



## Full wwPDB EM Validation Report ⓘ

Nov 5, 2022 – 11:27 AM EDT

PDB ID : 5VKQ  
EMDB ID : EMD-8702  
Title : Structure of a mechanotransduction ion channel *Drosophila* NOMPC in nanodisc  
Authors : Jin, P.; Bulkley, D.; Guo, Y.; Zhang, W.; Guo, Z.; Huynh, W.; Wu, S.; Meltzer, S.; Chen, T.; Jan, L.Y.; Jan, Y.-N.; Cheng, Y.  
Deposited on : 2017-04-22  
Resolution : 3.55 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

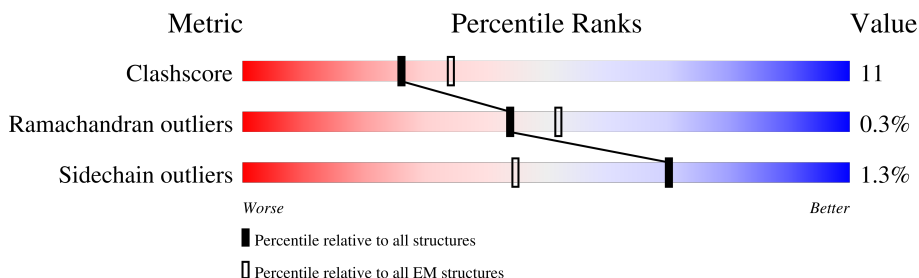
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.55 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	1732	
1	B	1732	
1	C	1732	
1	D	1732	

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	PCF	A	1803	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PCF	B	1808	-	-	X	-
2	PCF	C	1801	-	-	X	-
2	PCF	D	1801	-	-	X	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 41900 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.

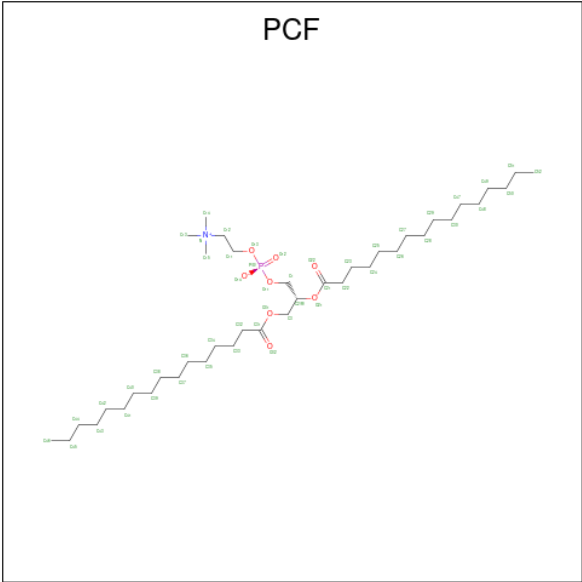
- Molecule 1 is a protein called No mechanoreceptor potential C isoform L.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1499	Total	C	N	O	S	0	0
			10217	6543	1834	1793	47		
1	B	1499	Total	C	N	O	S	0	0
			10217	6543	1834	1793	47		
1	C	1499	Total	C	N	O	S	0	0
			10217	6543	1834	1793	47		
1	D	1499	Total	C	N	O	S	0	0
			10217	6543	1834	1793	47		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1551	GLN	ASN	conflict	UNP E0A9E1
B	1551	GLN	ASN	conflict	UNP E0A9E1
C	1551	GLN	ASN	conflict	UNP E0A9E1
D	1551	GLN	ASN	conflict	UNP E0A9E1

- Molecule 2 is 1,2-DIACYL-SN-GLYCERO-3-PHOSHOCHOLINE (three-letter code: PCF) (formula: C<sub>40</sub>H<sub>80</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	P	0
			258	182	4	64	8	
			Total	C	N	O	P	
			258	182	4	64	8	
			Total	C	N	O	P	
2	A	1	Total	C	N	O	P	0
			258	182	4	64	8	
			Total	C	N	O	P	
			258	182	4	64	8	
			Total	C	N	O	P	
2	A	1	Total	C	N	O	P	0
			258	182	4	64	8	
			Total	C	N	O	P	
			258	182	4	64	8	
			Total	C	N	O	P	
2	A	1	Total	C	N	O	P	0
			258	182	4	64	8	
			Total	C	N	O	P	
			258	182	4	64	8	
			Total	C	N	O	P	
2	B	1	Total	C	N	O	P	0
			258	182	4	64	8	
			Total	C	N	O	P	
			258	182	4	64	8	
			Total	C	N	O	P	
2	B	1	Total	C	N	O	P	0
			258	182	4	64	8	
			Total	C	N	O	P	
			258	182	4	64	8	
			Total	C	N	O	P	
2	B	1	Total	C	N	O	P	0
			258	182	4	64	8	
			Total	C	N	O	P	
			258	182	4	64	8	
			Total	C	N	O	P	

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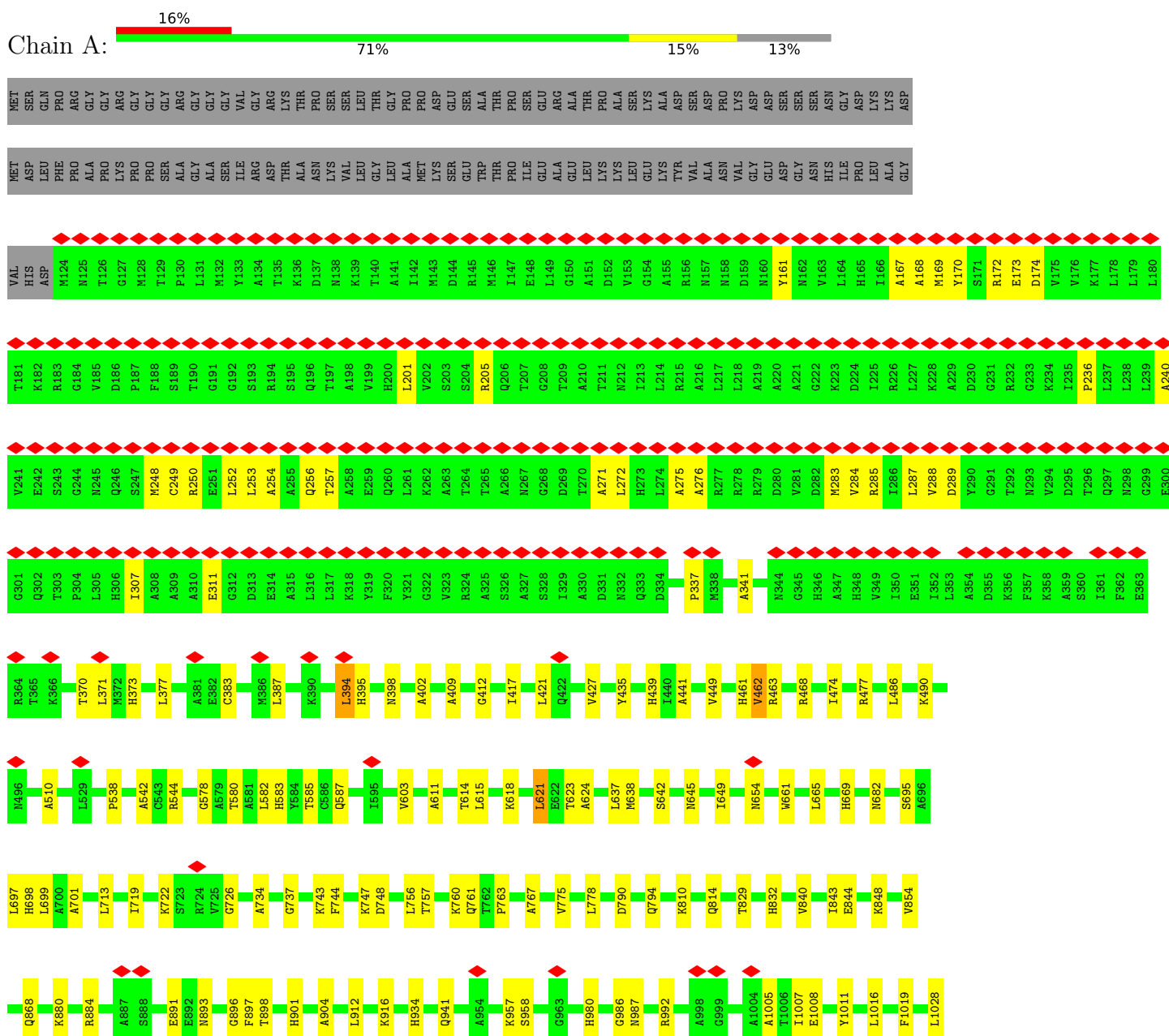
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Mol	Chain	Residues	Atoms					AltConf
2	B	1	Total	C	N	O	P	0
			258	182	4	64	8	
2	B	1	Total	C	N	O	P	0
			258	182	4	64	8	
2	C	1	Total	C	N	O	P	0
			258	182	4	64	8	
2	C	1	Total	C	N	O	P	0
			258	182	4	64	8	
2	C	1	Total	C	N	O	P	0
			258	182	4	64	8	
2	C	1	Total	C	N	O	P	0
			258	182	4	64	8	
2	C	1	Total	C	N	O	P	0
			258	182	4	64	8	
2	C	1	Total	C	N	O	P	0
			258	182	4	64	8	
2	D	1	Total	C	N	O	P	0
			258	182	4	64	8	
2	D	1	Total	C	N	O	P	0
			258	182	4	64	8	
2	D	1	Total	C	N	O	P	0
			258	182	4	64	8	
2	D	1	Total	C	N	O	P	0
			258	182	4	64	8	
2	D	1	Total	C	N	O	P	0
			258	182	4	64	8	
2	D	1	Total	C	N	O	P	0
			258	182	4	64	8	

### 3 Residue-property plots

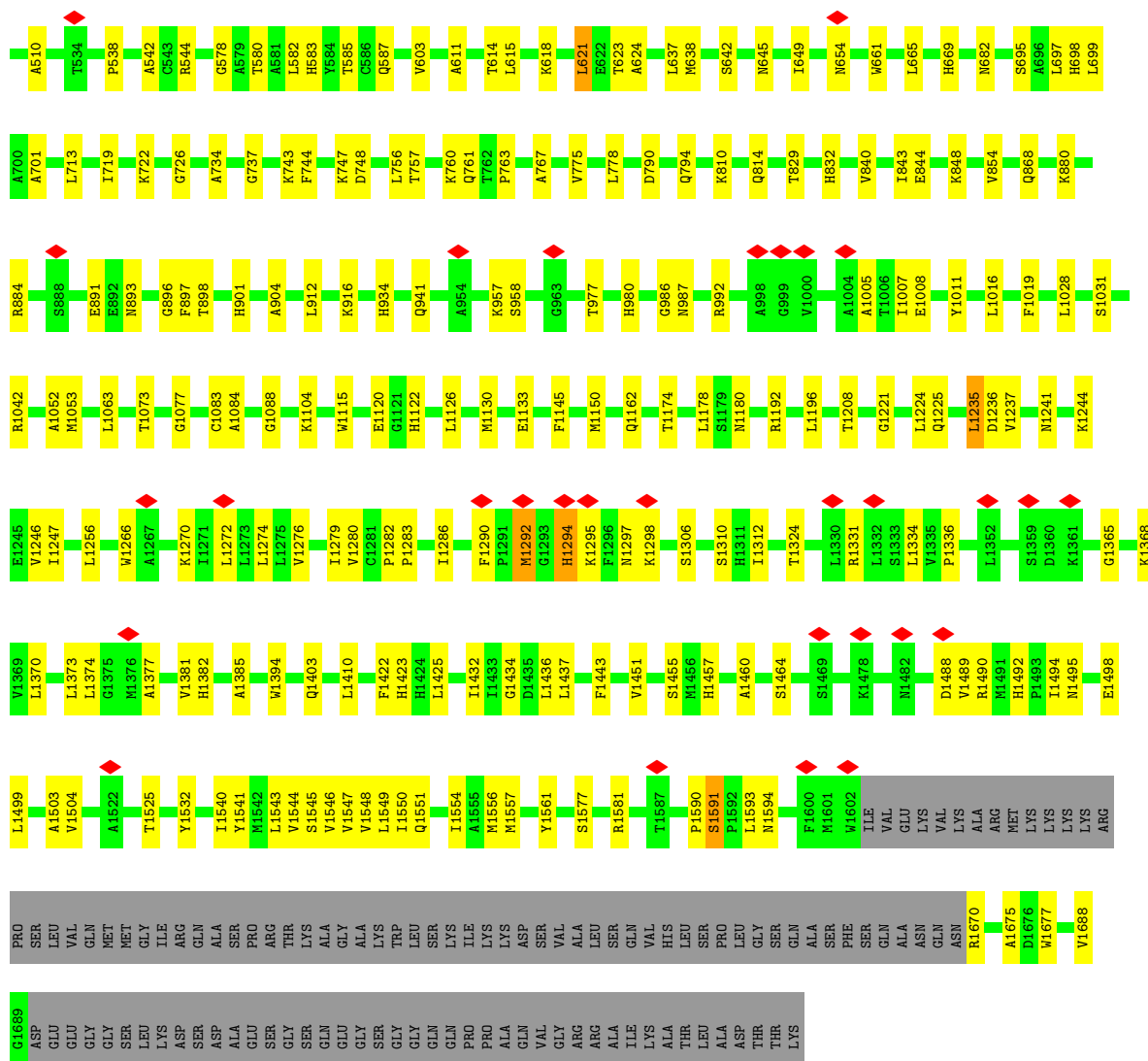
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: No mechanoreceptor potential C isoform L

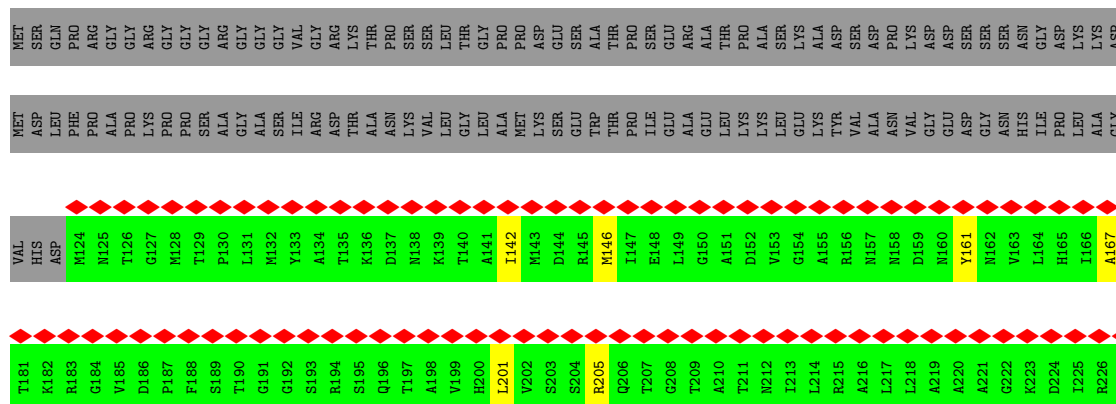








• Molecule 1: No mechanoreceptor potential C isoform L







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	175314	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	54	Depositor
Minimum defocus (nm)	-1400	Depositor
Maximum defocus (nm)	-3300	Depositor
Magnification	41132	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	60.021	Depositor
Minimum map value	-27.667	Depositor
Average map value	-0.243	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	10.0	Depositor
Map size ( $\text{\AA}$ )	486.24, 486.24, 486.24	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.2156, 1.2156, 1.2156	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0.31	0/10413	0.58	4/14270 (0.0%)
1	B	0.31	0/10413	0.58	4/14270 (0.0%)
1	C	0.31	0/10413	0.58	4/14270 (0.0%)
1	D	0.31	0/10413	0.58	4/14270 (0.0%)
All	All	0.31	0/41652	0.58	16/57080 (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	0	7
1	B	0	7
1	C	0	7
1	D	0	7
All	All	0	28

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1488	ASP	CB-CG-OD1	5.62	123.35	118.30
1	A	1488	ASP	CB-CG-OD1	5.61	123.34	118.30
1	D	1488	ASP	CB-CG-OD1	5.61	123.34	118.30
1	C	1488	ASP	CB-CG-OD1	5.54	123.28	118.30
1	C	621	LEU	CA-CB-CG	5.46	127.86	115.30
1	A	621	LEU	CA-CB-CG	5.45	127.84	115.30
1	B	621	LEU	CA-CB-CG	5.44	127.82	115.30
1	D	621	LEU	CA-CB-CG	5.43	127.80	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1593	LEU	CA-CB-CG	5.17	127.19	115.30
1	C	1593	LEU	CA-CB-CG	5.17	127.18	115.30
1	A	1593	LEU	CA-CB-CG	5.16	127.17	115.30
1	D	1593	LEU	CA-CB-CG	5.15	127.15	115.30
1	C	394	LEU	CA-CB-CG	5.03	126.86	115.30
1	D	394	LEU	CA-CB-CG	5.03	126.86	115.30
1	A	394	LEU	CA-CB-CG	5.02	126.84	115.30
1	B	394	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1266	TRP	Peptide
1	A	1590	PRO	Peptide
1	A	1591	SER	Peptide
1	A	394	LEU	Peptide
1	A	461	HIS	Peptide
1	A	957	LYS	Peptide
1	A	986	GLY	Peptide
1	B	1266	TRP	Peptide
1	B	1590	PRO	Peptide
1	B	1591	SER	Peptide
1	B	394	LEU	Peptide
1	B	461	HIS	Peptide
1	B	957	LYS	Peptide
1	B	986	GLY	Peptide
1	C	1266	TRP	Peptide
1	C	1590	PRO	Peptide
1	C	1591	SER	Peptide
1	C	394	LEU	Peptide
1	C	461	HIS	Peptide
1	C	957	LYS	Peptide
1	C	986	GLY	Peptide
1	D	1266	TRP	Peptide
1	D	1590	PRO	Peptide
1	D	1591	SER	Peptide
1	D	394	LEU	Peptide
1	D	461	HIS	Peptide
1	D	957	LYS	Peptide
1	D	986	GLY	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	10217	0	9270	204	0
1	B	10217	0	9270	205	0
1	C	10217	0	9270	216	0
1	D	10217	0	9270	215	0
2	A	258	0	309	77	0
2	B	258	0	309	75	0
2	C	258	0	309	85	0
2	D	258	0	309	82	0
All	All	41900	0	38316	900	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 11.

