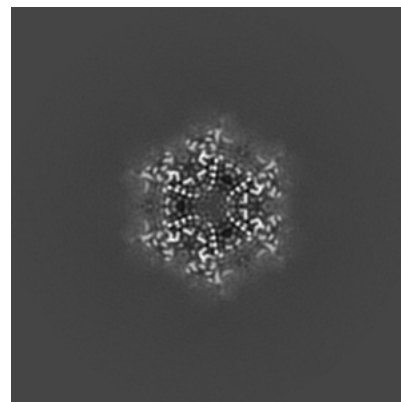
### 6.2.1 Primary map



X Index: 160

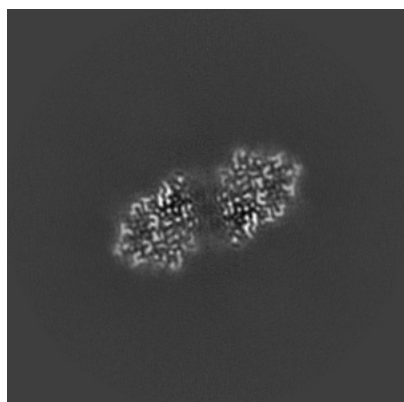


Y Index: 160

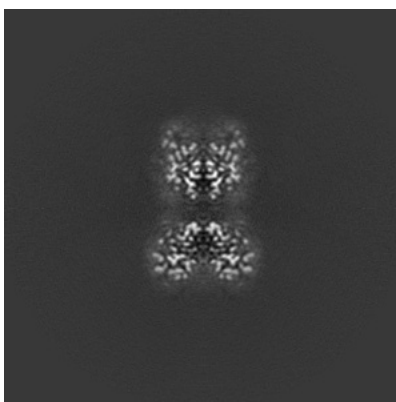


Z Index: 160

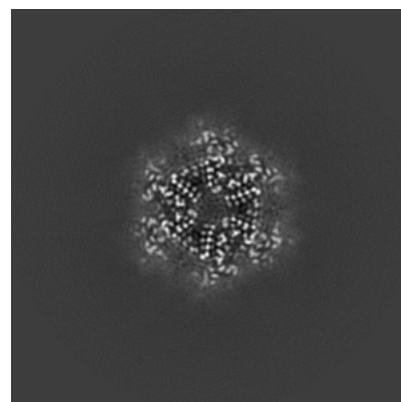
### 6.2.2 Raw map



X Index: 160



Y Index: 160

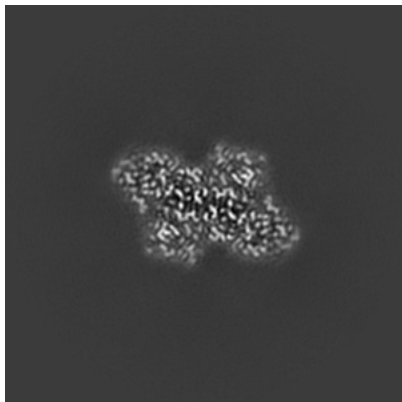


Z Index: 160

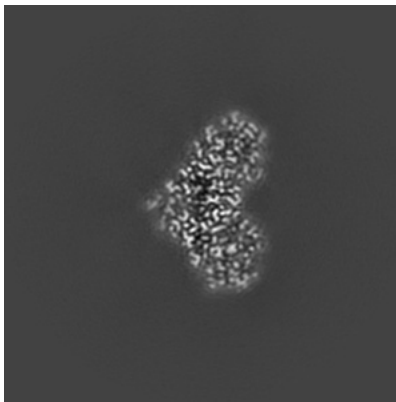
The images above show central slices of the map in three orthogonal directions.