All (900) 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:D:1532:TYR:CE2	2:D:1801:PCF:H222	1.24	1.68
1:C:1532:TYR:CE2	2:C:1801:PCF:H222	1.32	1.64
1:D:1532:TYR:CE1	2:D:1801:PCF:H21	1.32	1.62
1:A:1498:GLU:CB	2:B:1808:PCF:H351	1.30	1.57
1:D:1532:TYR:CD2	2:D:1801:PCF:H222	1.40	1.57
1:C:1498:GLU:CB	2:D:1801:PCF:H351	1.29	1.55
1:B:1532:TYR:CE2	2:B:1808:PCF:H222	1.41	1.54
1:C:1532:TYR:CZ	2:C:1801:PCF:H21	1.44	1.48
1:C:1532:TYR:CE1	2:C:1801:PCF:H21	1.46	1.47
1:A:1532:TYR:CE2	2:A:1803:PCF:H222	1.53	1.43
2:A:1803:PCF:H351	1:D:1498:GLU:CB	1.48	1.43
1:B:1498:GLU:CB	2:C:1801:PCF:H351	1.50	1.42
1:A:1532:TYR:CE1	2:A:1803:PCF:H21	1.55	1.39
1:D:1532:TYR:CE2	2:D:1801:PCF:C22	2.04	1.37
1:A:1532:TYR:CZ	2:A:1803:PCF:H21	1.59	1.35
1:C:1532:TYR:CD2	2:C:1801:PCF:H222	1.57	1.35
1:C:1532:TYR:CE2	2:C:1801:PCF:C22	2.10	1.34
1:B:1532:TYR:CE1	2:B:1808:PCF:H21	1.63	1.34
1:A:1532:TYR:CD2	2:A:1803:PCF:H222	1.65	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1489:VAL:HG21	2:A:1805:PCF:C13	1.62	1.28
1:D:1532:TYR:CZ	2:D:1801:PCF:H21	1.71	1.25
1:B:1532:TYR:CD2	2:B:1808:PCF:H222	1.74	1.22
1:C:1498:GLU:CB	2:D:1801:PCF:C35	2.20	1.19
1:A:1498:GLU:CB	2:B:1808:PCF:C35	2.21	1.17
1:D:1532:TYR:CZ	2:D:1801:PCF:C21	2.27	1.17
1:D:1532:TYR:CE1	2:D:1801:PCF:C2	2.28	1.16
1:D:1489:VAL:HG21	2:D:1803:PCF:H133	1.22	1.15
1:C:1489:VAL:HG21	2:C:1803:PCF:H133	1.19	1.14
1:B:1489:VAL:HG21	2:B:1802:PCF:H133	1.19	1.14
1:A:1532:TYR:CE2	2:A:1803:PCF:C22	2.29	1.13
2:D:1805:PCF:H361	2:D:1806:PCF:H241	1.27	1.13
1:B:1532:TYR:CE2	2:B:1808:PCF:C22	2.29	1.13
1:A:1489:VAL:CG2	2:A:1805:PCF:C13	2.27	1.12
1:D:1489:VAL:HG21	2:D:1803:PCF:C13	1.79	1.11
1:B:1489:VAL:HG21	2:B:1802:PCF:C13	1.80	1.11
1:C:1532:TYR:CZ	2:C:1801:PCF:C2	2.33	1.11
2:B:1804:PCF:H361	2:B:1805:PCF:H241	1.27	1.11
2:C:1805:PCF:C36	2:C:1806:PCF:H241	1.82	1.10
2:C:1805:PCF:H361	2:C:1806:PCF:H241	1.27	1.09
2:D:1805:PCF:C36	2:D:1806:PCF:H241	1.82	1.09
2:A:1807:PCF:H361	2:A:1808:PCF:H241	1.27	1.09
2:B:1804:PCF:C36	2:B:1805:PCF:H241	1.82	1.09
1:C:1489:VAL:HG21	2:C:1803:PCF:C13	1.82	1.08
2:A:1807:PCF:C36	2:A:1808:PCF:H241	1.82	1.08
1:C:1532:TYR:CE1	2:C:1801:PCF:C2	2.35	1.08
1:A:1282:PRO:O	1:A:1286:ILE:HG13	1.55	1.06
1:C:1282:PRO:O	1:C:1286:ILE:HG13	1.55	1.05
1:B:1282:PRO:O	1:B:1286:ILE:HG13	1.55	1.05
1:D:1532:TYR:CZ	2:D:1801:PCF:C22	2.39	1.04
1:D:1282:PRO:O	1:D:1286:ILE:HG13	1.55	1.04
1:A:1489:VAL:CG2	2:A:1805:PCF:H133	1.85	1.04
1:A:1489:VAL:HG21	2:A:1805:PCF:H133	1.07	1.03
1:B:1532:TYR:CZ	2:B:1808:PCF:H21	1.94	1.03
2:A:1803:PCF:C35	1:D:1498:GLU:CB	2.38	1.01
1:B:1422:PHE:HZ	2:B:1806:PCF:C34	1.73	1.00
1:C:1422:PHE:HZ	2:C:1807:PCF:C34	1.74	1.00
1:D:1422:PHE:HZ	2:D:1807:PCF:C34	1.73	1.00
1:D:1532:TYR:CE2	2:D:1801:PCF:C21	2.45	1.00
1:A:1422:PHE:HZ	2:A:1801:PCF:C34	1.74	0.99
1:B:1498:GLU:CB	2:C:1801:PCF:C35	2.40	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1532:TYR:CD2	2:D:1801:PCF:C22	2.33	0.99
1:A:1532:TYR:CE1	2:A:1803:PCF:C2	2.45	0.99
1:A:1532:TYR:CZ	2:A:1803:PCF:C2	2.46	0.98
1:C:1489:VAL:CG2	2:C:1803:PCF:C13	2.41	0.98
1:C:1489:VAL:CG2	2:C:1803:PCF:H133	1.92	0.98
1:D:1532:TYR:CZ	2:D:1801:PCF:H222	2.00	0.97
1:C:1492:HIS:CE1	2:C:1803:PCF:H222	1.99	0.97
1:C:1437:LEU:HB3	2:C:1806:PCF:H222	1.47	0.96
1:B:1532:TYR:CZ	2:B:1808:PCF:H222	2.00	0.95
1:B:1489:VAL:CG2	2:B:1802:PCF:H133	1.96	0.95
1:B:1489:VAL:CG2	2:B:1802:PCF:C13	2.44	0.95
1:D:1489:VAL:CG2	2:D:1803:PCF:C13	2.45	0.93
1:C:1532:TYR:CD2	2:C:1801:PCF:C22	2.44	0.92
1:D:1437:LEU:HB3	2:D:1806:PCF:H222	1.52	0.92
1:B:1532:TYR:CZ	2:B:1808:PCF:C22	2.52	0.92
1:C:1532:TYR:CE2	2:C:1801:PCF:C21	2.53	0.91
1:B:1532:TYR:CZ	2:B:1808:PCF:C21	2.54	0.90
1:D:1532:TYR:CZ	2:D:1801:PCF:C2	2.51	0.90
1:C:1532:TYR:CZ	2:C:1801:PCF:C21	2.55	0.90
1:A:1437:LEU:HB3	2:A:1808:PCF:H222	1.53	0.88
1:D:1489:VAL:CG2	2:D:1803:PCF:H133	2.01	0.87
1:D:1532:TYR:HE1	2:D:1801:PCF:H21	1.34	0.86
1:B:1437:LEU:HB3	2:B:1805:PCF:H222	1.57	0.86
1:D:1422:PHE:HZ	2:D:1807:PCF:H341	1.41	0.86
1:A:1422:PHE:HZ	2:A:1801:PCF:H341	1.41	0.85
1:B:1422:PHE:HZ	2:B:1806:PCF:H341	1.41	0.84
1:C:1422:PHE:HZ	2:C:1807:PCF:H341	1.41	0.83
1:A:1489:VAL:CG2	2:A:1805:PCF:H131	2.05	0.83
1:C:1532:TYR:CZ	2:C:1801:PCF:C22	2.62	0.83
2:B:1804:PCF:C36	2:B:1805:PCF:C24	2.58	0.82
1:A:1492:HIS:CE1	2:A:1805:PCF:H222	2.15	0.82
1:B:1492:HIS:CE1	2:B:1802:PCF:H222	2.15	0.82
1:A:1532:TYR:CE2	2:A:1803:PCF:C21	2.62	0.82
2:A:1807:PCF:C36	2:A:1808:PCF:C24	2.57	0.81
1:A:1532:TYR:CD2	2:A:1803:PCF:C22	2.54	0.81
1:C:1543:LEU:O	1:C:1547:VAL:HB	1.80	0.81
1:D:1543:LEU:O	1:D:1547:VAL:HB	1.80	0.81
2:D:1805:PCF:C36	2:D:1806:PCF:C24	2.58	0.81
1:A:1543:LEU:O	1:A:1547:VAL:HB	1.80	0.80
2:C:1805:PCF:C36	2:C:1806:PCF:C24	2.58	0.80
1:A:1422:PHE:CZ	2:A:1801:PCF:C34	2.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1543:LEU:O	1:B:1547:VAL:HB	1.80	0.80
1:D:1422:PHE:CZ	2:D:1807:PCF:C34	2.64	0.79
1:A:1489:VAL:HG23	2:A:1805:PCF:H131	1.65	0.78
2:A:1807:PCF:H362	2:A:1808:PCF:H232	1.66	0.78
1:B:1422:PHE:CZ	2:B:1806:PCF:C34	2.64	0.78
2:B:1804:PCF:H362	2:B:1805:PCF:H232	1.65	0.78
1:A:1492:HIS:HB3	2:B:1808:PCF:O14	1.83	0.77
2:A:1807:PCF:H361	2:A:1808:PCF:C24	2.13	0.77
1:D:1532:TYR:OH	2:D:1801:PCF:C21	2.32	0.77
1:A:1532:TYR:CZ	2:A:1803:PCF:C21	2.67	0.77
2:C:1805:PCF:H362	2:C:1806:PCF:H232	1.65	0.77
2:B:1804:PCF:H361	2:B:1805:PCF:C24	2.13	0.77
1:C:1422:PHE:CZ	2:C:1807:PCF:C34	2.64	0.77
1:C:1434:GLY:N	2:C:1805:PCF:O14	2.18	0.77
2:D:1805:PCF:H362	2:D:1806:PCF:H232	1.66	0.76
1:D:1492:HIS:ND1	2:D:1803:PCF:H111	2.01	0.76
1:C:1492:HIS:ND1	2:C:1803:PCF:H111	2.01	0.75
1:C:1528:TYR:HE2	2:C:1801:PCF:H131	1.51	0.75
1:A:1422:PHE:HZ	2:A:1801:PCF:H342	1.52	0.75
1:B:1492:HIS:ND1	2:B:1802:PCF:H111	2.02	0.75
1:B:1422:PHE:HZ	2:B:1806:PCF:H342	1.52	0.74
1:C:1422:PHE:HZ	2:C:1807:PCF:H342	1.52	0.74
1:D:1492:HIS:CE1	2:D:1803:PCF:H222	2.23	0.74
1:C:1532:TYR:OH	2:C:1801:PCF:O11	2.06	0.73
1:A:1532:TYR:OH	2:A:1803:PCF:O11	2.06	0.73
2:B:1804:PCF:H362	2:B:1805:PCF:C23	2.18	0.73
1:D:1422:PHE:HZ	2:D:1807:PCF:H342	1.52	0.73
2:A:1807:PCF:H362	2:A:1808:PCF:C23	2.18	0.72
1:A:1422:PHE:CZ	2:A:1801:PCF:H342	2.25	0.72
1:B:1422:PHE:CZ	2:B:1806:PCF:H342	2.25	0.72
1:C:1422:PHE:CZ	2:C:1807:PCF:H342	2.25	0.72
1:C:1532:TYR:OH	2:C:1801:PCF:C2	2.38	0.72
2:C:1805:PCF:H362	2:C:1806:PCF:C23	2.18	0.72
1:C:1422:PHE:CE2	2:C:1807:PCF:H321	2.25	0.71
1:D:1422:PHE:CE2	2:D:1807:PCF:H321	2.25	0.71
1:A:1422:PHE:CE2	2:A:1801:PCF:H321	2.25	0.71
1:D:1422:PHE:CZ	2:D:1807:PCF:H342	2.25	0.71
2:D:1805:PCF:H362	2:D:1806:PCF:C23	2.18	0.71
1:C:1272:LEU:HD21	2:C:1808:PCF:H222	1.73	0.71
1:A:1434:GLY:HA3	2:A:1807:PCF:O14	1.90	0.70
1:B:1422:PHE:CE2	2:B:1806:PCF:H321	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1272:LEU:HD21	2:D:1808:PCF:H222	1.73	0.70
1:A:1272:LEU:HD21	2:A:1802:PCF:H222	1.74	0.70
1:B:1422:PHE:CE2	2:B:1806:PCF:C32	2.75	0.70
1:C:1422:PHE:CE2	2:C:1807:PCF:C32	2.75	0.70
1:C:1532:TYR:OH	2:C:1801:PCF:H21	1.91	0.70
1:C:1437:LEU:HB3	2:C:1806:PCF:C22	2.21	0.70
1:A:1422:PHE:CE2	2:A:1801:PCF:C32	2.75	0.69
1:D:1422:PHE:CE2	2:D:1807:PCF:C32	2.75	0.69
1:C:1492:HIS:HE1	2:C:1803:PCF:H222	1.54	0.69
2:D:1805:PCF:H361	2:D:1806:PCF:C24	2.13	0.69
1:B:1272:LEU:HD21	2:B:1807:PCF:H222	1.73	0.69
1:C:1433:ILE:HG21	2:C:1805:PCF:O22	1.91	0.69
1:A:1492:HIS:ND1	2:A:1805:PCF:H111	2.07	0.69
1:B:1532:TYR:CE1	2:B:1808:PCF:C2	2.59	0.68
2:C:1805:PCF:H361	2:C:1806:PCF:C24	2.13	0.68
1:D:1489:VAL:CG2	2:D:1803:PCF:H131	2.22	0.68
1:B:1532:TYR:CD2	2:B:1808:PCF:C22	2.67	0.67
1:D:1532:TYR:CG	2:D:1801:PCF:H222	2.22	0.67
1:C:1489:VAL:CG2	2:C:1803:PCF:H131	2.26	0.66
1:D:1270:LYS:O	1:D:1274:LEU:HB2	1.95	0.66
1:A:1492:HIS:CB	2:B:1808:PCF:O14	2.43	0.66
1:C:1270:LYS:O	1:C:1274:LEU:HB2	1.95	0.66
1:C:1422:PHE:CZ	2:C:1807:PCF:H341	2.30	0.66
1:B:1270:LYS:O	1:B:1274:LEU:HB2	1.95	0.66
1:B:1489:VAL:CG2	2:B:1802:PCF:H131	2.25	0.66
1:A:1270:LYS:O	1:A:1274:LEU:HB2	1.95	0.65
1:A:1422:PHE:CZ	2:A:1801:PCF:H341	2.30	0.65
1:A:1528:TYR:HE2	2:A:1803:PCF:H131	1.61	0.65
1:A:1374:LEU:O	1:A:1377:ALA:HB3	1.97	0.65
1:B:1532:TYR:CE2	2:B:1808:PCF:C21	2.79	0.65
1:B:1374:LEU:O	1:B:1377:ALA:HB3	1.97	0.65
1:D:743:LYS:O	1:D:747:LYS:HB3	1.97	0.65
1:A:1532:TYR:CZ	2:A:1803:PCF:C22	2.81	0.64
1:A:695:SER:H	1:A:698:HIS:HD2	1.46	0.64
1:D:250:ARG:O	1:D:254:ALA:HB2	1.98	0.64
1:D:1434:GLY:HA3	2:D:1805:PCF:O14	1.97	0.64
1:A:250:ARG:O	1:A:254:ALA:HB2	1.98	0.64
1:C:1374:LEU:O	1:C:1377:ALA:HB3	1.97	0.64
1:D:695:SER:H	1:D:698:HIS:HD2	1.46	0.64
1:C:743:LYS:O	1:C:747:LYS:HB3	1.97	0.64
1:A:743:LYS:O	1:A:747:LYS:HB3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:ARG:O	1:C:254:ALA:HB2	1.98	0.64
1:C:1489:VAL:HG23	2:C:1803:PCF:H131	1.78	0.64
1:A:1434:GLY:N	2:A:1807:PCF:O14	2.31	0.64
1:B:695:SER:H	1:B:698:HIS:HD2	1.46	0.63
1:B:743:LYS:O	1:B:747:LYS:HB3	1.97	0.63
1:B:1224:LEU:HD22	1:B:1235:LEU:HD23	1.81	0.63
1:D:1374:LEU:O	1:D:1377:ALA:HB3	1.97	0.63
1:D:1224:LEU:HD22	1:D:1235:LEU:HD23	1.81	0.63
1:C:695:SER:H	1:C:698:HIS:HD2	1.46	0.63
1:A:1224:LEU:HD22	1:A:1235:LEU:HD23	1.81	0.63
1:B:1489:VAL:HG23	2:B:1802:PCF:H131	1.81	0.63
1:C:1224:LEU:HD22	1:C:1235:LEU:HD23	1.81	0.63
1:B:1532:TYR:CZ	2:B:1808:PCF:C2	2.79	0.63
1:B:250:ARG:O	1:B:254:ALA:HB2	1.98	0.62
1:B:1532:TYR:OH	2:B:1808:PCF:C21	2.47	0.62
1:D:1422:PHE:CZ	2:D:1807:PCF:H341	2.29	0.62
1:A:1492:HIS:HE1	2:A:1805:PCF:H222	1.64	0.62
1:A:1120:GLU:O	1:A:1122:HIS:ND1	2.31	0.62
1:B:1422:PHE:CZ	2:B:1806:PCF:H341	2.29	0.62
1:C:1492:HIS:ND1	2:C:1803:PCF:C11	2.62	0.62
1:C:1492:HIS:HB3	2:D:1801:PCF:O14	1.99	0.62
1:D:1334:LEU:HB3	1:D:1336:PRO:HD3	1.82	0.62
1:C:1489:VAL:HG23	2:C:1803:PCF:C13	2.30	0.62
1:C:1544:VAL:O	1:C:1548:VAL:HB	2.00	0.62
1:A:1434:GLY:CA	2:A:1807:PCF:O14	2.48	0.61
1:A:1544:VAL:O	1:A:1548:VAL:HB	2.00	0.61
1:B:1334:LEU:HB3	1:B:1336:PRO:HD3	1.82	0.61
1:D:1544:VAL:O	1:D:1548:VAL:HB	2.00	0.61
1:D:1528:TYR:HE2	2:D:1801:PCF:H131	1.65	0.61
1:A:1334:LEU:HB3	1:A:1336:PRO:HD3	1.82	0.61
2:A:1803:PCF:O14	1:D:1492:HIS:HB3	2.00	0.61
1:B:1544:VAL:O	1:B:1548:VAL:HB	2.00	0.61
1:B:1422:PHE:CZ	2:B:1806:PCF:C32	2.84	0.61
1:C:1334:LEU:HB3	1:C:1336:PRO:HD3	1.82	0.61
2:D:1806:PCF:H332	2:D:1806:PCF:H31	1.82	0.61
1:D:665:LEU:O	1:D:669:HIS:HB2	2.01	0.61
1:D:1422:PHE:CZ	2:D:1807:PCF:C32	2.84	0.61
1:A:665:LEU:O	1:A:669:HIS:HB2	2.01	0.61
1:A:1422:PHE:CZ	2:A:1801:PCF:C32	2.84	0.61
1:C:1532:TYR:HH	2:C:1801:PCF:C1	2.14	0.60
1:C:1422:PHE:CE2	2:C:1807:PCF:H322	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1554:ILE:HG12	1:D:1551:GLN:HB3	1.82	0.60
1:B:1410:LEU:HD11	1:C:1457:HIS:HB2	1.82	0.60
1:C:665:LEU:O	1:C:669:HIS:HB2	2.01	0.60
1:C:1422:PHE:HE2	2:C:1807:PCF:H321	1.65	0.60
1:A:1422:PHE:CE2	2:A:1801:PCF:H322	2.36	0.60
2:B:1805:PCF:H31	2:B:1805:PCF:H332	1.83	0.60
2:A:1808:PCF:H31	2:A:1808:PCF:H332	1.82	0.60
1:B:1422:PHE:CE2	2:B:1806:PCF:H322	2.36	0.60
1:D:1489:VAL:HG23	2:D:1803:PCF:H131	1.83	0.60
1:C:463:ARG:HH11	1:C:468:ARG:HG2	1.67	0.60
1:C:1422:PHE:CZ	2:C:1807:PCF:C32	2.84	0.60
1:D:1422:PHE:CE2	2:D:1807:PCF:H322	2.36	0.60
1:A:463:ARG:HH11	1:A:468:ARG:HG2	1.67	0.60
2:C:1806:PCF:H31	2:C:1806:PCF:H332	1.82	0.60
1:D:757:THR:H	1:D:761:GLN:H	1.50	0.59
1:B:665:LEU:O	1:B:669:HIS:HB2	2.01	0.59
1:A:1551:GLN:HB3	1:D:1554:ILE:HG12	1.82	0.59
1:B:463:ARG:HH11	1:B:468:ARG:HG2	1.67	0.59
1:C:1120:GLU:O	1:C:1122:HIS:ND1	2.31	0.59
1:A:757:THR:H	1:A:761:GLN:H	1.50	0.59
1:D:1492:HIS:ND1	2:D:1803:PCF:C11	2.65	0.59
1:A:1276:VAL:O	1:A:1280:VAL:HG22	2.03	0.59
1:A:1422:PHE:HE2	2:A:1801:PCF:H321	1.65	0.59
1:D:1276:VAL:O	1:D:1280:VAL:HG22	2.03	0.59
1:D:463:ARG:HH11	1:D:468:ARG:HG2	1.67	0.59
1:D:1422:PHE:HE2	2:D:1807:PCF:H321	1.65	0.59
2:B:1804:PCF:H341	2:B:1805:PCF:H221	1.85	0.59
2:D:1805:PCF:H341	2:D:1806:PCF:H221	1.85	0.59
1:B:1120:GLU:O	1:B:1122:HIS:ND1	2.31	0.59
2:C:1805:PCF:H341	2:C:1806:PCF:H221	1.85	0.59
2:A:1807:PCF:H341	2:A:1808:PCF:H221	1.85	0.58
1:C:1492:HIS:NE2	2:C:1803:PCF:H222	2.18	0.58
1:B:1276:VAL:O	1:B:1280:VAL:HG22	2.03	0.58
1:B:1492:HIS:ND1	2:B:1802:PCF:C11	2.65	0.58
1:B:1422:PHE:HE2	2:B:1806:PCF:C32	2.17	0.58
2:A:1807:PCF:H332	2:A:1807:PCF:H31	1.86	0.58
1:A:417:ILE:O	1:A:421:LEU:HB2	2.04	0.58
1:B:757:THR:H	1:B:761:GLN:H	1.50	0.58
1:B:1434:GLY:HA3	2:B:1804:PCF:O14	2.02	0.58
1:C:757:THR:H	1:C:761:GLN:H	1.50	0.58
1:C:395:HIS:CD2	1:D:457:GLY:HA2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1276:VAL:O	1:C:1280:VAL:HG22	2.03	0.58
1:B:1492:HIS:HE1	2:B:1802:PCF:H222	1.65	0.58
1:A:1422:PHE:HE2	2:A:1801:PCF:C32	2.17	0.58
1:B:1492:HIS:HB3	2:C:1801:PCF:O14	2.03	0.58
1:D:417:ILE:O	1:D:421:LEU:HB2	2.04	0.58
2:B:1804:PCF:H332	2:B:1804:PCF:H31	1.86	0.57
1:D:1052:ALA:HB1	1:D:1084:ALA:HB2	1.87	0.57
2:A:1807:PCF:H362	2:A:1808:PCF:C24	2.35	0.57
1:B:1422:PHE:HE2	2:B:1806:PCF:H321	1.65	0.57
1:B:417:ILE:O	1:B:421:LEU:HB2	2.04	0.57
1:C:383:CYS:O	1:C:387:LEU:HB2	2.05	0.57
2:A:1807:PCF:C36	2:A:1808:PCF:C23	2.83	0.57
1:B:1052:ALA:HB1	1:B:1084:ALA:HB2	1.87	0.57
2:D:1805:PCF:H31	2:D:1805:PCF:H332	1.86	0.57
1:C:417:ILE:O	1:C:421:LEU:HB2	2.04	0.56
1:C:1434:GLY:CA	2:C:1805:PCF:O14	2.53	0.56
1:D:1422:PHE:HE2	2:D:1807:PCF:C32	2.17	0.56
1:A:383:CYS:O	1:A:387:LEU:HB2	2.05	0.56
1:A:1052:ALA:HB1	1:A:1084:ALA:HB2	1.87	0.56
1:A:1433:ILE:HG21	2:A:1807:PCF:O22	2.04	0.56
1:A:1490:ARG:HH12	1:A:1525:THR:HG21	1.70	0.56
1:B:383:CYS:O	1:B:387:LEU:HB2	2.05	0.56
2:C:1805:PCF:H332	2:C:1805:PCF:H31	1.86	0.56
1:D:383:CYS:O	1:D:387:LEU:HB2	2.05	0.56
1:B:904:ALA:O	1:B:941:GLN:NE2	2.39	0.56
1:B:1490:ARG:HH12	1:B:1525:THR:HG21	1.70	0.56
1:C:1126:LEU:O	1:C:1130:MET:HB2	2.06	0.56
1:D:1282:PRO:O	1:D:1286:ILE:CG1	2.44	0.56
1:D:1423:HIS:CE1	2:D:1807:PCF:O22	2.59	0.56
2:D:1805:PCF:C36	2:D:1806:PCF:C23	2.83	0.56
1:C:1052:ALA:HB1	1:C:1084:ALA:HB2	1.87	0.56
1:C:661:TRP:HA	1:C:665:LEU:HD12	1.88	0.56
1:D:661:TRP:HA	1:D:665:LEU:HD12	1.88	0.56
1:D:904:ALA:O	1:D:941:GLN:NE2	2.39	0.56
1:A:1126:LEU:O	1:A:1130:MET:HB2	2.06	0.56
1:A:1423:HIS:CE1	2:A:1801:PCF:O22	2.59	0.56
1:D:1126:LEU:O	1:D:1130:MET:HB2	2.06	0.56
1:C:1434:GLY:HA3	2:C:1805:PCF:O14	2.06	0.56
1:A:1208:THR:HG22	1:A:1246:VAL:HA	1.88	0.56
2:B:1804:PCF:H362	2:B:1805:PCF:C24	2.35	0.56
1:C:904:ALA:O	1:C:941:GLN:NE2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:904:ALA:O	1:A:941:GLN:NE2	2.39	0.56
1:C:1208:THR:HG22	1:C:1246:VAL:HA	1.88	0.55
1:C:1423:HIS:CE1	2:C:1807:PCF:O22	2.59	0.55
1:D:1208:THR:HG22	1:D:1246:VAL:HA	1.88	0.55
1:B:1423:HIS:CE1	2:B:1806:PCF:O22	2.59	0.55
1:B:1591:SER:HA	1:B:1594:ASN:H	1.72	0.55
1:A:1591:SER:HA	1:A:1594:ASN:H	1.72	0.55
1:B:370:THR:HB	1:B:373:HIS:HD2	1.71	0.55
1:B:1208:THR:HG22	1:B:1246:VAL:HA	1.88	0.55
1:B:1282:PRO:O	1:B:1286:ILE:CG1	2.44	0.55
1:C:370:THR:HB	1:C:373:HIS:HD2	1.71	0.55
1:C:1532:TYR:OH	2:C:1801:PCF:C21	2.54	0.55
2:C:1805:PCF:H362	2:C:1806:PCF:C24	2.35	0.55
1:A:1282:PRO:O	1:A:1286:ILE:CG1	2.44	0.55
1:A:1437:LEU:HB3	2:A:1808:PCF:C22	2.33	0.55
1:B:1126:LEU:O	1:B:1130:MET:HB2	2.06	0.55
1:C:1490:ARG:HH12	1:C:1525:THR:HG21	1.70	0.55
1:C:1591:SER:HA	1:C:1594:ASN:H	1.72	0.55
2:D:1805:PCF:C37	2:D:1806:PCF:H241	2.36	0.55
1:A:580:THR:H	1:A:583:HIS:CD2	2.25	0.55
1:B:661:TRP:HA	1:B:665:LEU:HD12	1.88	0.55
1:D:370:THR:HB	1:D:373:HIS:HD2	1.71	0.55
1:D:1007:ILE:HD12	1:D:1011:TYR:HB2	1.88	0.55
2:A:1807:PCF:C37	2:A:1808:PCF:H241	2.36	0.55
1:C:462:VAL:O	1:C:463:ARG:NE	2.38	0.55
1:D:1490:ARG:HH12	1:D:1525:THR:HG21	1.70	0.55
1:A:370:THR:HB	1:A:373:HIS:HD2	1.71	0.55
1:A:462:VAL:O	1:A:463:ARG:NE	2.38	0.55
1:D:1451:VAL:O	1:D:1455:SER:HB3	2.07	0.55
1:A:1007:ILE:HD12	1:A:1011:TYR:HB2	1.88	0.55
1:A:661:TRP:HA	1:A:665:LEU:HD12	1.88	0.54
1:B:868:GLN:OE1	1:B:893:ASN:ND2	2.40	0.54
1:B:1007:ILE:HD12	1:B:1011:TYR:HB2	1.88	0.54
1:B:383:CYS:O	1:B:387:LEU:CB	2.56	0.54
1:C:383:CYS:O	1:C:387:LEU:CB	2.56	0.54
1:C:1007:ILE:HD12	1:C:1011:TYR:HB2	1.88	0.54
1:A:868:GLN:OE1	1:A:893:ASN:ND2	2.40	0.54
1:B:722:LYS:HB3	1:B:726:GLY:HA2	1.90	0.54
1:D:1422:PHE:CZ	2:D:1807:PCF:H321	2.43	0.54
1:D:1591:SER:HA	1:D:1594:ASN:H	1.72	0.54
1:C:868:GLN:OE1	1:C:893:ASN:ND2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:868:GLN:OE1	1:D:893:ASN:ND2	2.40	0.54
1:A:383:CYS:O	1:A:387:LEU:CB	2.56	0.54
1:A:1410:LEU:HD11	1:B:1457:HIS:HB2	1.88	0.54
1:C:1422:PHE:HE2	2:C:1807:PCF:C32	2.17	0.54
2:B:1804:PCF:C37	2:B:1805:PCF:H241	2.36	0.54
1:C:1422:PHE:CZ	2:C:1807:PCF:H321	2.43	0.54
1:A:236:PRO:O	1:A:240:ALA:HB3	2.08	0.54
1:B:669:HIS:HD2	1:B:699:LEU:HD22	1.74	0.54
1:C:1451:VAL:O	1:C:1455:SER:HB3	2.07	0.54
1:D:383:CYS:O	1:D:387:LEU:CB	2.56	0.54
1:D:580:THR:H	1:D:583:HIS:CD2	2.25	0.54
1:A:1451:VAL:O	1:A:1455:SER:HB3	2.07	0.53
1:A:1104:LYS:HE3	1:A:1133:GLU:HB3	1.90	0.53
1:B:1451:VAL:O	1:B:1455:SER:HB3	2.07	0.53
2:B:1804:PCF:C36	2:B:1805:PCF:C23	2.83	0.53
2:C:1805:PCF:C37	2:C:1806:PCF:H241	2.36	0.53
1:D:1120:GLU:O	1:D:1122:HIS:ND1	2.31	0.53
1:A:722:LYS:HB3	1:A:726:GLY:HA2	1.90	0.53
1:D:669:HIS:HD2	1:D:699:LEU:HD22	1.73	0.53
1:C:722:LYS:HB3	1:C:726:GLY:HA2	1.90	0.53
1:D:462:VAL:O	1:D:463:ARG:NE	2.38	0.53
1:B:580:THR:H	1:B:583:HIS:CD2	2.25	0.53
1:C:580:THR:H	1:C:583:HIS:CD2	2.25	0.53
2:C:1805:PCF:C36	2:C:1806:PCF:C23	2.83	0.53
1:D:236:PRO:O	1:D:240:ALA:HB3	2.08	0.53
1:D:486:LEU:O	1:D:490:LYS:N	2.41	0.53
1:D:1528:TYR:CE2	2:D:1801:PCF:H131	2.42	0.53
2:D:1805:PCF:H362	2:D:1806:PCF:C24	2.35	0.53
1:B:912:LEU:O	1:B:916:LYS:CB	2.57	0.53
1:D:1104:LYS:HE3	1:D:1133:GLU:HB3	1.90	0.53
1:B:1422:PHE:CZ	2:B:1806:PCF:H321	2.43	0.53
1:D:1495:ASN:O	1:D:1499:LEU:HB2	2.09	0.53
1:A:1422:PHE:CZ	2:A:1801:PCF:H321	2.43	0.53
1:B:236:PRO:O	1:B:240:ALA:HB3	2.08	0.53
1:C:912:LEU:O	1:C:916:LYS:CB	2.57	0.53
1:C:236:PRO:O	1:C:240:ALA:HB3	2.08	0.53
1:C:669:HIS:HD2	1:C:699:LEU:HD22	1.74	0.53
1:D:722:LYS:HB3	1:D:726:GLY:HA2	1.90	0.53
1:A:1495:ASN:O	1:A:1499:LEU:HB2	2.09	0.52
1:C:1532:TYR:CD1	2:C:1801:PCF:O31	2.61	0.52
1:D:170:TYR:O	1:D:174:ASP:CB	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:TYR:O	1:B:174:ASP:CB	2.58	0.52
1:D:743:LYS:HG3	1:D:778:LEU:HD21	1.91	0.52
1:B:462:VAL:O	1:B:463:ARG:NE	2.38	0.52
1:C:170:TYR:O	1:C:174:ASP:CB	2.58	0.52
1:C:810:LYS:O	1:C:814:GLN:CB	2.58	0.52
1:A:669:HIS:HD2	1:A:699:LEU:HD22	1.73	0.52
1:B:486:LEU:O	1:B:490:LYS:N	2.41	0.52
1:A:810:LYS:O	1:A:814:GLN:CB	2.58	0.52
1:D:912:LEU:O	1:D:916:LYS:CB	2.57	0.52
1:A:170:TYR:O	1:A:174:ASP:CB	2.58	0.52
1:A:912:LEU:O	1:A:916:LYS:CB	2.57	0.52
1:B:1174:THR:O	1:B:1178:LEU:HB3	2.10	0.52
1:C:1104:LYS:HE3	1:C:1133:GLU:HB3	1.90	0.52
1:C:1492:HIS:CE1	2:C:1803:PCF:C22	2.85	0.52
1:A:1532:TYR:OH	2:A:1803:PCF:C2	2.57	0.52
1:D:810:LYS:O	1:D:814:GLN:CB	2.58	0.52
1:D:544:ARG:NH1	1:D:587:GLN:OE1	2.43	0.52
1:A:544:ARG:NH1	1:A:587:GLN:OE1	2.43	0.52
1:B:538:PRO:O	1:B:542:ALA:HB2	2.10	0.52
1:C:734:ALA:HB1	1:C:767:ALA:HB2	1.92	0.52
1:C:1115:TRP:HD1	1:C:1145:PHE:HB2	1.75	0.52
1:C:1174:THR:O	1:C:1178:LEU:HB3	2.09	0.52
1:B:734:ALA:HB1	1:B:767:ALA:HB2	1.92	0.51
1:C:743:LYS:HG3	1:C:778:LEU:HD21	1.91	0.51
1:D:1174:THR:O	1:D:1178:LEU:HB3	2.09	0.51
1:A:743:LYS:HG3	1:A:778:LEU:HD21	1.91	0.51
1:B:743:LYS:HG3	1:B:778:LEU:HD21	1.91	0.51
1:B:1104:LYS:HE3	1:B:1133:GLU:HB3	1.90	0.51
1:C:538:PRO:O	1:C:542:ALA:HB2	2.10	0.51
1:C:1495:ASN:O	1:C:1499:LEU:HB2	2.09	0.51
1:A:249:CYS:O	1:A:253:LEU:CB	2.58	0.51
1:B:810:LYS:O	1:B:814:GLN:CB	2.58	0.51
1:B:1495:ASN:O	1:B:1499:LEU:HB2	2.09	0.51
1:D:249:CYS:O	1:D:253:LEU:CB	2.58	0.51
1:D:868:GLN:NE2	1:D:891:GLU:O	2.44	0.51
1:A:868:GLN:NE2	1:A:891:GLU:O	2.44	0.51
1:A:1174:THR:O	1:A:1178:LEU:HB3	2.09	0.51
1:B:868:GLN:NE2	1:B:891:GLU:O	2.44	0.51
1:B:1115:TRP:HD1	1:B:1145:PHE:HB2	1.75	0.51
1:D:538:PRO:O	1:D:542:ALA:HB2	2.10	0.51
1:B:544:ARG:NH1	1:B:587:GLN:OE1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:PRO:O	1:A:542:ALA:HB2	2.10	0.51
1:A:734:ALA:HB1	1:A:767:ALA:HB2	1.93	0.51
1:A:898:THR:OG1	1:A:901:HIS:ND1	2.36	0.51
2:A:1807:PCF:C34	2:A:1808:PCF:H221	2.41	0.51
1:B:638:MET:O	1:B:642:SER:CB	2.59	0.51
1:C:544:ARG:NH1	1:C:587:GLN:OE1	2.43	0.51
1:C:868:GLN:NE2	1:C:891:GLU:O	2.44	0.51
1:B:249:CYS:O	1:B:253:LEU:CB	2.58	0.51
1:C:638:MET:O	1:C:642:SER:CB	2.59	0.51
1:C:1282:PRO:O	1:C:1286:ILE:CG1	2.44	0.51
2:C:1805:PCF:C34	2:C:1806:PCF:H221	2.41	0.51
1:D:734:ALA:HB1	1:D:767:ALA:HB2	1.92	0.51
1:A:1554:ILE:HG12	1:B:1551:GLN:HB3	1.93	0.51
1:C:249:CYS:O	1:C:253:LEU:CB	2.58	0.51
2:D:1805:PCF:C34	2:D:1806:PCF:H221	2.41	0.51
1:D:253:LEU:O	1:D:257:THR:CB	2.59	0.51
1:A:1115:TRP:HD1	1:A:1145:PHE:HB2	1.75	0.51
1:C:368:GLY:HA2	1:D:490:LYS:HE2	1.93	0.51
2:A:1803:PCF:O14	1:D:1492:HIS:CB	2.59	0.50
1:C:756:LEU:HB3	1:C:760:LYS:HA	1.93	0.50
1:D:638:MET:O	1:D:642:SER:CB	2.59	0.50
1:D:756:LEU:HB3	1:D:760:LYS:HA	1.93	0.50
1:B:1370:LEU:HD23	1:B:1373:LEU:HD12	1.93	0.50
1:B:1554:ILE:HG12	1:C:1551:GLN:HB3	1.93	0.50
2:B:1804:PCF:C34	2:B:1805:PCF:H221	2.41	0.50
1:A:756:LEU:HB3	1:A:760:LYS:HA	1.93	0.50
1:B:582:LEU:HD11	1:B:611:ALA:HB1	1.94	0.50
1:B:1532:TYR:HE1	2:B:1808:PCF:H21	1.55	0.50
1:C:538:PRO:O	1:C:542:ALA:CB	2.60	0.50
1:D:582:LEU:HD11	1:D:611:ALA:HB1	1.94	0.50
1:D:1115:TRP:HD1	1:D:1145:PHE:HB2	1.75	0.50
1:D:1532:TYR:CG	2:D:1801:PCF:C22	2.89	0.50
1:C:253:LEU:O	1:C:257:THR:CB	2.59	0.50
1:C:486:LEU:O	1:C:490:LYS:N	2.41	0.50
1:C:1370:LEU:HD23	1:C:1373:LEU:HD12	1.94	0.50
1:D:538:PRO:O	1:D:542:ALA:CB	2.60	0.50
1:A:582:LEU:HD11	1:A:611:ALA:HB1	1.94	0.50
1:B:253:LEU:O	1:B:257:THR:CB	2.59	0.50
1:B:756:LEU:HB3	1:B:760:LYS:HA	1.93	0.50
1:A:398:ASN:HD22	1:A:402:ALA:HB3	1.77	0.50
1:A:538:PRO:O	1:A:542:ALA:CB	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:638:MET:O	1:A:642:SER:CB	2.59	0.50
1:D:398:ASN:HD22	1:D:402:ALA:HB3	1.77	0.50
1:C:582:LEU:HD11	1:C:611:ALA:HB1	1.94	0.50
1:C:1444:LEU:HD23	2:C:1806:PCF:H381	1.93	0.50
1:C:1532:TYR:CE1	2:C:1801:PCF:O31	2.65	0.50
1:A:253:LEU:O	1:A:257:THR:CB	2.59	0.50
1:B:398:ASN:HD22	1:B:402:ALA:HB3	1.77	0.50
1:B:1394:TRP:CH2	2:B:1801:PCF:H131	2.47	0.50
1:C:398:ASN:HD22	1:C:402:ALA:HB3	1.77	0.50
1:D:829:THR:H	1:D:832:HIS:HD2	1.60	0.49
1:D:1434:GLY:CA	2:D:1805:PCF:O14	2.60	0.49
1:A:829:THR:H	1:A:832:HIS:HD2	1.60	0.49
1:C:829:THR:H	1:C:832:HIS:HD2	1.60	0.49
1:B:538:PRO:O	1:B:542:ALA:CB	2.60	0.49
1:B:829:THR:H	1:B:832:HIS:HD2	1.60	0.49
1:B:1675:ALA:HB3	1:B:1677:TRP:CE2	2.48	0.49
1:C:1498:GLU:CB	2:D:1801:PCF:C36	2.90	0.49
1:D:168:ALA:O	1:D:172:ARG:CB	2.61	0.49
1:A:412:GLY:HA2	1:A:449:VAL:HG21	1.94	0.49
1:A:486:LEU:O	1:A:490:LYS:N	2.41	0.49
1:A:1675:ALA:HB3	1:A:1677:TRP:CE2	2.48	0.49
1:C:1528:TYR:CE2	2:C:1801:PCF:H131	2.38	0.49
1:D:412:GLY:HA2	1:D:449:VAL:HG21	1.94	0.49
1:D:1675:ALA:HB3	1:D:1677:TRP:CE2	2.48	0.49
1:B:168:ALA:O	1:B:172:ARG:CB	2.61	0.49
1:B:898:THR:OG1	1:B:901:HIS:ND1	2.36	0.49
1:A:168:ALA:O	1:A:172:ARG:CB	2.61	0.49
1:A:1370:LEU:HD23	1:A:1373:LEU:HD12	1.94	0.49
1:A:1492:HIS:ND1	2:A:1805:PCF:C11	2.75	0.49
2:A:1807:PCF:H291	1:B:1540:ILE:HG21	1.95	0.49
1:B:412:GLY:HA2	1:B:449:VAL:HG21	1.94	0.49
1:C:1403:GLN:NE2	1:D:1460:ALA:O	2.46	0.49
1:D:1394:TRP:CH2	2:D:1802:PCF:H131	2.48	0.49
1:C:1237:VAL:O	1:C:1241:ASN:N	2.44	0.49
1:D:1370:LEU:HD23	1:D:1373:LEU:HD12	1.94	0.49
1:D:1434:GLY:N	2:D:1805:PCF:O14	2.46	0.49
1:C:1441:ALA:CB	2:C:1806:PCF:H32	2.44	0.48
1:D:1237:VAL:O	1:D:1241:ASN:N	2.45	0.48
1:C:168:ALA:O	1:C:172:ARG:CB	2.61	0.48
1:A:1443:PHE:HE1	1:A:1549:LEU:HB3	1.79	0.48
1:B:1443:PHE:HE1	1:B:1549:LEU:HB3	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1808:PCF:O22	2:A:1808:PCF:H112	2.14	0.48
1:C:1126:LEU:O	1:C:1130:MET:CB	2.61	0.48
1:C:1675:ALA:HB3	1:C:1677:TRP:CE2	2.48	0.48
1:A:1126:LEU:O	1:A:1130:MET:CB	2.61	0.48
1:D:169:MET:O	1:D:173:GLU:CB	2.62	0.48
1:D:1126:LEU:O	1:D:1130:MET:CB	2.61	0.48
1:B:1492:HIS:CB	2:C:1801:PCF:O14	2.62	0.48
1:C:412:GLY:HA2	1:C:449:VAL:HG21	1.94	0.48
1:C:1443:PHE:HE1	1:C:1549:LEU:HB3	1.79	0.48
2:C:1806:PCF:O22	2:C:1806:PCF:H112	2.14	0.48
1:D:1532:TYR:CE1	2:D:1801:PCF:C22	2.93	0.48
2:D:1806:PCF:O22	2:D:1806:PCF:H112	2.14	0.48
1:A:272:LEU:O	1:A:276:ALA:HB2	2.14	0.48
1:C:1016:LEU:HA	1:C:1019:PHE:HD2	1.79	0.48
1:C:1410:LEU:HD11	1:D:1457:HIS:HB2	1.95	0.48
1:B:409:ALA:HB1	1:B:441:ALA:HB2	1.96	0.47
1:B:1237:VAL:O	1:B:1241:ASN:N	2.44	0.47
1:C:169:MET:O	1:C:173:GLU:CB	2.62	0.47
1:D:898:THR:OG1	1:D:901:HIS:ND1	2.36	0.47
1:D:1532:TYR:CE2	2:D:1801:PCF:O22	2.66	0.47
1:D:1532:TYR:OH	2:D:1801:PCF:C2	2.60	0.47
1:A:1492:HIS:CG	2:B:1808:PCF:O14	2.67	0.47
2:B:1805:PCF:O22	2:B:1805:PCF:H112	2.14	0.47
1:D:272:LEU:O	1:D:276:ALA:HB2	2.14	0.47
1:D:1437:LEU:HB3	2:D:1806:PCF:C22	2.36	0.47
1:D:1443:PHE:HE1	1:D:1549:LEU:HB3	1.79	0.47
1:B:1126:LEU:O	1:B:1130:MET:CB	2.61	0.47
1:B:1377:ALA:O	1:B:1381:VAL:N	2.48	0.47
1:A:1377:ALA:O	1:A:1381:VAL:N	2.48	0.47
1:B:893:ASN:H	1:B:897:PHE:H	1.62	0.47
1:C:1162:GLN:HE22	1:C:1688:VAL:HG11	1.80	0.47
1:C:1492:HIS:CB	2:D:1801:PCF:O14	2.62	0.47
1:A:169:MET:O	1:A:173:GLU:CB	2.62	0.47
1:B:272:LEU:O	1:B:276:ALA:HB2	2.14	0.47
1:B:1016:LEU:HA	1:B:1019:PHE:HD2	1.79	0.47
1:C:1377:ALA:O	1:C:1381:VAL:N	2.48	0.47
1:D:409:ALA:HB1	1:D:441:ALA:HB2	1.96	0.47
1:D:1377:ALA:O	1:D:1381:VAL:N	2.48	0.47
1:A:236:PRO:O	1:A:240:ALA:CB	2.63	0.47
1:A:1237:VAL:O	1:A:1241:ASN:N	2.45	0.47
1:D:236:PRO:O	1:D:240:ALA:CB	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:638:MET:O	1:D:642:SER:HB3	2.15	0.47
1:D:893:ASN:HB2	1:D:896:GLY:H	1.79	0.47
1:D:1016:LEU:HA	1:D:1019:PHE:HD2	1.79	0.47
1:B:169:MET:O	1:B:173:GLU:CB	2.62	0.47
1:B:1256:LEU:HD21	1:B:1577:SER:HA	1.97	0.47
1:B:1492:HIS:HD2	1:B:1494:ILE:HG22	1.80	0.47
1:C:272:LEU:O	1:C:276:ALA:HB2	2.14	0.47
1:C:1290:PHE:HB3	1:C:1292:MET:HG3	1.97	0.47
1:D:1162:GLN:HE22	1:D:1688:VAL:HG11	1.80	0.47
1:A:1016:LEU:HA	1:A:1019:PHE:HD2	1.79	0.47
1:A:1256:LEU:HD21	1:A:1577:SER:HA	1.97	0.47
1:A:1290:PHE:HB3	1:A:1292:MET:HG3	1.97	0.47
1:B:1561:TYR:CZ	1:C:1556:MET:HG2	2.49	0.47
1:C:1492:HIS:HD2	1:C:1494:ILE:HG22	1.80	0.47
1:C:1493:PRO:HG3	2:C:1803:PCF:H12	1.97	0.47
1:D:1492:HIS:HE1	2:D:1803:PCF:H222	1.73	0.47
1:A:474:ILE:HG12	1:A:477:ARG:HH12	1.80	0.47
1:A:638:MET:O	1:A:642:SER:HB3	2.15	0.47
1:A:763:PRO:O	1:A:767:ALA:HB2	2.15	0.47
1:B:1162:GLN:HE22	1:B:1688:VAL:HG11	1.80	0.47
1:D:1290:PHE:HB3	1:D:1292:MET:HG3	1.97	0.47
1:A:744:PHE:O	1:A:748:ASP:CB	2.63	0.46
1:A:893:ASN:H	1:A:897:PHE:H	1.62	0.46
1:B:236:PRO:O	1:B:240:ALA:CB	2.63	0.46
1:B:1504:VAL:HG22	1:B:1550:ILE:HD11	1.97	0.46
2:D:1805:PCF:O22	2:D:1805:PCF:H11	2.15	0.46
1:A:409:ALA:HB1	1:A:441:ALA:HB2	1.96	0.46
1:C:421:LEU:HD11	1:C:427:VAL:HG13	1.97	0.46
1:C:638:MET:O	1:C:642:SER:HB3	2.15	0.46
1:D:421:LEU:HD11	1:D:427:VAL:HG13	1.97	0.46
1:A:893:ASN:HB2	1:A:896:GLY:H	1.79	0.46
1:B:763:PRO:O	1:B:767:ALA:HB2	2.15	0.46
2:B:1804:PCF:H11	2:B:1804:PCF:O22	2.15	0.46
1:D:744:PHE:O	1:D:748:ASP:CB	2.63	0.46
1:A:1236:ASP:OD1	1:A:1581:ARG:NH1	2.49	0.46
1:A:1492:HIS:HD2	1:A:1494:ILE:HG22	1.80	0.46
1:A:1504:VAL:HG22	1:A:1550:ILE:HD11	1.97	0.46
1:D:1492:HIS:HD2	1:D:1494:ILE:HG22	1.80	0.46
1:A:435:TYR:HD1	1:A:439:HIS:HB3	1.81	0.46
1:C:236:PRO:O	1:C:240:ALA:CB	2.63	0.46
1:C:252:LEU:O	1:C:256:GLN:CB	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:HIS:O	1:C:377:LEU:N	2.49	0.46
1:C:409:ALA:HB1	1:C:441:ALA:HB2	1.96	0.46
1:C:744:PHE:O	1:C:748:ASP:CB	2.63	0.46
1:C:763:PRO:O	1:C:767:ALA:HB2	2.15	0.46
1:C:474:ILE:HG12	1:C:477:ARG:HH12	1.80	0.46
1:C:893:ASN:H	1:C:897:PHE:H	1.63	0.46
1:D:763:PRO:O	1:D:767:ALA:HB2	2.15	0.46
1:B:744:PHE:O	1:B:748:ASP:CB	2.63	0.46