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

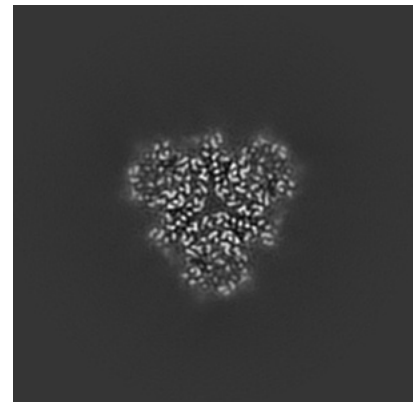
### 6.3.1 Primary map



X Index: 140

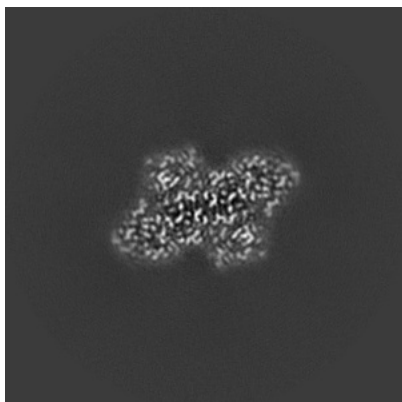


Y Index: 181

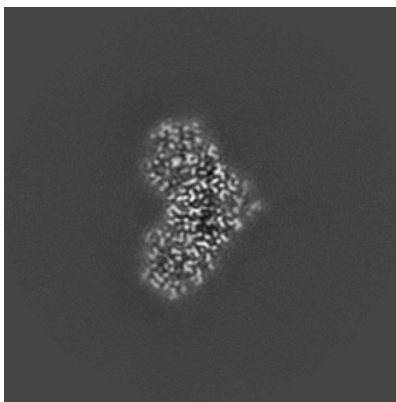


Z Index: 168

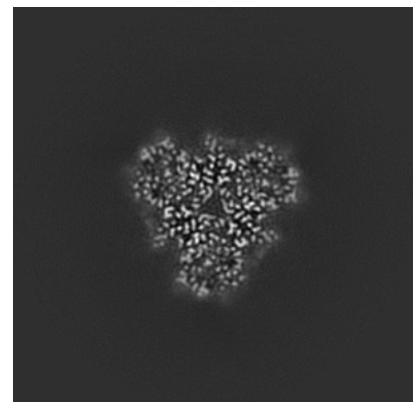
### 6.3.2 Raw map



X Index: 180



Y Index: 181



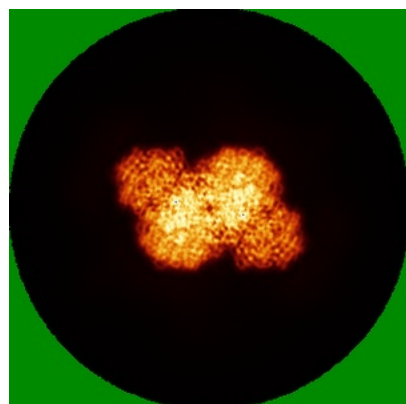
Z Index: 150

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

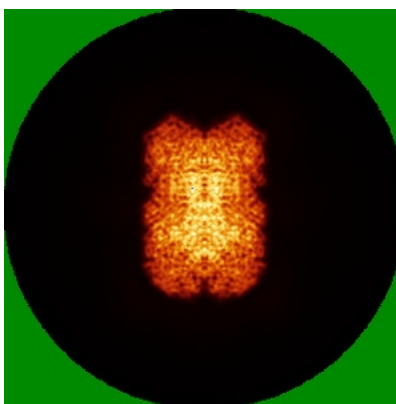