1:B:893:ASN:HB2	1:B:896:GLY:H	1.79	0.46
1:B:1290:PHE:HB3	1:B:1292:MET:HG3	1.97	0.46
1:D:1504:VAL:HG22	1:D:1550:ILE:HD11	1.97	0.46
1:A:1162:GLN:HE22	1:A:1688:VAL:HG11	1.80	0.46
1:B:474:ILE:HG12	1:B:477:ARG:HH12	1.80	0.46
1:B:1236:ASP:OD1	1:B:1581:ARG:NH1	2.49	0.46
1:C:1236:ASP:OD1	1:C:1581:ARG:NH1	2.49	0.46
1:A:1489:VAL:HG23	2:A:1805:PCF:C13	2.25	0.46
1:D:252:LEU:O	1:D:256:GLN:CB	2.64	0.46
1:D:373:HIS:O	1:D:377:LEU:N	2.49	0.46
1:D:893:ASN:H	1:D:897:PHE:H	1.62	0.46
1:A:252:LEU:O	1:A:256:GLN:CB	2.64	0.46
1:A:421:LEU:HD11	1:A:427:VAL:HG13	1.97	0.46
1:B:142:ILE:O	1:B:146:MET:N	2.42	0.46
1:B:201:LEU:O	1:B:205:ARG:CB	2.64	0.46
1:B:1425:LEU:O	1:C:1442:ARG:NE	2.46	0.46
1:C:893:ASN:HB2	1:C:896:GLY:H	1.79	0.46
1:D:201:LEU:O	1:D:205:ARG:CB	2.64	0.46
1:D:1236:ASP:OD1	1:D:1581:ARG:NH1	2.49	0.46
1:D:1256:LEU:HD21	1:D:1577:SER:HA	1.97	0.46
1:A:1073:THR:HB	1:A:1077:GLY:HA2	1.98	0.45
1:A:1279:ILE:HD11	1:A:1312:ILE:HG21	1.99	0.45
1:B:421:LEU:HD11	1:B:427:VAL:HG13	1.97	0.45
1:B:697:LEU:O	1:B:701:ALA:CB	2.64	0.45
1:C:582:LEU:O	1:C:585:THR:OG1	2.29	0.45
1:C:697:LEU:O	1:C:701:ALA:CB	2.64	0.45
1:D:474:ILE:HG12	1:D:477:ARG:HH12	1.80	0.45
1:B:638:MET:O	1:B:642:SER:HB3	2.15	0.45
1:C:435:TYR:HD1	1:C:439:HIS:HB3	1.81	0.45
1:D:307:ILE:O	1:D:311:GLU:CB	2.65	0.45
1:A:737:GLY:HA2	1:A:775:VAL:HG21	1.98	0.45
2:A:1807:PCF:O22	2:A:1807:PCF:H11	2.15	0.45
1:B:284:VAL:O	1:B:288:VAL:CB	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:435:TYR:HD1	1:D:439:HIS:HB3	1.81	0.45
1:A:307:ILE:O	1:A:311:GLU:CB	2.65	0.45
1:A:697:LEU:O	1:A:701:ALA:CB	2.64	0.45
1:A:1457:HIS:HB2	1:D:1410:LEU:HD11	1.98	0.45
1:B:252:LEU:O	1:B:256:GLN:CB	2.64	0.45
1:C:307:ILE:O	1:C:311:GLU:CB	2.65	0.45
2:C:1805:PCF:O22	2:C:1805:PCF:H11	2.15	0.45
1:D:284:VAL:O	1:D:288:VAL:CB	2.65	0.45
1:A:284:VAL:O	1:A:288:VAL:CB	2.65	0.45
1:C:1088:GLY:HA3	1:C:1122:HIS:CD2	2.52	0.45
1:D:737:GLY:HA2	1:D:775:VAL:HG21	1.98	0.45
1:D:1436:LEU:HD22	1:D:1557:MET:HG2	1.99	0.45
1:A:201:LEU:O	1:A:205:ARG:CB	2.64	0.45
1:A:980:HIS:CE1	1:A:1005:ALA:HB1	2.52	0.45
1:B:307:ILE:O	1:B:311:GLU:CB	2.65	0.45
1:B:1279:ILE:HD11	1:B:1312:ILE:HG21	1.99	0.45
1:C:1256:LEU:HD21	1:C:1577:SER:HA	1.97	0.45
1:A:1403:GLN:NE2	1:B:1460:ALA:O	2.49	0.45
1:C:284:VAL:O	1:C:288:VAL:CB	2.65	0.45
1:C:980:HIS:CE1	1:C:1005:ALA:HB1	2.52	0.45
1:C:1436:LEU:HD22	1:C:1557:MET:HG2	1.99	0.45
1:C:1504:VAL:HG22	1:C:1550:ILE:HD11	1.97	0.45
1:D:161:TYR:HA	1:D:167:ALA:HA	1.99	0.45
1:D:697:LEU:O	1:D:701:ALA:CB	2.64	0.45
1:A:1436:LEU:HD22	1:A:1557:MET:HG2	1.99	0.45
1:B:1073:THR:HB	1:B:1077:GLY:HA2	1.98	0.45
1:C:1279:ILE:HD11	1:C:1312:ILE:HG21	1.98	0.45
1:D:1150:MET:HG3	1:D:1196:LEU:HD23	1.99	0.45
1:D:1279:ILE:HD11	1:D:1312:ILE:HG21	1.98	0.45
1:B:737:GLY:HA2	1:B:775:VAL:HG21	1.98	0.45
1:B:1088:GLY:HA3	1:B:1122:HIS:CD2	2.52	0.45
1:C:161:TYR:HA	1:C:167:ALA:HA	1.99	0.45
1:C:713:LEU:HD21	1:C:719:ILE:HG23	1.99	0.45
1:C:737:GLY:HA2	1:C:775:VAL:HG21	1.98	0.45
1:D:980:HIS:CE1	1:D:1005:ALA:HB1	2.52	0.45
1:A:1150:MET:HG3	1:A:1196:LEU:HD23	1.99	0.45
1:C:201:LEU:O	1:C:205:ARG:CB	2.64	0.45
1:C:1437:LEU:HD13	2:C:1805:PCF:H341	1.99	0.45
1:A:373:HIS:O	1:A:377:LEU:N	2.49	0.44
1:D:1073:THR:HB	1:D:1077:GLY:HA2	1.98	0.44
1:A:713:LEU:HD21	1:A:719:ILE:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1088:GLY:HA3	1:A:1122:HIS:CD2	2.52	0.44
1:B:1324:THR:HG21	2:C:1803:PCF:O32	2.18	0.44
1:B:1434:GLY:CA	2:B:1804:PCF:O14	2.66	0.44
1:B:1495:ASN:O	1:B:1499:LEU:CB	2.65	0.44
1:C:1306:SER:O	1:C:1310:SER:CB	2.66	0.44
1:A:1306:SER:O	1:A:1310:SER:CB	2.66	0.44
1:A:1436:LEU:HD23	1:A:1436:LEU:HA	1.87	0.44
2:A:1805:PCF:O32	1:D:1324:THR:HG21	2.18	0.44
1:B:1150:MET:HG3	1:B:1196:LEU:HD23	1.99	0.44
1:D:1088:GLY:HA3	1:D:1122:HIS:CD2	2.52	0.44
1:D:1244:LYS:HA	1:D:1247:ILE:HG22	2.00	0.44
1:D:1433:ILE:HG21	2:D:1805:PCF:O22	2.17	0.44
1:A:161:TYR:HA	1:A:167:ALA:HA	1.99	0.44
1:B:435:TYR:HD1	1:B:439:HIS:HB3	1.81	0.44
1:B:1436:LEU:HD22	1:B:1557:MET:HG2	1.99	0.44
1:D:1221:GLY:O	1:D:1225:GLN:CB	2.66	0.44
1:B:161:TYR:HA	1:B:167:ALA:HA	1.99	0.44
1:B:1221:GLY:O	1:B:1225:GLN:CB	2.66	0.44
1:C:1244:LYS:HA	1:C:1247:ILE:HG22	2.00	0.44
1:C:1495:ASN:O	1:C:1499:LEU:CB	2.65	0.44
1:A:1221:GLY:O	1:A:1225:GLN:CB	2.66	0.44
1:B:980:HIS:CE1	1:B:1005:ALA:HB1	2.52	0.44
1:C:1073:THR:HB	1:C:1077:GLY:HA2	1.98	0.44
1:C:1150:MET:HG3	1:C:1196:LEU:HD23	1.99	0.44
1:B:373:HIS:O	1:B:377:LEU:N	2.49	0.44
1:D:1365:GLY:O	1:D:1368:LYS:HB2	2.18	0.44
1:D:1495:ASN:O	1:D:1499:LEU:CB	2.65	0.44
1:B:1503:ALA:HB3	1:B:1541:TYR:HE2	1.83	0.44
1:C:1324:THR:HG21	2:D:1803:PCF:O32	2.18	0.44
1:C:1441:ALA:HB1	2:C:1806:PCF:H32	2.00	0.44
1:A:934:HIS:CE1	1:A:958:SER:HB3	2.53	0.43
1:B:713:LEU:HD21	1:B:719:ILE:HG23	1.99	0.43
1:B:934:HIS:CE1	1:B:958:SER:HB3	2.53	0.43
1:B:1403:GLN:NE2	1:C:1460:ALA:O	2.51	0.43
1:A:880:LYS:O	1:A:884:ARG:CB	2.66	0.43
1:A:1324:THR:HG21	2:B:1802:PCF:O32	2.18	0.43
1:A:1365:GLY:O	1:A:1368:LYS:HB2	2.18	0.43
1:B:880:LYS:O	1:B:884:ARG:CB	2.66	0.43
1:B:1008:GLU:O	1:B:1042:ARG:NH1	2.49	0.43
1:D:1503:ALA:HB3	1:D:1541:TYR:HE2	1.83	0.43
1:A:1492:HIS:CD2	1:A:1494:ILE:HG22	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1495:ASN:O	1:A:1499:LEU:CB	2.65	0.43
1:B:763:PRO:O	1:B:767:ALA:CB	2.66	0.43
2:A:1808:PCF:H332	2:A:1808:PCF:C3	2.48	0.43
1:C:1221:GLY:O	1:C:1225:GLN:CB	2.66	0.43
1:D:510:ALA:HB1	1:D:542:ALA:HB2	2.00	0.43
1:D:713:LEU:HD21	1:D:719:ILE:HG23	1.99	0.43
1:D:992:ARG:HE	1:D:1028:LEU:HD21	1.83	0.43
1:A:510:ALA:HB1	1:A:542:ALA:HB2	2.00	0.43
1:B:1282:PRO:N	1:B:1283:PRO:CD	2.82	0.43
1:B:1306:SER:O	1:B:1310:SER:CB	2.66	0.43
1:C:763:PRO:O	1:C:767:ALA:CB	2.66	0.43
1:C:1365:GLY:O	1:C:1368:LYS:HB2	2.18	0.43
1:B:582:LEU:O	1:B:585:THR:OG1	2.29	0.43
1:B:1365:GLY:O	1:B:1368:LYS:HB2	2.18	0.43
1:D:285:ARG:O	1:D:289:ASP:CB	2.67	0.43
1:A:271:ALA:O	1:A:275:ALA:CB	2.67	0.43
1:A:285:ARG:O	1:A:289:ASP:CB	2.67	0.43
1:B:283:MET:O	1:B:287:LEU:CB	2.67	0.43
1:B:1244:LYS:HA	1:B:1247:ILE:HG22	2.00	0.43
1:C:283:MET:O	1:C:287:LEU:CB	2.67	0.43
1:C:992:ARG:HE	1:C:1028:LEU:HD21	1.83	0.43
1:D:763:PRO:O	1:D:767:ALA:CB	2.66	0.43
1:D:1306:SER:O	1:D:1310:SER:CB	2.66	0.43
1:A:1244:LYS:HA	1:A:1247:ILE:HG22	2.00	0.43
1:B:578:GLY:HA3	1:B:618:LYS:H	1.84	0.43
1:C:1501:PHE:HZ	1:D:1543:LEU:HD12	1.84	0.43
1:D:880:LYS:O	1:D:884:ARG:CB	2.66	0.43
1:D:1282:PRO:N	1:D:1283:PRO:CD	2.82	0.43
1:A:697:LEU:O	1:A:701:ALA:HB3	2.19	0.43
1:A:763:PRO:O	1:A:767:ALA:CB	2.66	0.43
1:B:271:ALA:O	1:B:275:ALA:CB	2.67	0.43
2:B:1805:PCF:H332	2:B:1805:PCF:C3	2.48	0.43
1:C:271:ALA:O	1:C:275:ALA:CB	2.67	0.43
1:C:1503:ALA:HB3	1:C:1541:TYR:HE2	1.83	0.43
1:D:142:ILE:O	1:D:146:MET:N	2.42	0.43
1:D:844:GLU:O	1:D:848:LYS:CB	2.67	0.43
1:A:1503:ALA:HB3	1:A:1541:TYR:HE2	1.83	0.43
1:C:844:GLU:O	1:C:848:LYS:CB	2.67	0.43
1:D:271:ALA:O	1:D:275:ALA:CB	2.67	0.43
1:A:283:MET:O	1:A:287:LEU:CB	2.67	0.42
1:A:578:GLY:HA3	1:A:618:LYS:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:623:THR:OG1	1:B:624:ALA:N	2.52	0.42
1:B:645:ASN:HB2	1:B:649:ILE:HG13	2.01	0.42
1:B:844:GLU:O	1:B:848:LYS:CB	2.67	0.42
1:C:510:ALA:HB1	1:C:542:ALA:HB2	2.00	0.42
1:C:623:THR:OG1	1:C:624:ALA:N	2.52	0.42
1:C:1492:HIS:CD2	1:C:1494:ILE:HG22	2.53	0.42
1:A:603:VAL:HG21	1:A:637:LEU:HD22	2.01	0.42
1:C:697:LEU:O	1:C:701:ALA:HB3	2.19	0.42
1:D:934:HIS:CE1	1:D:958:SER:HB3	2.53	0.42
1:D:1492:HIS:CD2	1:D:1494:ILE:HG22	2.53	0.42
1:A:992:ARG:HE	1:A:1028:LEU:HD21	1.83	0.42
1:A:1282:PRO:N	1:A:1283:PRO:CD	2.82	0.42
1:B:285:ARG:O	1:B:289:ASP:CB	2.67	0.42
1:C:898:THR:OG1	1:C:901:HIS:ND1	2.36	0.42
1:C:934:HIS:CE1	1:C:958:SER:HB3	2.53	0.42
1:C:1282:PRO:N	1:C:1283:PRO:CD	2.82	0.42
1:D:1464:SER:HB3	1:D:1490:ARG:HH11	1.84	0.42
1:A:623:THR:OG1	1:A:624:ALA:N	2.52	0.42
1:A:645:ASN:HB2	1:A:649:ILE:HG13	2.01	0.42
1:B:697:LEU:O	1:B:701:ALA:HB3	2.19	0.42
1:C:880:LYS:O	1:C:884:ARG:CB	2.66	0.42
1:C:1053:MET:HB3	1:C:1083:CYS:HB3	2.02	0.42
1:D:370:THR:HB	1:D:373:HIS:CD2	2.54	0.42
1:D:623:THR:OG1	1:D:624:ALA:N	2.52	0.42
1:A:1464:SER:HB3	1:A:1490:ARG:HH11	1.85	0.42
1:D:283:MET:O	1:D:287:LEU:CB	2.67	0.42
1:D:697:LEU:O	1:D:701:ALA:HB3	2.19	0.42
1:B:992:ARG:HE	1:B:1028:LEU:HD21	1.83	0.42
1:B:1180:ASN:HB2	1:B:1241:ASN:OD1	2.20	0.42
1:B:1282:PRO:HD2	1:B:1283:PRO:HD3	2.01	0.42
1:B:1545:SER:OG	1:B:1546:VAL:N	2.53	0.42
2:B:1808:PCF:H132	2:B:1808:PCF:H112	1.84	0.42
1:C:1464:SER:HB3	1:C:1490:ARG:HH11	1.85	0.42
1:A:1008:GLU:O	1:A:1042:ARG:NH1	2.49	0.42
1:A:1053:MET:HB3	1:A:1083:CYS:HB3	2.02	0.42
1:A:1180:ASN:HB2	1:A:1241:ASN:OD1	2.20	0.42
1:C:578:GLY:HA3	1:C:618:LYS:H	1.84	0.42
1:D:614:THR:OG1	1:D:615:LEU:N	2.53	0.42
1:B:1492:HIS:CD2	1:B:1494:ILE:HG22	2.53	0.42
1:C:285:ARG:O	1:C:289:ASP:CB	2.67	0.42
1:C:1180:ASN:HB2	1:C:1241:ASN:OD1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1282:PRO:HD2	1:C:1283:PRO:HD3	2.01	0.42
1:D:645:ASN:HB2	1:D:649:ILE:HG13	2.01	0.42
1:A:395:HIS:CD2	1:B:457:GLY:HA2	2.55	0.42
1:A:844:GLU:O	1:A:848:LYS:CB	2.67	0.42
1:B:510:ALA:HB1	1:B:542:ALA:HB2	2.00	0.42
1:D:603:VAL:HG21	1:D:637:LEU:HD22	2.01	0.42
2:D:1801:PCF:H322	2:D:1801:PCF:H31	1.85	0.42
1:A:1382:HIS:O	1:A:1385:ALA:HB3	2.20	0.42
1:C:1545:SER:OG	1:C:1546:VAL:N	2.53	0.42
1:D:248:MET:O	1:D:252:LEU:CB	2.68	0.42
1:D:1540:ILE:HG12	2:D:1801:PCF:H412	2.02	0.42
1:D:1545:SER:OG	1:D:1546:VAL:N	2.53	0.42
2:D:1806:PCF:H332	2:D:1806:PCF:C3	2.48	0.42
1:A:580:THR:H	1:A:583:HIS:HD2	1.67	0.41
1:A:582:LEU:O	1:A:585:THR:OG1	2.29	0.41
1:A:1532:TYR:HH	2:A:1803:PCF:C1	2.32	0.41
1:B:603:VAL:HG21	1:B:637:LEU:HD22	2.01	0.41
1:C:1382:HIS:O	1:C:1385:ALA:HB3	2.20	0.41
1:C:1532:TYR:OH	2:C:1801:PCF:C1	2.66	0.41
2:C:1803:PCF:H112	2:C:1803:PCF:H132	1.84	0.41
1:D:1008:GLU:O	1:D:1042:ARG:NH1	2.49	0.41
1:D:1532:TYR:OH	2:D:1801:PCF:O11	2.34	0.41
1:A:614:THR:OG1	1:A:615:LEU:N	2.53	0.41
1:A:1282:PRO:HD2	1:A:1283:PRO:HD3	2.01	0.41
1:B:337:PRO:O	1:B:341:ALA:CB	2.68	0.41
1:C:337:PRO:O	1:C:341:ALA:CB	2.68	0.41
1:C:614:THR:OG1	1:C:615:LEU:N	2.53	0.41
1:C:1436:LEU:HD23	1:C:1436:LEU:HA	1.87	0.41
2:D:1807:PCF:H332	2:D:1807:PCF:C3	2.50	0.41
1:A:248:MET:O	1:A:252:LEU:CB	2.68	0.41
1:A:1547:VAL:HG23	1:D:1505:PHE:HE1	1.85	0.41
1:D:578:GLY:HA3	1:D:618:LYS:H	1.84	0.41
1:B:248:MET:O	1:B:252:LEU:CB	2.68	0.41
1:B:1434:GLY:N	2:B:1804:PCF:O14	2.53	0.41
1:C:248:MET:O	1:C:252:LEU:CB	2.68	0.41
1:C:840:VAL:HA	1:C:843:ILE:HG22	2.02	0.41
2:C:1806:PCF:H332	2:C:1806:PCF:C3	2.48	0.41
1:D:337:PRO:O	1:D:341:ALA:CB	2.68	0.41
1:D:840:VAL:HA	1:D:843:ILE:HG22	2.02	0.41
1:D:1382:HIS:O	1:D:1385:ALA:HB3	2.20	0.41
1:B:1432:ILE:HG21	1:B:1561:TYR:HD1	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1464:SER:HB3	1:B:1490:ARG:HH11	1.84	0.41
1:C:645:ASN:HB2	1:C:649:ILE:HG13	2.01	0.41
1:C:1432:ILE:HG21	1:C:1561:TYR:HD1	1.85	0.41
2:C:1803:PCF:P	2:C:1803:PCF:O22	2.79	0.41
1:A:790:ASP:H	1:A:794:GLN:H	1.69	0.41
1:B:580:THR:H	1:B:583:HIS:HD2	1.67	0.41
1:D:1053:MET:HB3	1:D:1083:CYS:HB3	2.02	0.41
1:A:1545:SER:OG	1:A:1546:VAL:N	2.53	0.41
2:B:1804:PCF:H332	2:B:1804:PCF:C3	2.51	0.41
1:C:790:ASP:H	1:C:794:GLN:H	1.69	0.41
1:D:1432:ILE:HG21	1:D:1561:TYR:HD1	1.85	0.41
1:A:722:LYS:NZ	1:D:1031:SER:O	2.32	0.41
1:B:1436:LEU:HA	1:B:1436:LEU:HD23	1.86	0.41
2:B:1808:PCF:H322	2:B:1808:PCF:H31	1.85	0.41
1:A:337:PRO:O	1:A:341:ALA:CB	2.68	0.41
1:A:840:VAL:HA	1:A:843:ILE:HG22	2.02	0.41
1:A:1432:ILE:HG21	1:A:1561:TYR:HD1	1.85	0.41
1:A:1561:TYR:CZ	1:B:1556:MET:HG2	2.56	0.41
2:A:1801:PCF:C3	2:A:1801:PCF:H332	2.50	0.41
2:A:1807:PCF:H332	2:A:1807:PCF:C3	2.51	0.41
1:B:614:THR:OG1	1:B:615:LEU:N	2.53	0.41
1:B:790:ASP:H	1:B:794:GLN:H	1.69	0.41
1:B:1031:SER:O	1:C:722:LYS:NZ	2.36	0.41
1:B:1382:HIS:O	1:B:1385:ALA:HB3	2.20	0.41
1:B:1422:PHE:CZ	2:B:1806:PCF:H322	2.56	0.41
1:B:1492:HIS:NE2	2:B:1802:PCF:H222	2.36	0.41
2:B:1802:PCF:O22	2:B:1802:PCF:P	2.79	0.41
1:C:603:VAL:HG21	1:C:637:LEU:HD22	2.02	0.41
1:D:790:ASP:H	1:D:794:GLN:H	1.69	0.41
1:D:1180:ASN:HB2	1:D:1241:ASN:OD1	2.20	0.41
1:D:1282:PRO:HD2	1:D:1283:PRO:HD3	2.01	0.41
1:D:1536:ILE:HD11	2:D:1801:PCF:C27	2.50	0.41
2:D:1801:PCF:H132	2:D:1801:PCF:H112	1.84	0.41
1:A:1532:TYR:CE1	2:A:1803:PCF:C1	3.03	0.41
2:A:1803:PCF:H112	2:A:1803:PCF:H132	1.84	0.41
1:B:713:LEU:HD23	1:B:713:LEU:HA	1.94	0.41
1:B:840:VAL:HA	1:B:843:ILE:HG22	2.02	0.41
1:B:1053:MET:HB3	1:B:1083:CYS:HB3	2.02	0.41
1:B:1294:HIS:CE1	1:B:1298:LYS:HG3	2.56	0.41
2:A:1805:PCF:P	2:A:1805:PCF:O22	2.79	0.40
2:B:1806:PCF:H332	2:B:1806:PCF:C3	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:ILE:O	1:C:146:MET:N	2.42	0.40
2:A:1805:PCF:H132	2:A:1805:PCF:H112	1.84	0.40
2:B:1802:PCF:H112	2:B:1802:PCF:H132	1.84	0.40
1:D:1294:HIS:CE1	1:D:1298:LYS:HG3	2.56	0.40
1:A:1498:GLU:CB	2:B:1808:PCF:O32	2.69	0.40
2:A:1803:PCF:O14	1:D:1492:HIS:CG	2.75	0.40
1:B:977:THR:H	1:B:980:HIS:HD2	1.69	0.40
1:C:977:THR:H	1:C:980:HIS:HD2	1.69	0.40
2:C:1805:PCF:H332	2:C:1805:PCF:C3	2.51	0.40
1:D:977:THR:H	1:D:980:HIS:HD2	1.70	0.40
1:A:1543:LEU:HD12	1:D:1501:PHE:HZ	1.86	0.40
1:C:397:PRO:HG2	1:D:491:SER:HB3	2.04	0.40
2:D:1803:PCF:O22	2:D:1803:PCF:P	2.79	0.40
1:A:1294:HIS:CE1	1:A:1298:LYS:HG3	2.56	0.40
1:A:1532:TYR:CD1	2:A:1803:PCF:O31	2.75	0.40
1:B:237:LEU:O	1:B:241:VAL:CB	2.70	0.40
2:C:1807:PCF:C3	2:C:1807:PCF:H332	2.50	0.40
1:D:237:LEU:O	1:D:241:VAL:CB	2.70	0.40
1:D:309:ALA:HB1	1:D:341:ALA:HB2	2.04	0.40
1:D:580:THR:H	1:D:583:HIS:HD2	1.67	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1495/1732 (86%)	1357 (91%)	133 (9%)	5 (0%)	41	74
1	B	1495/1732 (86%)	1357 (91%)	133 (9%)	5 (0%)	41	74
1	C	1495/1732 (86%)	1357 (91%)	133 (9%)	5 (0%)	41	74
1	D	1495/1732 (86%)	1357 (91%)	133 (9%)	5 (0%)	41	74
All	All	5980/6928 (86%)	5428 (91%)	532 (9%)	20 (0%)	44	74

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	987	ASN
1	B	987	ASN
1	C	987	ASN
1	D	987	ASN
1	A	371	LEU
1	A	1295	LYS
1	B	371	LEU
1	B	462	VAL
1	B	1295	LYS
1	C	371	LEU
1	C	462	VAL
1	C	1295	LYS
1	D	371	LEU
1	D	1295	LYS
1	A	462	VAL
1	A	1294	HIS
1	B	1294	HIS
1	C	1294	HIS
1	D	462	VAL
1	D	1294	HIS

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	836/1421 (59%)	825 (99%)	11 (1%)	69	87
1	B	836/1421 (59%)	825 (99%)	11 (1%)	69	87
1	C	836/1421 (59%)	825 (99%)	11 (1%)	69	87
1	D	836/1421 (59%)	825 (99%)	11 (1%)	69	87
All	All	3344/5684 (59%)	3300 (99%)	44 (1%)	70	87

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	621	LEU
1	A	654	ASN
1	A	682	ASN
1	A	854	VAL
1	A	1063	LEU
1	A	1192	ARG
1	A	1235	LEU
1	A	1292	MET
1	A	1297	ASN
1	A	1331	ARG
1	A	1670	ARG
1	B	621	LEU
1	B	654	ASN
1	B	682	ASN
1	B	854	VAL
1	B	1063	LEU
1	B	1192	ARG
1	B	1235	LEU
1	B	1292	MET
1	B	1297	ASN
1	B	1331	ARG
1	B	1670	ARG
1	C	621	LEU
1	C	654	ASN
1	C	682	ASN
1	C	854	VAL
1	C	1063	LEU
1	C	1192	ARG
1	C	1235	LEU
1	C	1292	MET
1	C	1297	ASN
1	C	1331	ARG
1	C	1670	ARG
1	D	621	LEU
1	D	654	ASN
1	D	682	ASN
1	D	854	VAL
1	D	1063	LEU
1	D	1192	ARG
1	D	1235	LEU
1	D	1292	MET
1	D	1297	ASN
1	D	1331	ARG

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Mol	Chain	Res	Type
1	D	1670	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	398	ASN
1	A	514	ASN
1	A	654	ASN
1	A	669	HIS
1	A	832	HIS
1	A	837	GLN
1	A	980	HIS
1	A	1162	GLN
1	A	1241	ASN
1	A	1243	GLN
1	A	1253	GLN
1	A	1297	ASN
1	A	1403	GLN
1	A	1423	HIS
1	B	398	ASN
1	B	514	ASN
1	B	654	ASN
1	B	669	HIS
1	B	832	HIS
1	B	837	GLN
1	B	980	HIS
1	B	1162	GLN
1	B	1241	ASN
1	B	1243	GLN
1	B	1253	GLN
1	B	1297	ASN
1	B	1423	HIS
1	C	398	ASN
1	C	514	ASN
1	C	654	ASN
1	C	669	HIS
1	C	832	HIS
1	C	837	GLN
1	C	980	HIS
1	C	1162	GLN
1	C	1241	ASN
1	C	1243	GLN