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

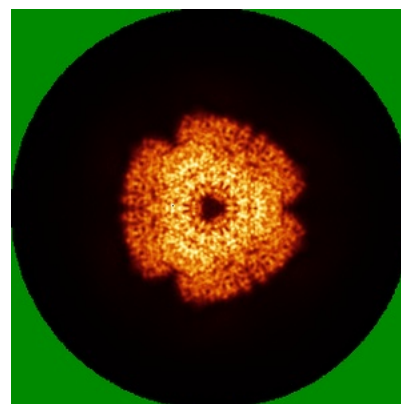
### 6.4.1 Primary map



X

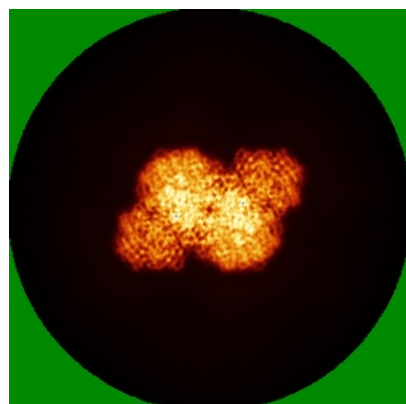


Y

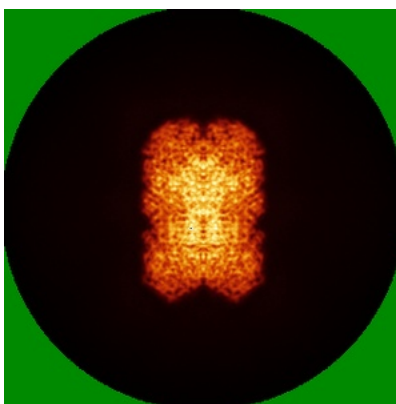


Z

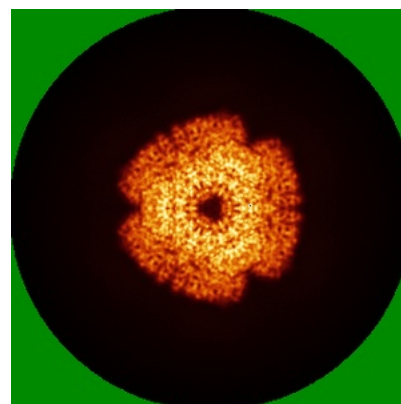
### 6.4.2 Raw map



X



Y

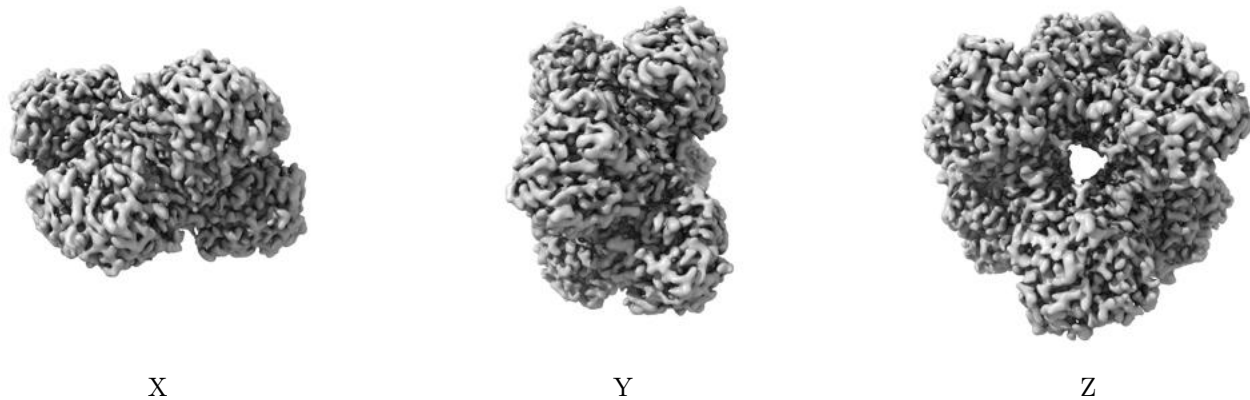


Z

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.

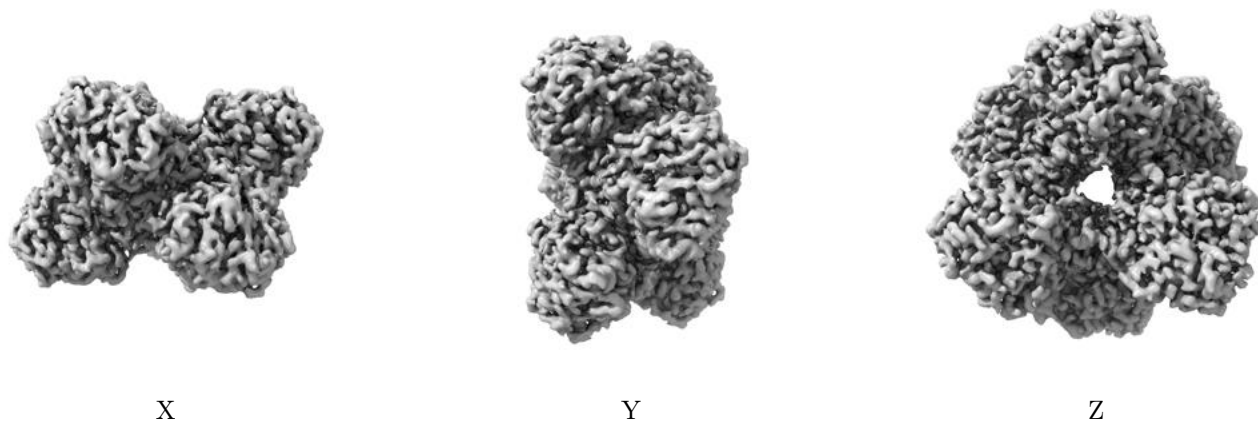
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00552. 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.

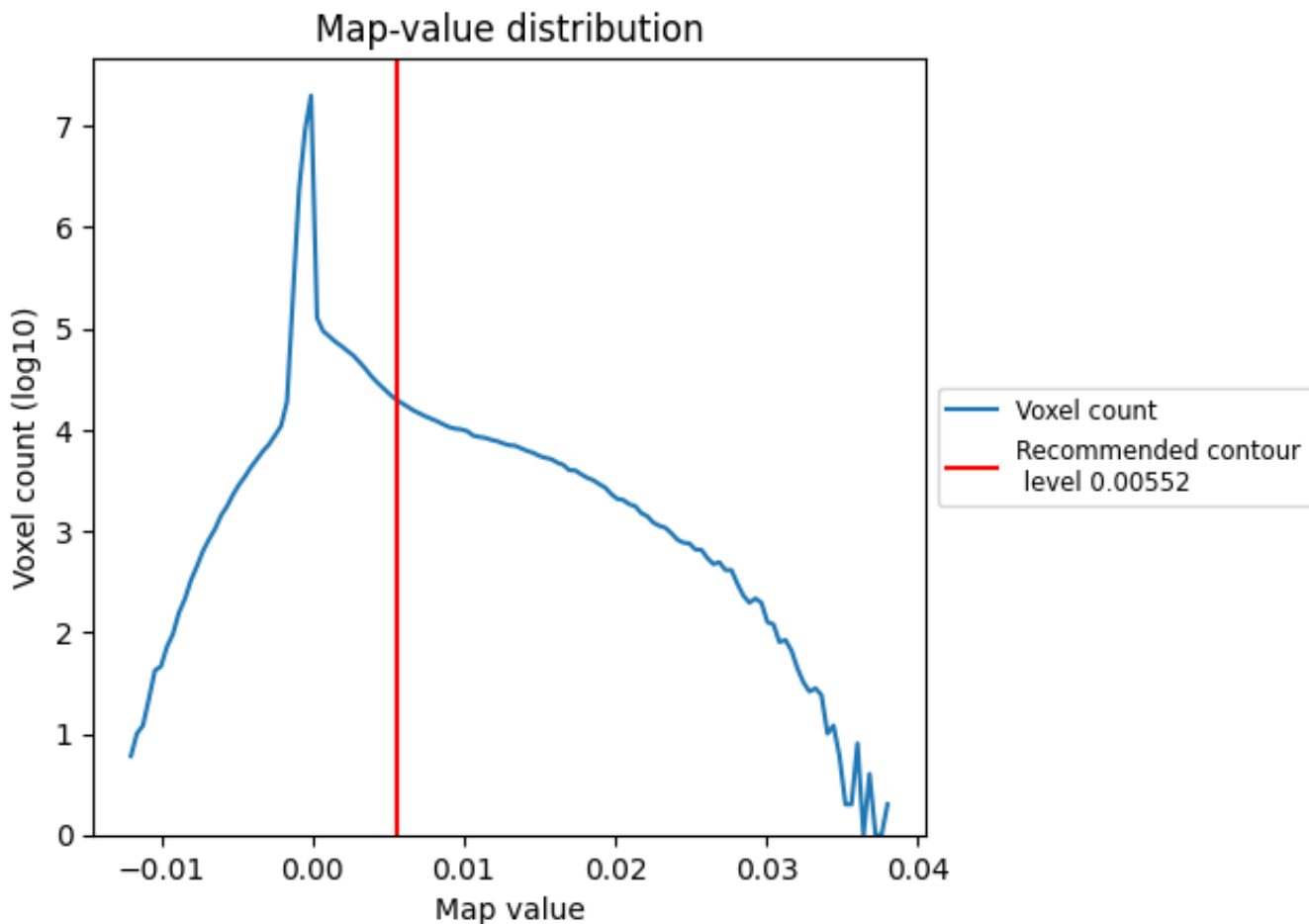
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

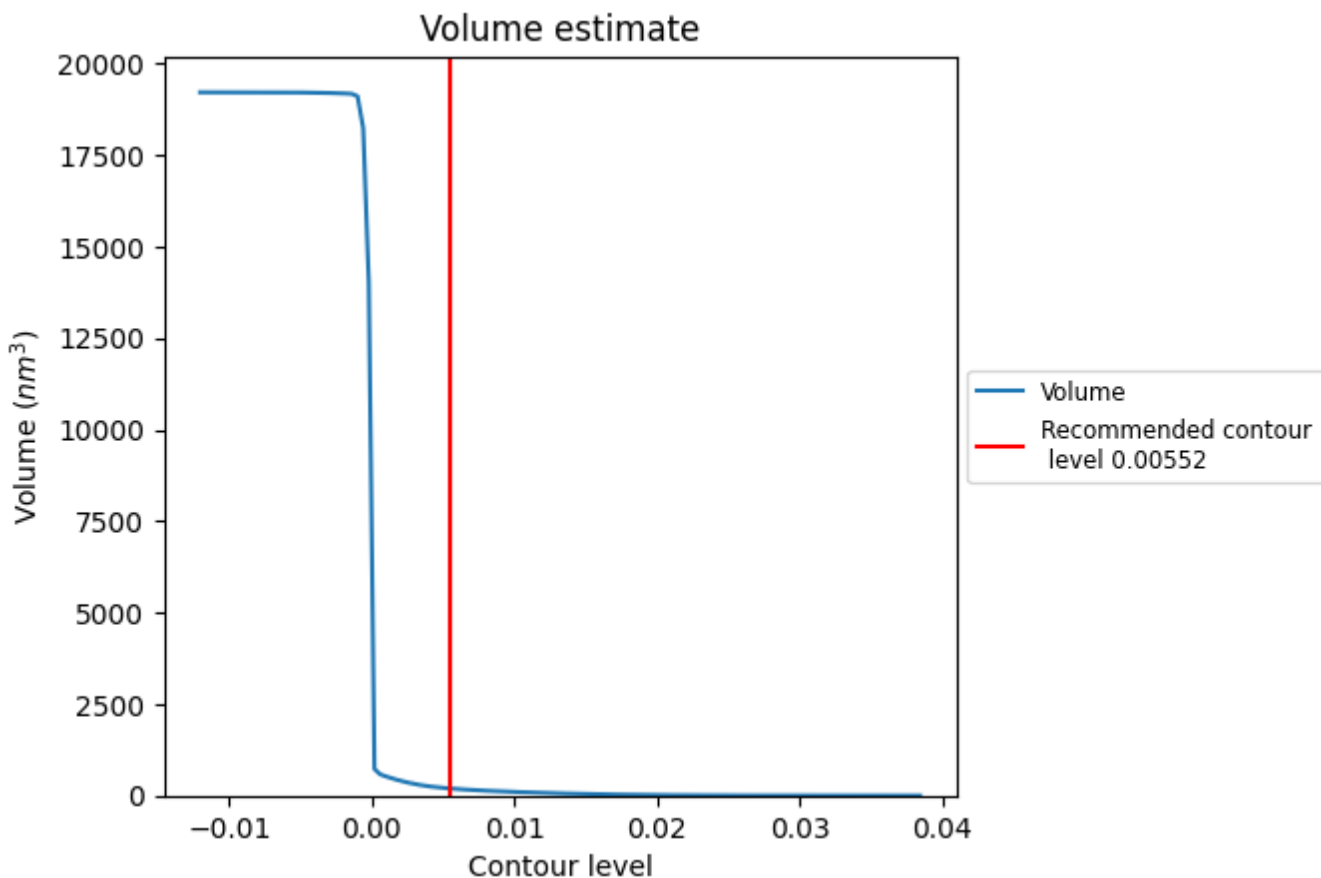
This section contains the results of statistical analysis of the map.