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Mol	Chain	Res	Type
1	C	1253	GLN
1	C	1297	ASN
1	C	1423	HIS
1	D	398	ASN
1	D	514	ASN
1	D	654	ASN
1	D	669	HIS
1	D	832	HIS
1	D	837	GLN
1	D	980	HIS
1	D	1162	GLN
1	D	1241	ASN
1	D	1243	GLN
1	D	1253	GLN
1	D	1297	ASN
1	D	1423	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

32 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	PCF	D	1807	-	36,36,49	0.68	0	40,41,57	1.01	2 (5%)
2	PCF	B	1808	-	41,41,49	0.64	0	47,49,57	0.86	0
2	PCF	D	1803	-	34,34,49	0.69	0	40,42,57	0.91	1 (2%)
2	PCF	B	1805	-	31,31,49	0.87	1 (3%)	37,39,57	1.10	2 (5%)
2	PCF	A	1808	-	31,31,49	0.87	1 (3%)	37,39,57	1.10	2 (5%)
2	PCF	D	1808	-	27,27,49	0.78	0	31,32,57	1.01	1 (3%)
2	PCF	C	1806	-	31,31,49	0.88	1 (3%)	37,39,57	1.10	2 (5%)
2	PCF	B	1804	-	29,29,49	0.74	0	33,34,57	1.07	2 (6%)
2	PCF	C	1802	-	35,35,49	0.69	0	41,43,57	0.92	1 (2%)
2	PCF	A	1804	-	35,35,49	0.68	0	41,43,57	0.92	1 (2%)
2	PCF	B	1802	-	34,34,49	0.68	0	40,42,57	0.91	1 (2%)
2	PCF	B	1803	-	17,17,49	1.11	1 (5%)	19,21,57	0.94	1 (5%)
2	PCF	C	1808	-	27,27,49	0.78	0	31,32,57	1.01	1 (3%)
2	PCF	A	1802	-	27,27,49	0.78	0	31,32,57	1.01	1 (3%)
2	PCF	D	1806	-	31,31,49	0.87	1 (3%)	37,39,57	1.10	2 (5%)
2	PCF	B	1801	-	35,35,49	0.69	0	41,43,57	0.92	1 (2%)
2	PCF	A	1805	-	34,34,49	0.69	0	40,42,57	0.92	1 (2%)
2	PCF	C	1803	-	34,34,49	0.68	0	40,42,57	0.91	1 (2%)
2	PCF	C	1805	-	29,29,49	0.74	0	33,34,57	1.07	2 (6%)
2	PCF	D	1805	-	29,29,49	0.74	0	33,34,57	1.08	2 (6%)
2	PCF	C	1801	-	41,41,49	0.64	0	47,49,57	0.86	0
2	PCF	B	1807	-	27,27,49	0.78	0	31,32,57	1.01	1 (3%)
2	PCF	A	1801	-	36,36,49	0.68	0	40,41,57	1.00	2 (5%)
2	PCF	C	1804	-	17,17,49	1.12	1 (5%)	19,21,57	0.94	1 (5%)
2	PCF	D	1801	-	41,41,49	0.64	0	47,49,57	0.86	0
2	PCF	D	1804	-	17,17,49	1.12	1 (5%)	19,21,57	0.93	1 (5%)
2	PCF	C	1807	-	36,36,49	0.68	0	40,41,57	1.00	2 (5%)
2	PCF	B	1806	-	36,36,49	0.68	0	40,41,57	1.01	2 (5%)
2	PCF	D	1802	-	35,35,49	0.69	0	41,43,57	0.92	1 (2%)
2	PCF	A	1806	-	17,17,49	1.11	1 (5%)	19,21,57	0.94	1 (5%)
2	PCF	A	1807	-	29,29,49	0.74	0	33,34,57	1.08	2 (6%)
2	PCF	A	1803	-	41,41,49	0.64	0	47,49,57	0.86	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PCF	D	1807	-	-	14/38/38/53	-
2	PCF	B	1808	-	-	23/45/45/53	-
2	PCF	D	1803	-	-	19/38/38/53	-
2	PCF	B	1805	-	-	13/35/35/53	-
2	PCF	A	1808	-	-	13/35/35/53	-
2	PCF	D	1808	-	-	6/29/29/53	-
2	PCF	C	1806	-	-	13/35/35/53	-
2	PCF	B	1804	-	-	13/31/31/53	-
2	PCF	C	1802	-	-	21/39/39/53	-
2	PCF	A	1804	-	-	21/39/39/53	-
2	PCF	B	1802	-	-	19/38/38/53	-
2	PCF	B	1803	-	-	10/18/18/53	-
2	PCF	C	1808	-	-	6/29/29/53	-
2	PCF	A	1802	-	-	6/29/29/53	-
2	PCF	D	1806	-	-	13/35/35/53	-
2	PCF	B	1801	-	-	21/39/39/53	-
2	PCF	A	1805	-	-	19/38/38/53	-
2	PCF	C	1803	-	-	19/38/38/53	-
2	PCF	C	1805	-	-	13/31/31/53	-
2	PCF	D	1805	-	-	13/31/31/53	-
2	PCF	C	1801	-	-	23/45/45/53	-
2	PCF	B	1807	-	-	6/29/29/53	-
2	PCF	A	1801	-	-	14/38/38/53	-
2	PCF	C	1804	-	-	10/18/18/53	-
2	PCF	D	1801	-	-	23/45/45/53	-
2	PCF	D	1804	-	-	10/18/18/53	-
2	PCF	C	1807	-	-	14/38/38/53	-
2	PCF	B	1806	-	-	14/38/38/53	-
2	PCF	D	1802	-	-	21/39/39/53	-
2	PCF	A	1806	-	-	10/18/18/53	-
2	PCF	A	1807	-	-	13/31/31/53	-
2	PCF	A	1803	-	-	23/45/45/53	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1804	PCF	O21-C2	-2.80	1.43	1.46
2	C	1804	PCF	O21-C2	-2.75	1.43	1.46
2	B	1803	PCF	O21-C2	-2.74	1.43	1.46
2	A	1806	PCF	O21-C2	-2.71	1.43	1.46
2	C	1806	PCF	O21-C2	-2.46	1.40	1.46
2	A	1808	PCF	O21-C2	-2.43	1.40	1.46
2	B	1805	PCF	O21-C2	-2.43	1.40	1.46
2	D	1806	PCF	O21-C2	-2.42	1.40	1.46

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1805	PCF	C2-O21-C21	-3.34	109.56	117.79
2	B	1802	PCF	C2-O21-C21	-3.34	109.57	117.79
2	C	1803	PCF	C2-O21-C21	-3.34	109.58	117.79
2	D	1803	PCF	C2-O21-C21	-3.33	109.59	117.79
2	B	1801	PCF	C2-O21-C21	-3.27	109.74	117.79
2	A	1804	PCF	C2-O21-C21	-3.27	109.75	117.79
2	C	1802	PCF	C2-O21-C21	-3.26	109.76	117.79
2	D	1802	PCF	C2-O21-C21	-3.26	109.76	117.79
2	A	1808	PCF	O31-C31-C32	3.08	121.58	111.91
2	B	1805	PCF	O31-C31-C32	3.08	121.57	111.91
2	C	1806	PCF	O31-C31-C32	3.08	121.57	111.91
2	D	1806	PCF	O31-C31-C32	3.06	121.52	111.91
2	C	1807	PCF	O21-C21-C22	2.23	116.31	111.50
2	B	1806	PCF	O21-C21-C22	2.23	116.31	111.50
2	D	1807	PCF	O21-C21-C22	2.23	116.30	111.50
2	A	1801	PCF	O21-C21-C22	2.22	116.29	111.50
2	A	1807	PCF	O11-P-O12	2.12	112.43	106.47
2	B	1804	PCF	O11-P-O12	2.12	112.41	106.47
2	C	1805	PCF	O11-P-O12	2.11	112.40	106.47
2	D	1805	PCF	O11-P-O12	2.11	112.38	106.47
2	C	1807	PCF	O11-P-O12	2.10	112.38	106.47
2	D	1807	PCF	O11-P-O12	2.10	112.37	106.47
2	A	1801	PCF	O11-P-O12	2.10	112.36	106.47
2	B	1806	PCF	O11-P-O12	2.10	112.36	106.47
2	D	1805	PCF	C2-O21-C21	-2.10	112.63	117.79
2	B	1804	PCF	C2-O21-C21	-2.09	112.64	117.79
2	C	1805	PCF	C2-O21-C21	-2.09	112.64	117.79
2	A	1807	PCF	C2-O21-C21	-2.09	112.65	117.79
2	C	1806	PCF	C3-O31-C31	-2.06	109.51	117.12
2	A	1808	PCF	C3-O31-C31	-2.05	109.52	117.12
2	D	1806	PCF	C3-O31-C31	-2.05	109.53	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1805	PCF	C3-O31-C31	-2.05	109.53	117.12
2	B	1807	PCF	O11-P-O12	2.05	112.21	106.47
2	C	1804	PCF	C3-O31-C31	-2.05	109.55	117.12
2	B	1803	PCF	C3-O31-C31	-2.04	109.56	117.12
2	D	1808	PCF	O11-P-O12	2.04	112.20	106.47
2	C	1808	PCF	O11-P-O12	2.04	112.20	106.47
2	A	1802	PCF	O11-P-O12	2.03	112.18	106.47
2	A	1806	PCF	C3-O31-C31	-2.03	109.60	117.12
2	D	1804	PCF	C3-O31-C31	-2.03	109.61	117.12

There are no chirality outliers.

All (476) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1801	PCF	C1-O11-P-O13
2	A	1801	PCF	C22-C21-O21-C2
2	A	1803	PCF	C11-O13-P-O12
2	A	1803	PCF	O13-C11-C12-N
2	A	1803	PCF	O22-C21-O21-C2
2	A	1803	PCF	C22-C21-O21-C2
2	A	1804	PCF	C11-O13-P-O12
2	A	1804	PCF	C11-O13-P-O14
2	A	1804	PCF	O13-C11-C12-N
2	A	1804	PCF	C22-C21-O21-C2
2	A	1805	PCF	C1-O11-P-O14
2	A	1805	PCF	C11-O13-P-O14
2	A	1805	PCF	C22-C21-O21-C2
2	A	1806	PCF	C1-O11-P-O13
2	A	1806	PCF	C1-O11-P-O14
2	A	1806	PCF	C1-C2-O21-C21
2	A	1806	PCF	C3-C2-O21-C21
2	A	1806	PCF	O22-C21-O21-C2
2	A	1807	PCF	C1-O11-P-O13
2	A	1808	PCF	C11-O13-P-O11
2	A	1808	PCF	C11-O13-P-O12
2	A	1808	PCF	C11-O13-P-O14
2	A	1808	PCF	C12-C11-O13-P
2	B	1801	PCF	C11-O13-P-O12
2	B	1801	PCF	C11-O13-P-O14
2	B	1801	PCF	O13-C11-C12-N
2	B	1801	PCF	C22-C21-O21-C2
2	B	1802	PCF	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
2	B	1802	PCF	C11-O13-P-O14
2	B	1802	PCF	C22-C21-O21-C2
2	B	1803	PCF	C1-O11-P-O13
2	B	1803	PCF	C1-O11-P-O14
2	B	1803	PCF	C1-C2-O21-C21
2	B	1803	PCF	C3-C2-O21-C21
2	B	1803	PCF	O22-C21-O21-C2
2	B	1804	PCF	C1-O11-P-O13
2	B	1805	PCF	C11-O13-P-O11
2	B	1805	PCF	C11-O13-P-O12
2	B	1805	PCF	C11-O13-P-O14
2	B	1805	PCF	C12-C11-O13-P
2	B	1806	PCF	C1-O11-P-O13
2	B	1806	PCF	C22-C21-O21-C2
2	B	1808	PCF	C11-O13-P-O12
2	B	1808	PCF	O13-C11-C12-N
2	B	1808	PCF	O22-C21-O21-C2
2	B	1808	PCF	C22-C21-O21-C2
2	C	1801	PCF	C11-O13-P-O12
2	C	1801	PCF	O13-C11-C12-N
2	C	1801	PCF	O22-C21-O21-C2
2	C	1801	PCF	C22-C21-O21-C2
2	C	1802	PCF	C11-O13-P-O12
2	C	1802	PCF	C11-O13-P-O14
2	C	1802	PCF	O13-C11-C12-N
2	C	1802	PCF	C22-C21-O21-C2
2	C	1803	PCF	C1-O11-P-O14
2	C	1803	PCF	C11-O13-P-O14
2	C	1803	PCF	C22-C21-O21-C2
2	C	1804	PCF	C1-O11-P-O13
2	C	1804	PCF	C1-O11-P-O14
2	C	1804	PCF	C1-C2-O21-C21
2	C	1804	PCF	C3-C2-O21-C21
2	C	1804	PCF	O22-C21-O21-C2
2	C	1805	PCF	C1-O11-P-O13
2	C	1806	PCF	C11-O13-P-O11
2	C	1806	PCF	C11-O13-P-O12
2	C	1806	PCF	C11-O13-P-O14
2	C	1806	PCF	C12-C11-O13-P
2	C	1807	PCF	C1-O11-P-O13
2	C	1807	PCF	C22-C21-O21-C2
2	D	1801	PCF	C11-O13-P-O12

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Mol	Chain	Res	Type	Atoms
2	D	1801	PCF	O13-C11-C12-N
2	D	1801	PCF	O22-C21-O21-C2
2	D	1801	PCF	C22-C21-O21-C2
2	D	1802	PCF	C11-O13-P-O12
2	D	1802	PCF	C11-O13-P-O14
2	D	1802	PCF	O13-C11-C12-N
2	D	1802	PCF	C22-C21-O21-C2
2	D	1803	PCF	C1-O11-P-O14
2	D	1803	PCF	C11-O13-P-O14
2	D	1803	PCF	C22-C21-O21-C2
2	D	1804	PCF	C1-O11-P-O13
2	D	1804	PCF	C1-O11-P-O14
2	D	1804	PCF	C1-C2-O21-C21
2	D	1804	PCF	C3-C2-O21-C21
2	D	1804	PCF	O22-C21-O21-C2
2	D	1805	PCF	C1-O11-P-O13
2	D	1806	PCF	C11-O13-P-O11
2	D	1806	PCF	C11-O13-P-O12
2	D	1806	PCF	C11-O13-P-O14
2	D	1806	PCF	C12-C11-O13-P
2	D	1807	PCF	C1-O11-P-O13
2	D	1807	PCF	C22-C21-O21-C2
2	A	1801	PCF	O32-C31-O31-C3
2	A	1807	PCF	O32-C31-O31-C3
2	A	1808	PCF	O32-C31-O31-C3
2	B	1804	PCF	O32-C31-O31-C3
2	B	1805	PCF	O32-C31-O31-C3
2	B	1806	PCF	O32-C31-O31-C3
2	C	1805	PCF	O32-C31-O31-C3
2	C	1806	PCF	O32-C31-O31-C3
2	C	1807	PCF	O32-C31-O31-C3
2	D	1805	PCF	O32-C31-O31-C3
2	D	1806	PCF	O32-C31-O31-C3
2	D	1807	PCF	O32-C31-O31-C3
2	A	1801	PCF	C32-C31-O31-C3
2	A	1807	PCF	C32-C31-O31-C3
2	A	1808	PCF	C32-C31-O31-C3
2	B	1804	PCF	C32-C31-O31-C3
2	B	1805	PCF	C32-C31-O31-C3
2	B	1806	PCF	C32-C31-O31-C3
2	C	1805	PCF	C32-C31-O31-C3
2	C	1806	PCF	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
2	C	1807	PCF	C32-C31-O31-C3
2	D	1805	PCF	C32-C31-O31-C3
2	D	1806	PCF	C32-C31-O31-C3
2	D	1807	PCF	C32-C31-O31-C3
2	A	1803	PCF	O32-C31-O31-C3
2	A	1804	PCF	O32-C31-O31-C3
2	B	1801	PCF	O32-C31-O31-C3
2	B	1808	PCF	O32-C31-O31-C3
2	C	1801	PCF	O32-C31-O31-C3
2	C	1802	PCF	O32-C31-O31-C3
2	D	1801	PCF	O32-C31-O31-C3
2	D	1802	PCF	O32-C31-O31-C3
2	A	1801	PCF	O22-C21-O21-C2
2	A	1805	PCF	O22-C21-O21-C2
2	B	1802	PCF	O22-C21-O21-C2
2	B	1806	PCF	O22-C21-O21-C2
2	C	1803	PCF	O22-C21-O21-C2
2	C	1807	PCF	O22-C21-O21-C2
2	D	1803	PCF	O22-C21-O21-C2
2	D	1807	PCF	O22-C21-O21-C2
2	A	1803	PCF	C32-C31-O31-C3
2	A	1804	PCF	C32-C31-O31-C3
2	B	1801	PCF	C32-C31-O31-C3
2	B	1808	PCF	C32-C31-O31-C3
2	C	1801	PCF	C32-C31-O31-C3
2	C	1802	PCF	C32-C31-O31-C3
2	D	1801	PCF	C32-C31-O31-C3
2	D	1802	PCF	C32-C31-O31-C3
2	A	1804	PCF	O22-C21-O21-C2
2	B	1801	PCF	O22-C21-O21-C2
2	C	1802	PCF	O22-C21-O21-C2
2	D	1802	PCF	O22-C21-O21-C2
2	A	1806	PCF	C32-C31-O31-C3
2	B	1803	PCF	C32-C31-O31-C3
2	C	1804	PCF	C32-C31-O31-C3
2	D	1804	PCF	C32-C31-O31-C3
2	A	1806	PCF	O32-C31-O31-C3
2	B	1803	PCF	O32-C31-O31-C3
2	C	1804	PCF	O32-C31-O31-C3
2	D	1804	PCF	O32-C31-O31-C3
2	A	1805	PCF	C32-C31-O31-C3
2	B	1802	PCF	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
2	C	1803	PCF	C32-C31-O31-C3
2	D	1803	PCF	C32-C31-O31-C3
2	A	1807	PCF	O22-C21-O21-C2
2	B	1804	PCF	O22-C21-O21-C2
2	C	1805	PCF	O22-C21-O21-C2
2	D	1805	PCF	O22-C21-O21-C2
2	A	1805	PCF	O32-C31-O31-C3
2	B	1802	PCF	O32-C31-O31-C3
2	C	1803	PCF	O32-C31-O31-C3
2	D	1803	PCF	O32-C31-O31-C3
2	A	1805	PCF	C21-C22-C23-C24
2	B	1802	PCF	C21-C22-C23-C24
2	C	1803	PCF	C21-C22-C23-C24
2	D	1803	PCF	C21-C22-C23-C24
2	A	1803	PCF	C21-C22-C23-C24
2	A	1804	PCF	C21-C22-C23-C24
2	B	1801	PCF	C21-C22-C23-C24
2	B	1808	PCF	C21-C22-C23-C24
2	C	1801	PCF	C21-C22-C23-C24
2	C	1802	PCF	C21-C22-C23-C24
2	D	1801	PCF	C21-C22-C23-C24
2	D	1802	PCF	C21-C22-C23-C24
2	A	1807	PCF	C22-C21-O21-C2
2	B	1804	PCF	C22-C21-O21-C2
2	C	1805	PCF	C22-C21-O21-C2
2	D	1805	PCF	C22-C21-O21-C2
2	A	1803	PCF	C1-O11-P-O13
2	A	1803	PCF	C11-O13-P-O11
2	A	1804	PCF	C11-O13-P-O11
2	A	1805	PCF	C1-O11-P-O13
2	A	1808	PCF	C1-O11-P-O13
2	B	1801	PCF	C11-O13-P-O11
2	B	1802	PCF	C1-O11-P-O13
2	B	1805	PCF	C1-O11-P-O13
2	B	1808	PCF	C1-O11-P-O13
2	B	1808	PCF	C11-O13-P-O11
2	C	1801	PCF	C1-O11-P-O13
2	C	1801	PCF	C11-O13-P-O11
2	C	1802	PCF	C11-O13-P-O11
2	C	1803	PCF	C1-O11-P-O13
2	C	1806	PCF	C1-O11-P-O13
2	D	1801	PCF	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
2	D	1801	PCF	C11-O13-P-O11
2	D	1802	PCF	C11-O13-P-O11
2	D	1803	PCF	C1-O11-P-O13
2	D	1806	PCF	C1-O11-P-O13
2	A	1805	PCF	C26-C27-C28-C29
2	B	1802	PCF	C26-C27-C28-C29
2	C	1803	PCF	C26-C27-C28-C29
2	D	1803	PCF	C26-C27-C28-C29
2	A	1805	PCF	C22-C23-C24-C25
2	B	1802	PCF	C22-C23-C24-C25
2	C	1803	PCF	C22-C23-C24-C25
2	D	1803	PCF	C22-C23-C24-C25
2	B	1802	PCF	C25-C26-C27-C28
2	C	1803	PCF	C25-C26-C27-C28
2	D	1803	PCF	C25-C26-C27-C28
2	A	1805	PCF	C25-C26-C27-C28
2	B	1801	PCF	C25-C26-C27-C28
2	A	1804	PCF	C25-C26-C27-C28
2	C	1802	PCF	C25-C26-C27-C28
2	D	1802	PCF	C25-C26-C27-C28
2	B	1808	PCF	C32-C33-C34-C35
2	A	1803	PCF	C32-C33-C34-C35
2	C	1801	PCF	C32-C33-C34-C35
2	D	1801	PCF	C32-C33-C34-C35
2	A	1804	PCF	C23-C24-C25-C26
2	B	1801	PCF	C23-C24-C25-C26
2	C	1802	PCF	C23-C24-C25-C26
2	D	1802	PCF	C23-C24-C25-C26
2	A	1803	PCF	C41-C42-C43-C44
2	B	1808	PCF	C41-C42-C43-C44
2	C	1801	PCF	C41-C42-C43-C44
2	D	1801	PCF	C41-C42-C43-C44
2	A	1802	PCF	C32-C31-O31-C3
2	B	1807	PCF	C32-C31-O31-C3
2	C	1808	PCF	C32-C31-O31-C3
2	D	1808	PCF	C32-C31-O31-C3
2	B	1808	PCF	C24-C25-C26-C27
2	C	1801	PCF	C24-C25-C26-C27
2	D	1801	PCF	C24-C25-C26-C27
2	A	1803	PCF	C24-C25-C26-C27
2	A	1803	PCF	C42-C43-C44-C45
2	B	1808	PCF	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
2	C	1801	PCF	C42-C43-C44-C45
2	D	1801	PCF	C42-C43-C44-C45
2	A	1803	PCF	C34-C35-C36-C37
2	B	1808	PCF	C34-C35-C36-C37
2	C	1801	PCF	C34-C35-C36-C37
2	D	1801	PCF	C34-C35-C36-C37
2	A	1804	PCF	C26-C27-C28-C29
2	B	1801	PCF	C26-C27-C28-C29
2	C	1802	PCF	C26-C27-C28-C29
2	D	1802	PCF	C26-C27-C28-C29
2	A	1802	PCF	O32-C31-O31-C3
2	B	1807	PCF	O32-C31-O31-C3
2	C	1808	PCF	O32-C31-O31-C3
2	D	1808	PCF	O32-C31-O31-C3
2	A	1805	PCF	C32-C33-C34-C35
2	B	1802	PCF	C32-C33-C34-C35
2	C	1803	PCF	C32-C33-C34-C35
2	D	1803	PCF	C32-C33-C34-C35
2	C	1802	PCF	C22-C23-C24-C25
2	D	1802	PCF	C22-C23-C24-C25
2	A	1804	PCF	C22-C23-C24-C25
2	B	1801	PCF	C22-C23-C24-C25
2	A	1805	PCF	C27-C28-C29-C30
2	B	1802	PCF	C27-C28-C29-C30
2	C	1803	PCF	C27-C28-C29-C30
2	D	1803	PCF	C27-C28-C29-C30
2	A	1801	PCF	C1-O11-P-O12
2	A	1802	PCF	C1-O11-P-O12
2	A	1807	PCF	C1-O11-P-O12
2	B	1804	PCF	C1-O11-P-O12
2	B	1806	PCF	C1-O11-P-O12
2	B	1807	PCF	C1-O11-P-O12
2	C	1805	PCF	C1-O11-P-O12
2	C	1807	PCF	C1-O11-P-O12
2	C	1808	PCF	C1-O11-P-O12
2	D	1805	PCF	C1-O11-P-O12
2	D	1807	PCF	C1-O11-P-O12
2	D	1808	PCF	C1-O11-P-O12
2	A	1803	PCF	O21-C2-C3-O31
2	B	1808	PCF	O21-C2-C3-O31
2	C	1801	PCF	O21-C2-C3-O31
2	D	1801	PCF	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
2	A	1807	PCF	C31-C32-C33-C34
2	B	1804	PCF	C31-C32-C33-C34
2	C	1805	PCF	C31-C32-C33-C34
2	D	1805	PCF	C31-C32-C33-C34
2	A	1804	PCF	C31-C32-C33-C34
2	B	1801	PCF	C31-C32-C33-C34
2	C	1802	PCF	C31-C32-C33-C34
2	D	1802	PCF	C31-C32-C33-C34
2	A	1803	PCF	C2-C1-O11-P
2	B	1808	PCF	C2-C1-O11-P
2	C	1801	PCF	C2-C1-O11-P
2	D	1801	PCF	C2-C1-O11-P
2	A	1808	PCF	C2-C1-O11-P
2	B	1805	PCF	C2-C1-O11-P
2	C	1806	PCF	C2-C1-O11-P
2	D	1806	PCF	C2-C1-O11-P
2	A	1801	PCF	C27-C28-C29-C30
2	C	1807	PCF	C27-C28-C29-C30
2	D	1807	PCF	C27-C28-C29-C30
2	B	1806	PCF	C27-C28-C29-C30
2	A	1807	PCF	C1-O11-P-O14
2	B	1804	PCF	C1-O11-P-O14
2	C	1805	PCF	C1-O11-P-O14
2	D	1805	PCF	C1-O11-P-O14
2	A	1804	PCF	C35-C36-C37-C38
2	B	1801	PCF	C35-C36-C37-C38
2	C	1802	PCF	C35-C36-C37-C38
2	D	1802	PCF	C35-C36-C37-C38
2	A	1803	PCF	C1-O11-P-O12
2	A	1803	PCF	C11-O13-P-O14
2	A	1805	PCF	C11-O13-P-O12
2	A	1808	PCF	C1-O11-P-O14
2	B	1802	PCF	C11-O13-P-O12
2	B	1805	PCF	C1-O11-P-O14
2	B	1808	PCF	C1-O11-P-O12
2	B	1808	PCF	C11-O13-P-O14
2	C	1801	PCF	C1-O11-P-O12
2	C	1801	PCF	C11-O13-P-O14
2	C	1803	PCF	C11-O13-P-O12
2	C	1806	PCF	C1-O11-P-O14
2	D	1801	PCF	C1-O11-P-O12
2	D	1801	PCF	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
2	D	1803	PCF	C11-O13-P-O12
2	D	1806	PCF	C1-O11-P-O14
2	A	1803	PCF	C25-C26-C27-C28
2	B	1808	PCF	C25-C26-C27-C28
2	C	1801	PCF	C25-C26-C27-C28
2	D	1801	PCF	C25-C26-C27-C28
2	A	1805	PCF	O13-C11-C12-N
2	B	1802	PCF	O13-C11-C12-N
2	C	1803	PCF	O13-C11-C12-N
2	D	1803	PCF	O13-C11-C12-N
2	B	1808	PCF	C38-C39-C40-C41
2	C	1801	PCF	C38-C39-C40-C41
2	D	1801	PCF	C38-C39-C40-C41
2	A	1803	PCF	C38-C39-C40-C41
2	A	1804	PCF	C2-C1-O11-P
2	B	1801	PCF	C2-C1-O11-P
2	C	1802	PCF	C2-C1-O11-P
2	D	1802	PCF	C2-C1-O11-P
2	A	1805	PCF	C11-O13-P-O11
2	B	1802	PCF	C11-O13-P-O11
2	C	1803	PCF	C11-O13-P-O11
2	D	1803	PCF	C11-O13-P-O11
2	A	1803	PCF	C1-C2-C3-O31
2	B	1808	PCF	C1-C2-C3-O31
2	C	1801	PCF	C1-C2-C3-O31
2	D	1801	PCF	C1-C2-C3-O31
2	B	1808	PCF	C23-C24-C25-C26
2	B	1801	PCF	C33-C34-C35-C36
2	C	1802	PCF	C33-C34-C35-C36
2	D	1801	PCF	C23-C24-C25-C26
2	D	1802	PCF	C33-C34-C35-C36
2	A	1803	PCF	C23-C24-C25-C26
2	A	1804	PCF	C33-C34-C35-C36
2	C	1801	PCF	C23-C24-C25-C26
2	A	1801	PCF	C1-C2-O21-C21
2	A	1801	PCF	C3-C2-O21-C21
2	B	1806	PCF	C1-C2-O21-C21
2	B	1806	PCF	C3-C2-O21-C21
2	C	1807	PCF	C1-C2-O21-C21
2	C	1807	PCF	C3-C2-O21-C21
2	D	1807	PCF	C1-C2-O21-C21
2	D	1807	PCF	C3-C2-O21-C21

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Mol	Chain	Res	Type	Atoms
2	A	1807	PCF	C27-C28-C29-C30
2	B	1804	PCF	C27-C28-C29-C30
2	C	1805	PCF	C27-C28-C29-C30
2	D	1805	PCF	C27-C28-C29-C30
2	B	1805	PCF	O21-C21-C22-C23
2	C	1806	PCF	O21-C21-C22-C23
2	D	1806	PCF	O21-C21-C22-C23
2	A	1808	PCF	O21-C21-C22-C23
2	A	1807	PCF	O21-C21-C22-C23
2	B	1804	PCF	O21-C21-C22-C23
2	C	1805	PCF	O21-C21-C22-C23
2	D	1805	PCF	O21-C21-C22-C23
2	D	1808	PCF	O31-C31-C32-C33
2	A	1802	PCF	C1-O11-P-O14
2	B	1807	PCF	C1-O11-P-O14
2	C	1808	PCF	C1-O11-P-O14
2	D	1808	PCF	C1-O11-P-O14
2	A	1802	PCF	O31-C31-C32-C33
2	A	1808	PCF	O31-C31-C32-C33
2	B	1805	PCF	O31-C31-C32-C33
2	B	1807	PCF	O31-C31-C32-C33
2	C	1806	PCF	O31-C31-C32-C33
2	C	1808	PCF	O31-C31-C32-C33
2	D	1806	PCF	O31-C31-C32-C33
2	A	1804	PCF	O21-C21-C22-C23
2	A	1807	PCF	O31-C31-C32-C33
2	B	1801	PCF	O21-C21-C22-C23
2	C	1802	PCF	O21-C21-C22-C23
2	C	1805	PCF	O31-C31-C32-C33
2	D	1802	PCF	O21-C21-C22-C23
2	A	1801	PCF	O31-C31-C32-C33
2	B	1804	PCF	O31-C31-C32-C33
2	B	1806	PCF	O31-C31-C32-C33
2	C	1807	PCF	O31-C31-C32-C33
2	D	1805	PCF	O31-C31-C32-C33
2	D	1807	PCF	O31-C31-C32-C33
2	A	1806	PCF	C1-O11-P-O12
2	B	1803	PCF	C1-O11-P-O12
2	C	1804	PCF	C1-O11-P-O12
2	D	1804	PCF	C1-O11-P-O12
2	A	1801	PCF	O21-C21-C22-C23
2	B	1806	PCF	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
2	C	1807	PCF	O21-C21-C22-C23
2	D	1807	PCF	O21-C21-C22-C23
2	A	1805	PCF	O21-C21-C22-C23
2	B	1802	PCF	O21-C21-C22-C23
2	C	1803	PCF	O21-C21-C22-C23
2	D	1803	PCF	O21-C21-C22-C23
2	B	1806	PCF	O32-C31-C32-C33
2	C	1807	PCF	O32-C31-C32-C33
2	D	1807	PCF	O32-C31-C32-C33
2	A	1801	PCF	O32-C31-C32-C33
2	C	1802	PCF	C27-C28-C29-C30
2	B	1801	PCF	C27-C28-C29-C30
2	D	1802	PCF	C27-C28-C29-C30
2	A	1804	PCF	C27-C28-C29-C30
2	A	1802	PCF	O32-C31-C32-C33
2	B	1807	PCF	O32-C31-C32-C33
2	C	1808	PCF	O32-C31-C32-C33
2	D	1808	PCF	O32-C31-C32-C33
2	A	1801	PCF	C29-C30-C47-C48
2	C	1807	PCF	C29-C30-C47-C48
2	A	1808	PCF	O32-C31-C32-C33
2	B	1806	PCF	C29-C30-C47-C48
2	D	1807	PCF	C29-C30-C47-C48
2	B	1805	PCF	O32-C31-C32-C33
2	C	1806	PCF	O32-C31-C32-C33
2	D	1806	PCF	O32-C31-C32-C33
2	C	1805	PCF	O32-C31-C32-C33
2	A	1804	PCF	O22-C21-C22-C23
2	A	1807	PCF	O32-C31-C32-C33
2	B	1801	PCF	O22-C21-C22-C23
2	B	1804	PCF	O32-C31-C32-C33
2	D	1805	PCF	O32-C31-C32-C33
2	C	1802	PCF	O22-C21-C22-C23
2	D	1802	PCF	O22-C21-C22-C23
2	A	1804	PCF	C1-O11-P-O12
2	A	1808	PCF	C1-O11-P-O12
2	B	1801	PCF	C1-O11-P-O12
2	B	1805	PCF	C1-O11-P-O12
2	C	1802	PCF	C1-O11-P-O12
2	C	1806	PCF	C1-O11-P-O12
2	D	1802	PCF	C1-O11-P-O12
2	D	1806	PCF	C1-O11-P-O12

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Mol	Chain	Res	Type	Atoms
2	B	1806	PCF	O22-C21-C22-C23
2	C	1807	PCF	O22-C21-C22-C23
2	D	1807	PCF	O22-C21-C22-C23
2	A	1801	PCF	O22-C21-C22-C23
2	A	1805	PCF	C24-C25-C26-C27
2	D	1803	PCF	C24-C25-C26-C27
2	A	1807	PCF	C1-C2-O21-C21
2	B	1804	PCF	C1-C2-O21-C21
2	C	1805	PCF	C1-C2-O21-C21
2	D	1805	PCF	C1-C2-O21-C21
2	B	1802	PCF	C24-C25-C26-C27
2	C	1803	PCF	C24-C25-C26-C27
2	A	1806	PCF	O31-C31-C32-C33
2	B	1803	PCF	O31-C31-C32-C33
2	C	1804	PCF	O31-C31-C32-C33
2	D	1804	PCF	O31-C31-C32-C33
2	A	1803	PCF	O21-C21-C22-C23
2	B	1808	PCF	O21-C21-C22-C23
2	C	1801	PCF	O21-C21-C22-C23
2	D	1801	PCF	O21-C21-C22-C23
2	A	1805	PCF	O22-C21-C22-C23
2	A	1806	PCF	O32-C31-C32-C33
2	B	1802	PCF	O22-C21-C22-C23
2	B	1803	PCF	O32-C31-C32-C33
2	C	1803	PCF	O22-C21-C22-C23
2	C	1804	PCF	O32-C31-C32-C33
2	D	1803	PCF	O22-C21-C22-C23
2	D	1804	PCF	O32-C31-C32-C33

There are no ring outliers.

26 monomers are involved in 319 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1807	PCF	15	0
2	B	1808	PCF	22	0
2	D	1803	PCF	12	0
2	B	1805	PCF	15	0
2	A	1808	PCF	16	0
2	D	1808	PCF	1	0
2	C	1806	PCF	19	0
2	B	1804	PCF	17	0
2	B	1802	PCF	14	0

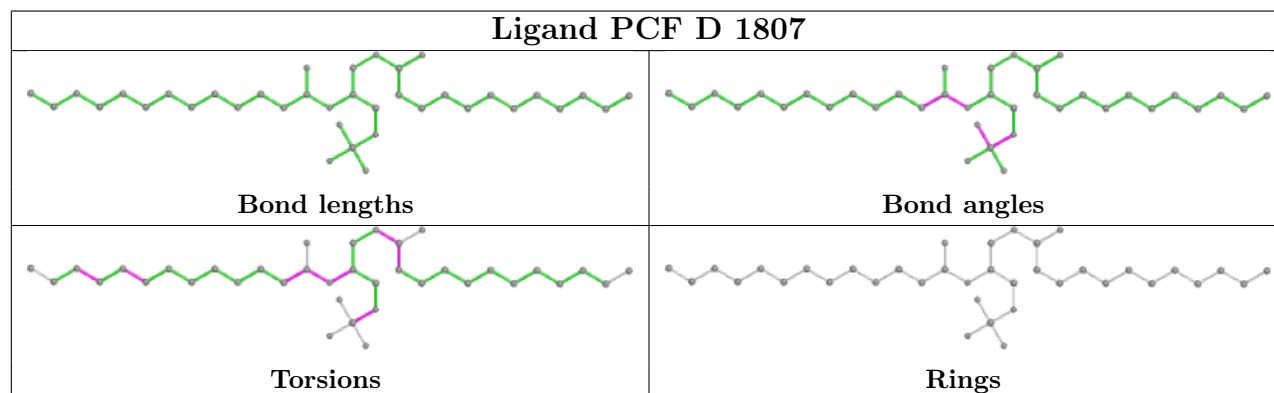
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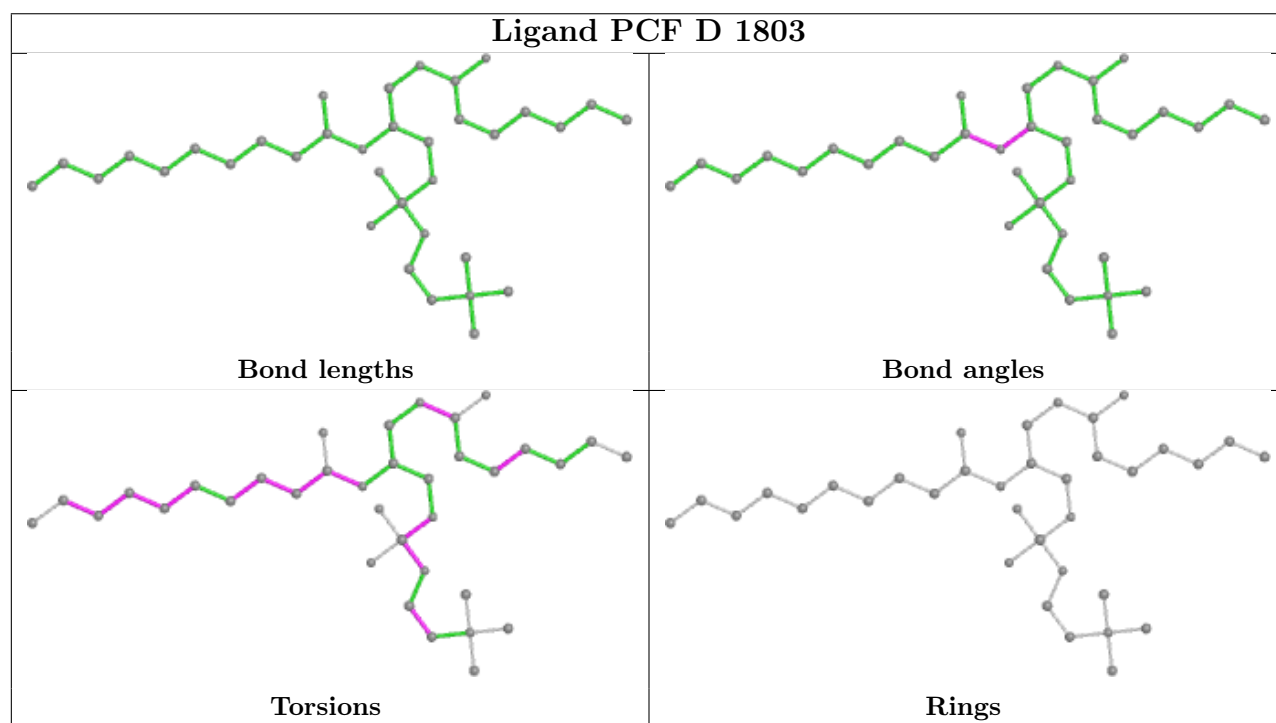
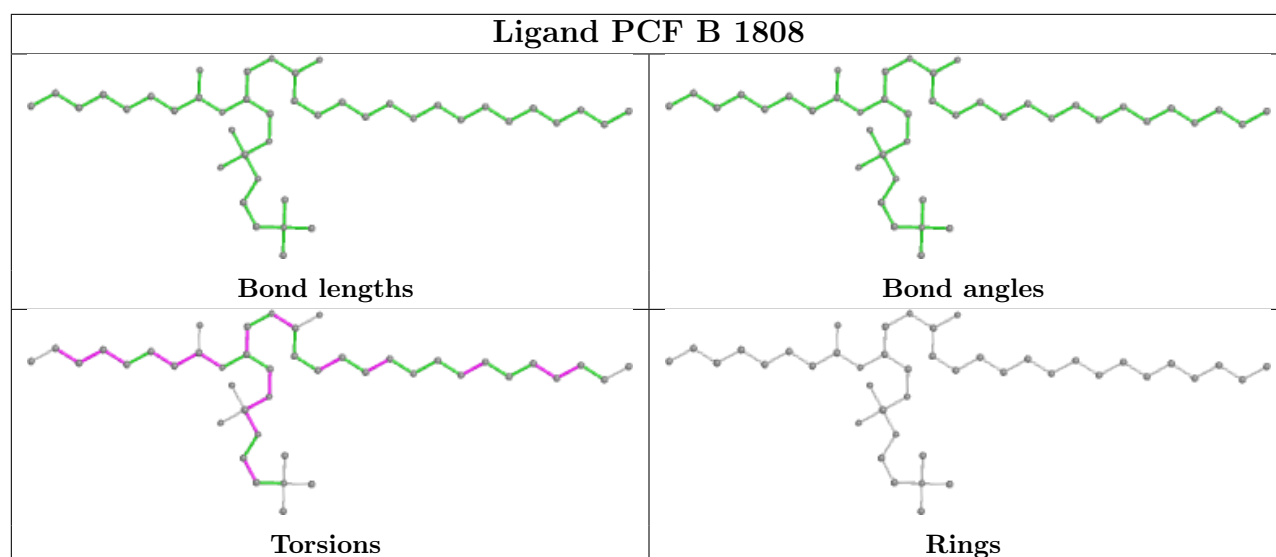