### 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.

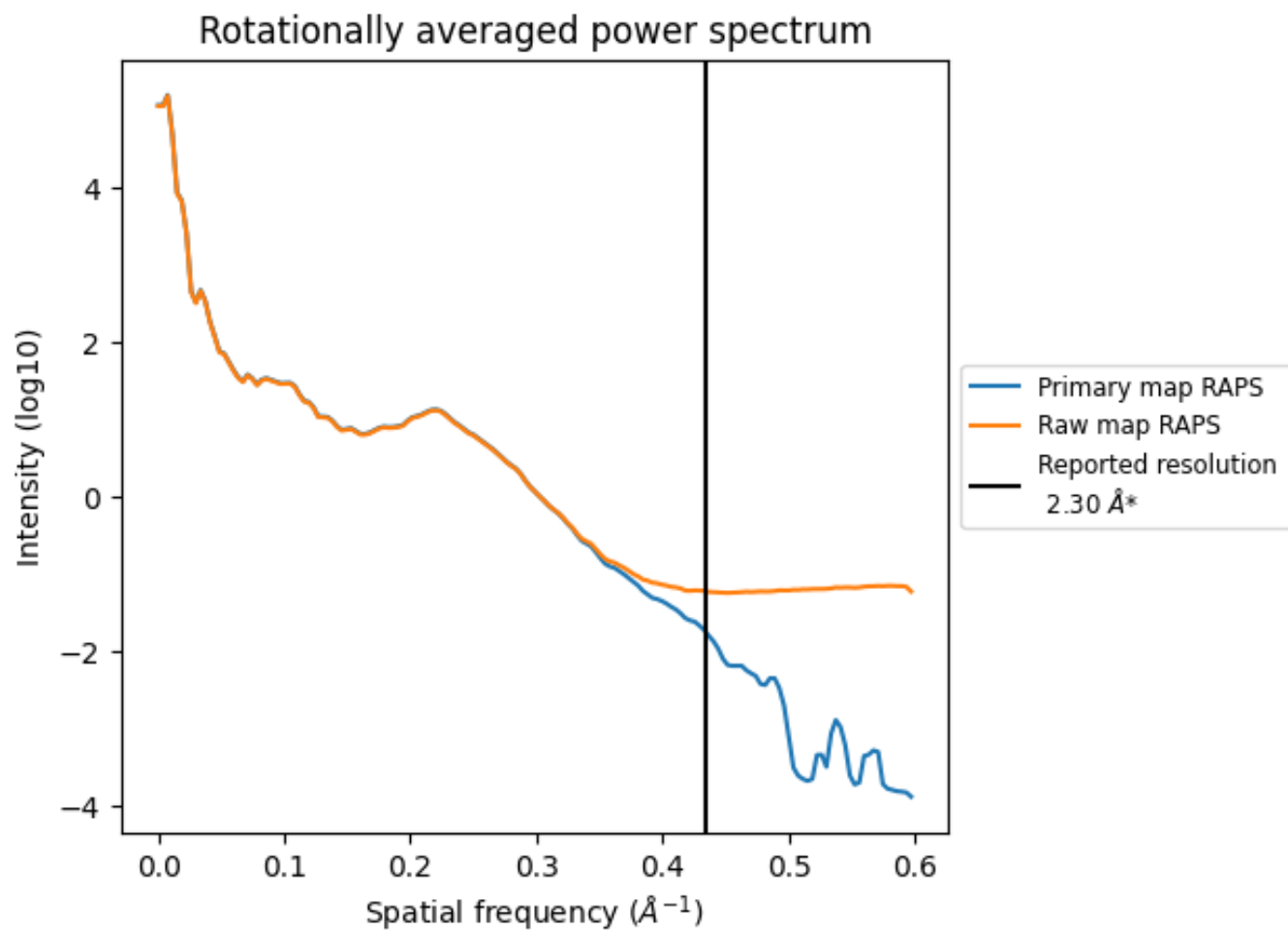
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 192 nm<sup>3</sup>; this corresponds to an approximate mass of 174 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](#)

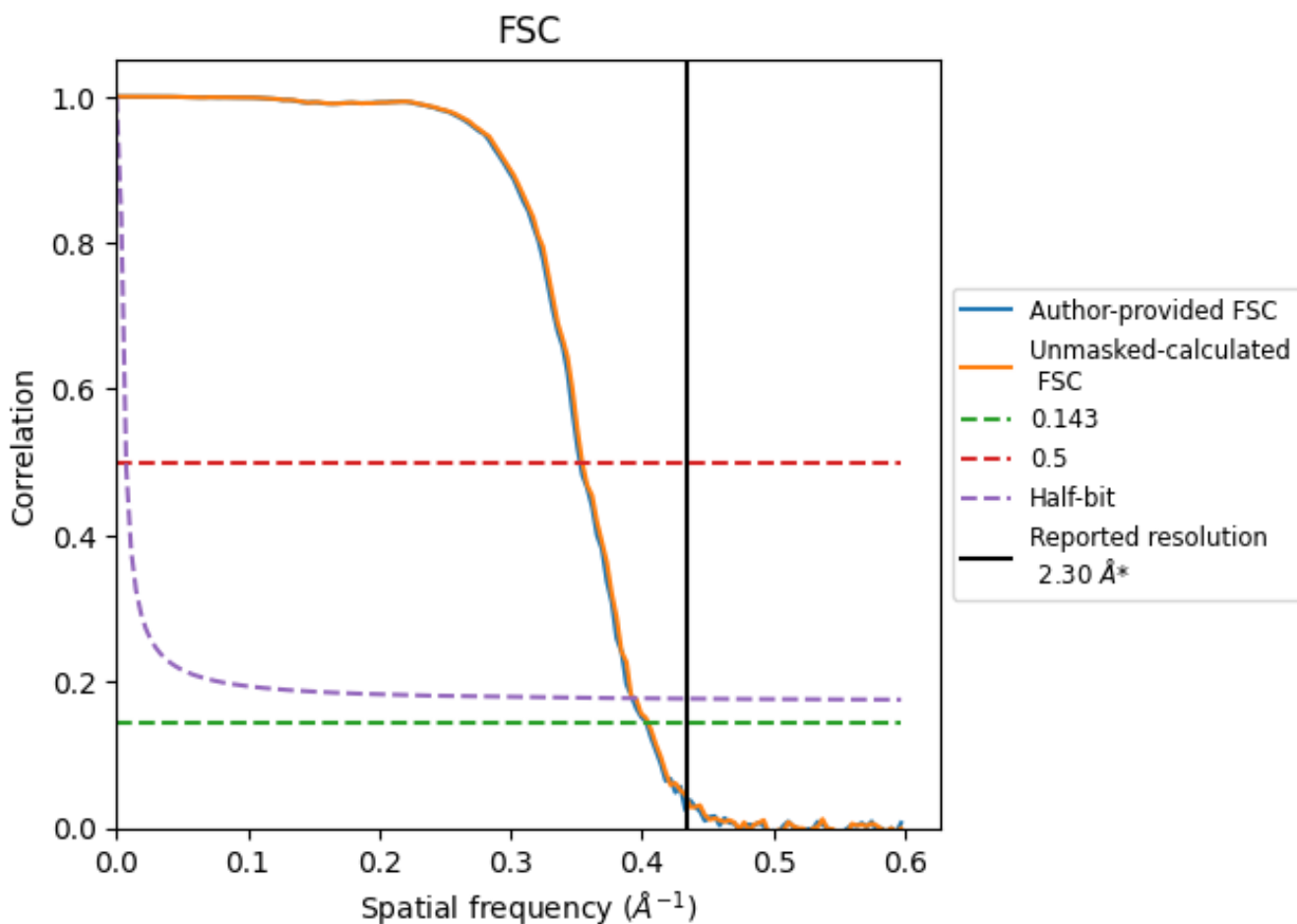


\*Reported resolution corresponds to spatial frequency of 0.435 Å<sup>-1</sup>

## 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 0.435 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

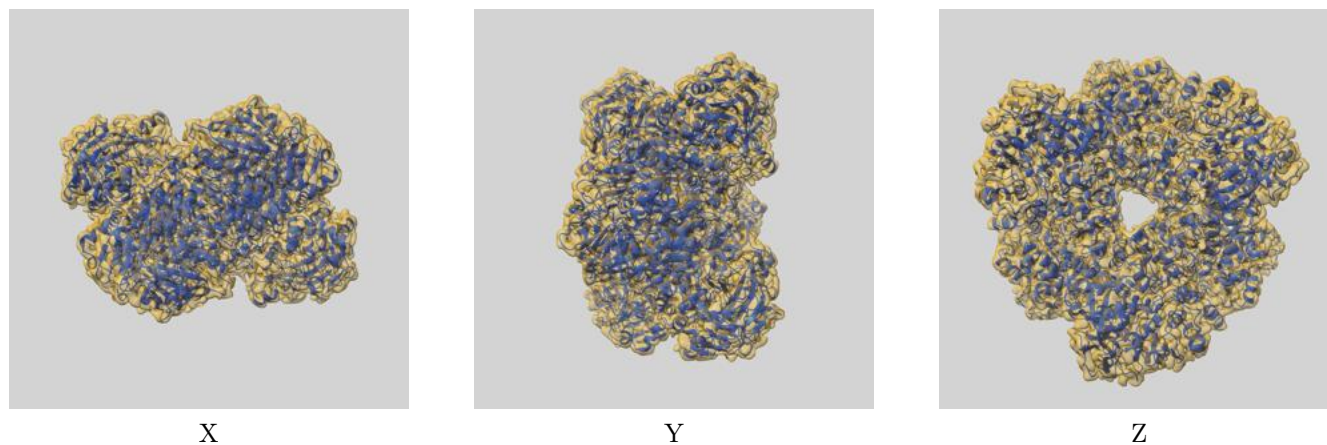
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.30	-	-
Author-provided FSC curve	2.48	2.83	2.55
Unmasked-calculated*	2.47	2.82	2.53

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

This section contains information regarding the fit between EMDB map EMD-17324 and PDB model 8P02. Per-residue inclusion information can be found in section 3 on page 8.

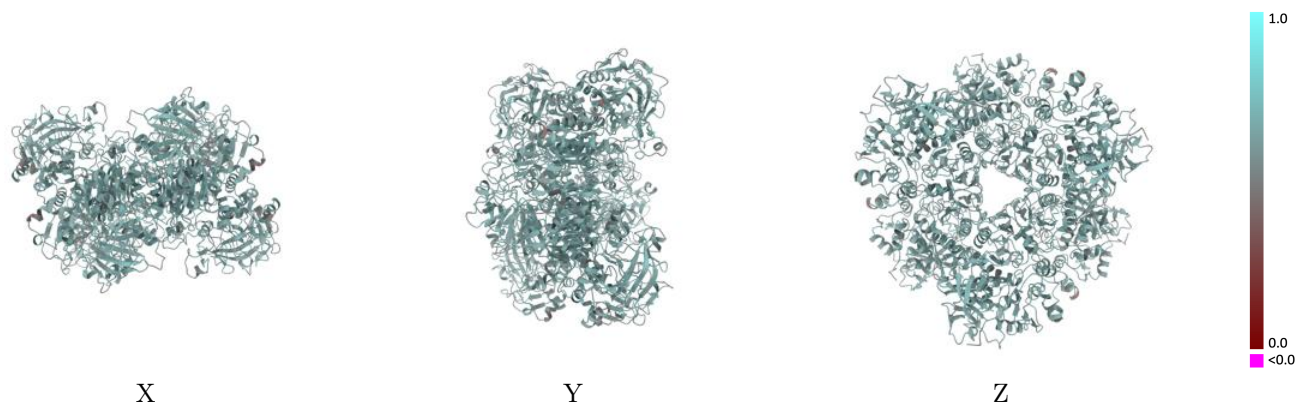
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.00552 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.

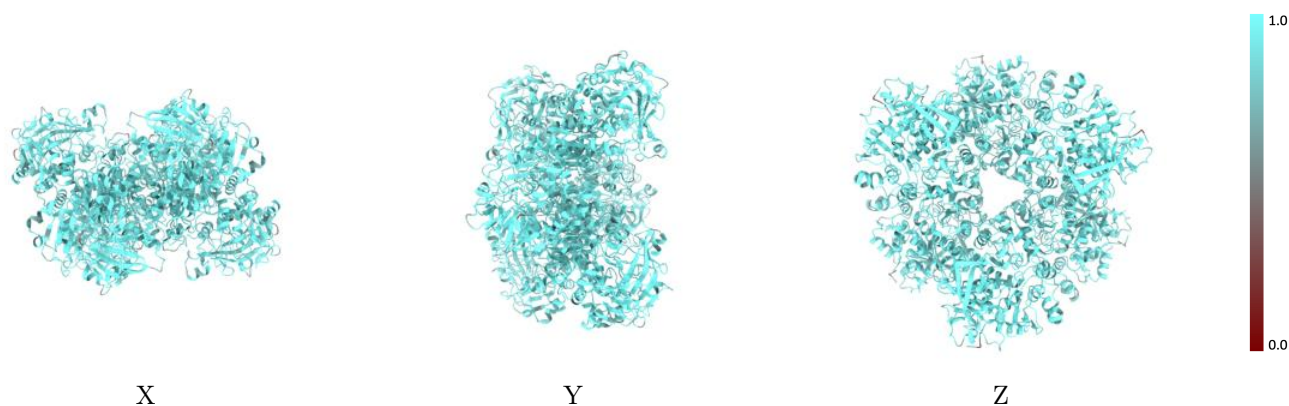


## 9.2 Q-score mapped to coordinate model [i](#)



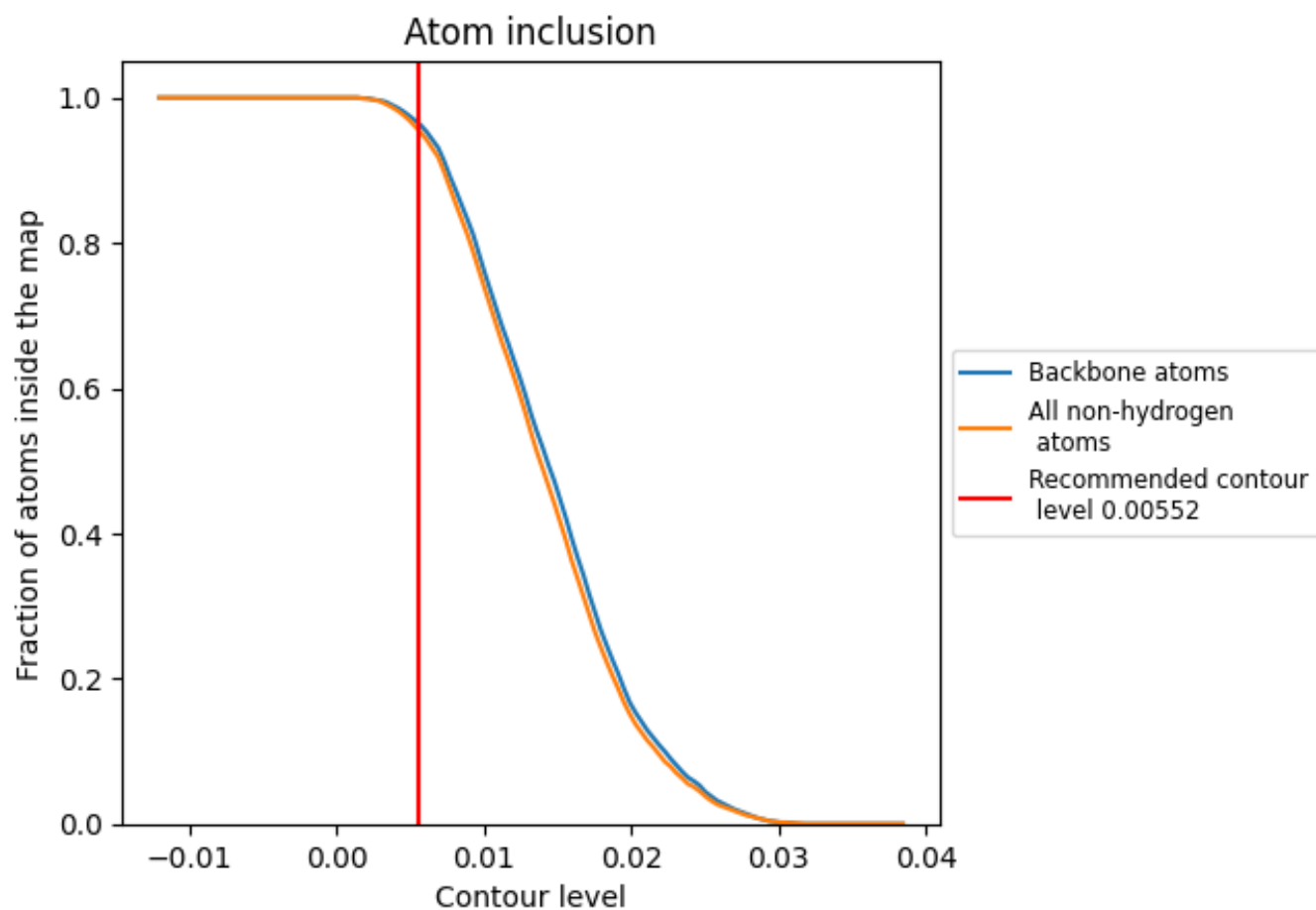
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00552).















## 9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.00552) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9560	 0.6090
A	 0.9570	 0.6090
B	 0.9580	 0.6080
C	 0.9590	 0.6100
D	 0.9570	 0.6100
E	 0.9590	 0.6080
F	 0.9590	 0.6080