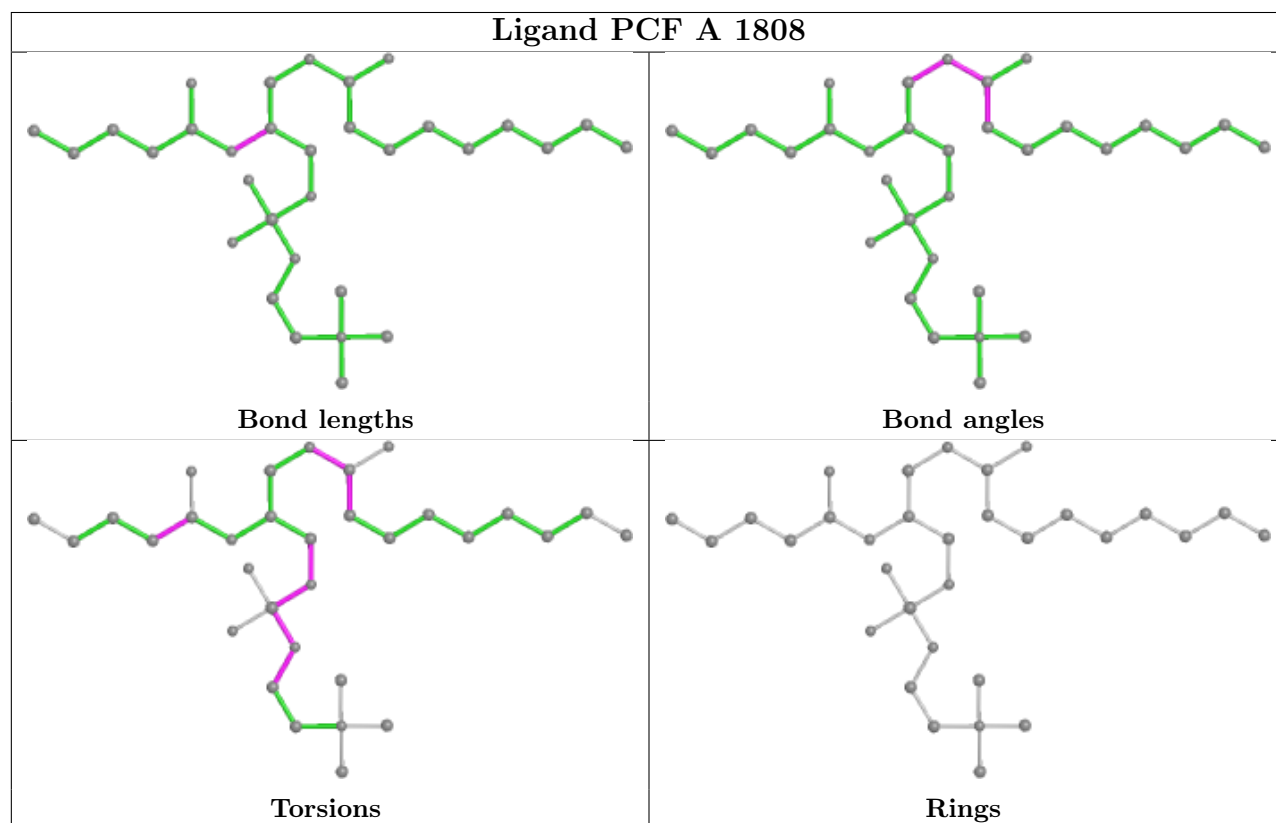
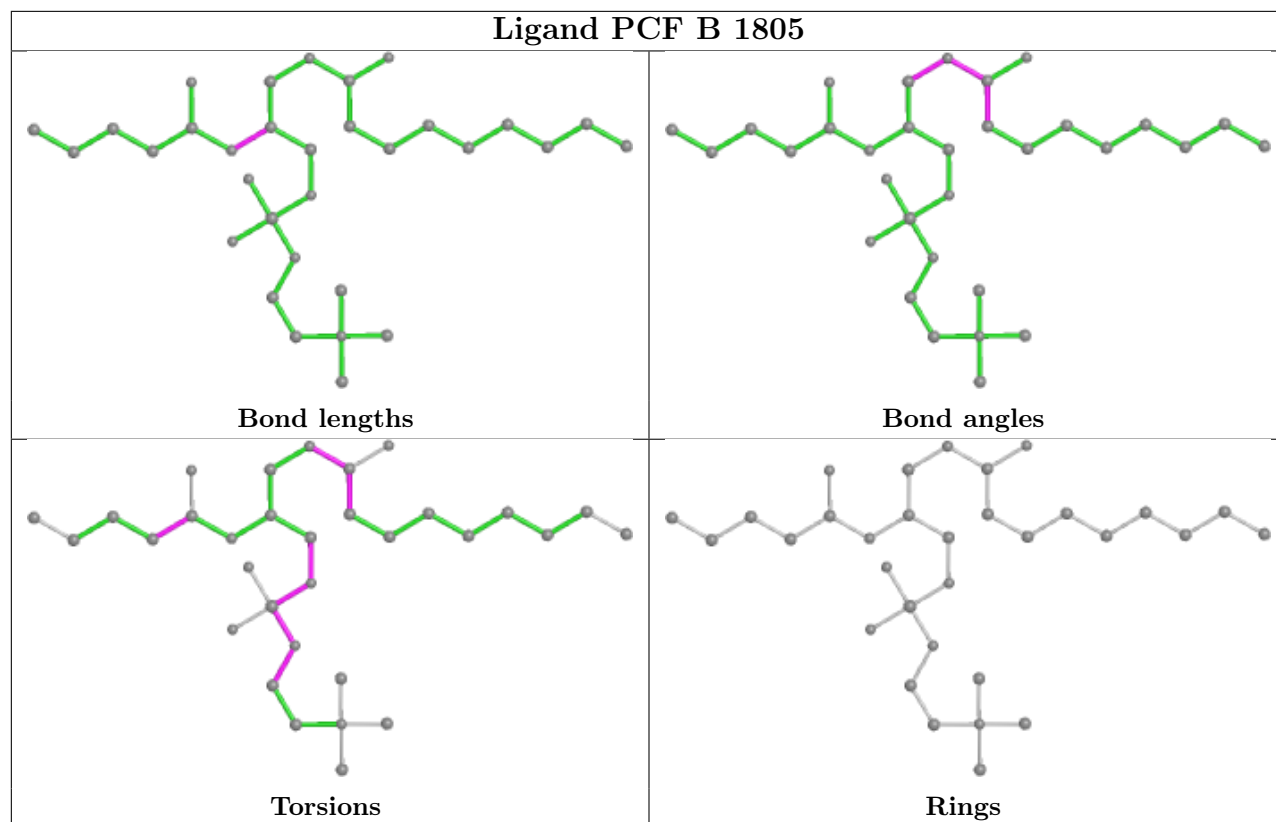
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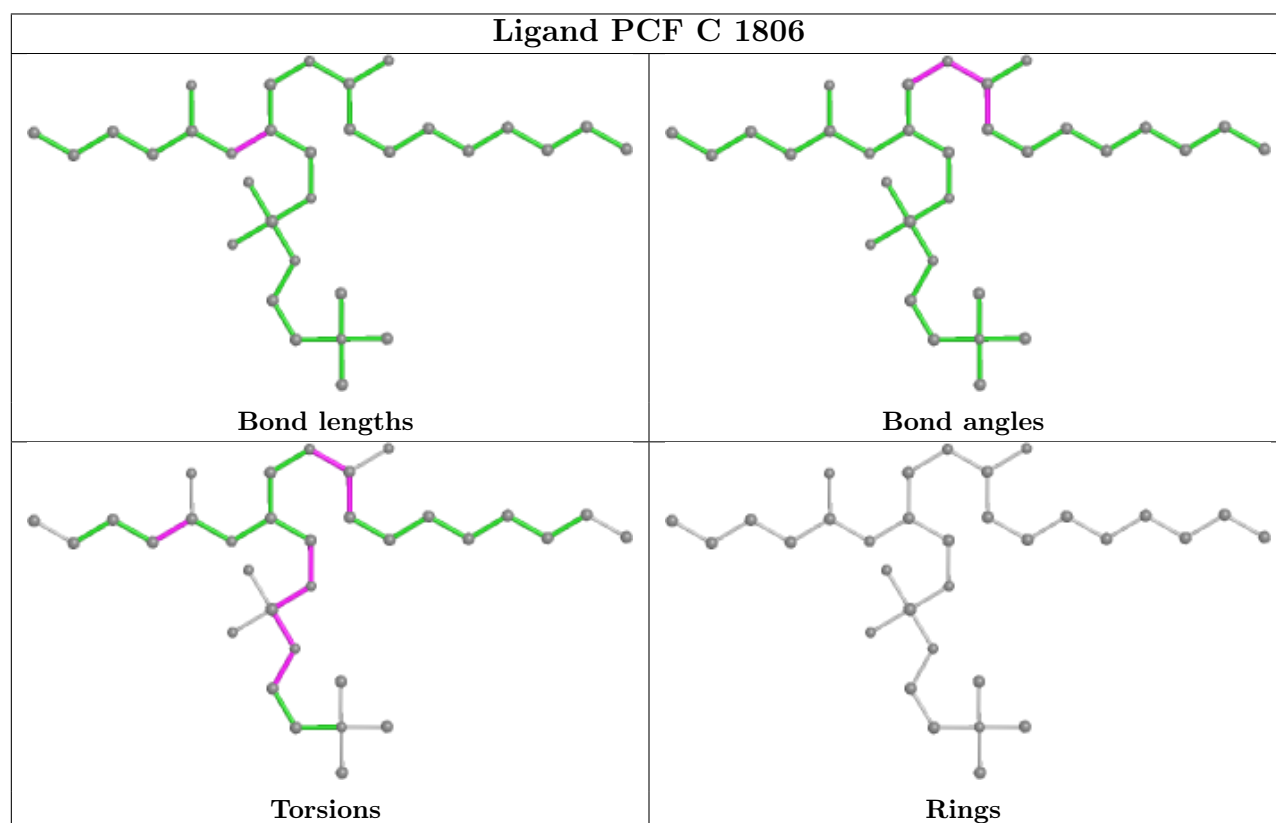
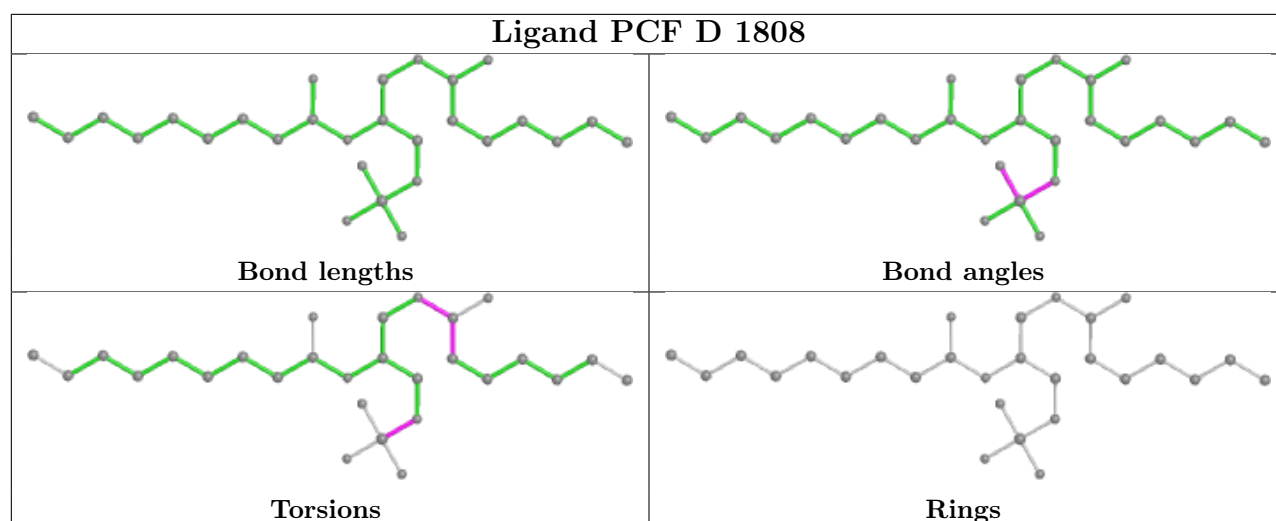
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1808	PCF	1	0
2	A	1802	PCF	1	0
2	D	1806	PCF	16	0
2	B	1801	PCF	1	0
2	A	1805	PCF	14	0
2	C	1803	PCF	17	0
2	C	1805	PCF	19	0
2	D	1805	PCF	17	0
2	C	1801	PCF	25	0
2	B	1807	PCF	1	0
2	A	1801	PCF	15	0
2	D	1801	PCF	31	0
2	C	1807	PCF	15	0
2	B	1806	PCF	16	0
2	D	1802	PCF	1	0
2	A	1807	PCF	19	0
2	A	1803	PCF	23	0

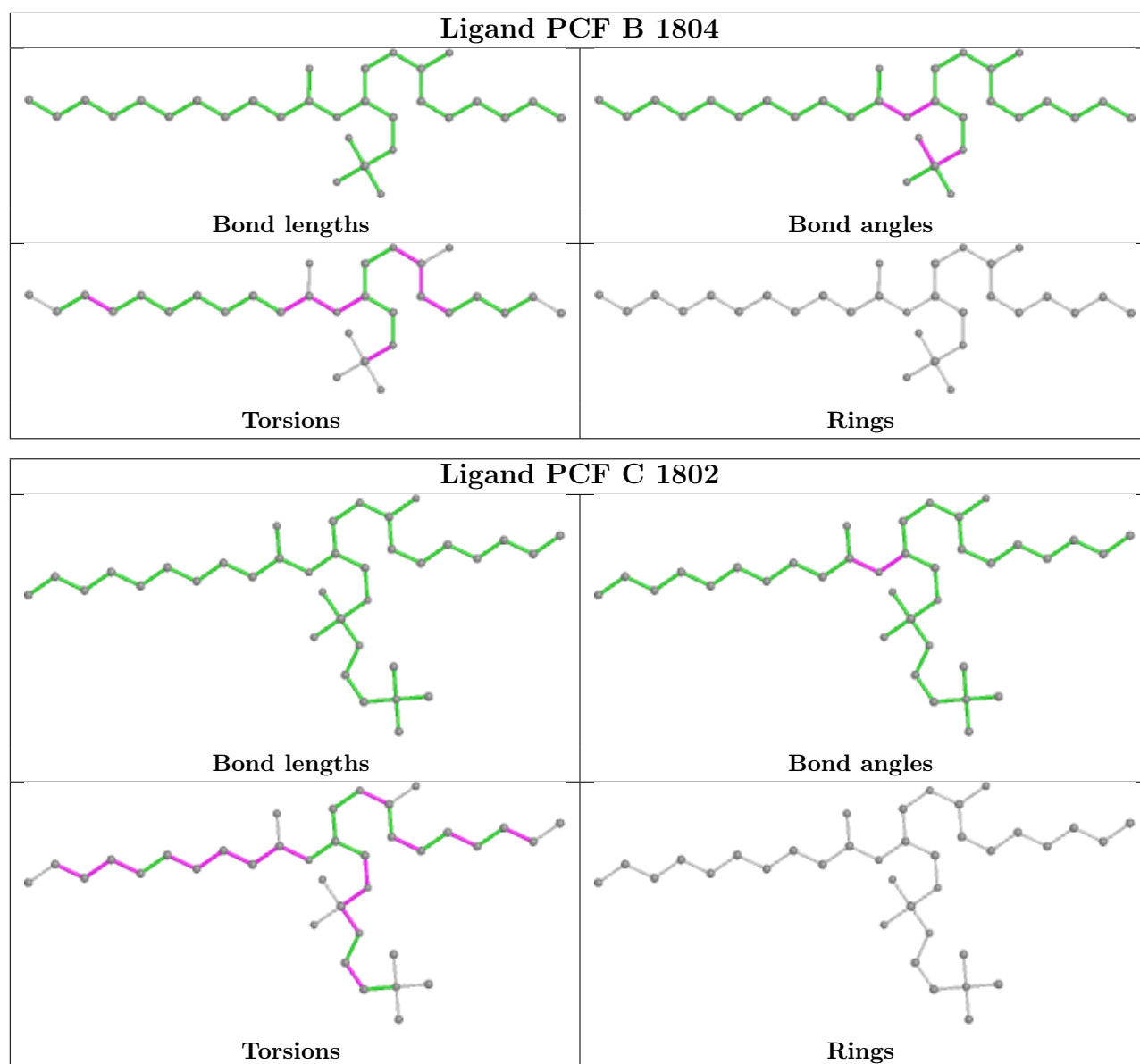
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

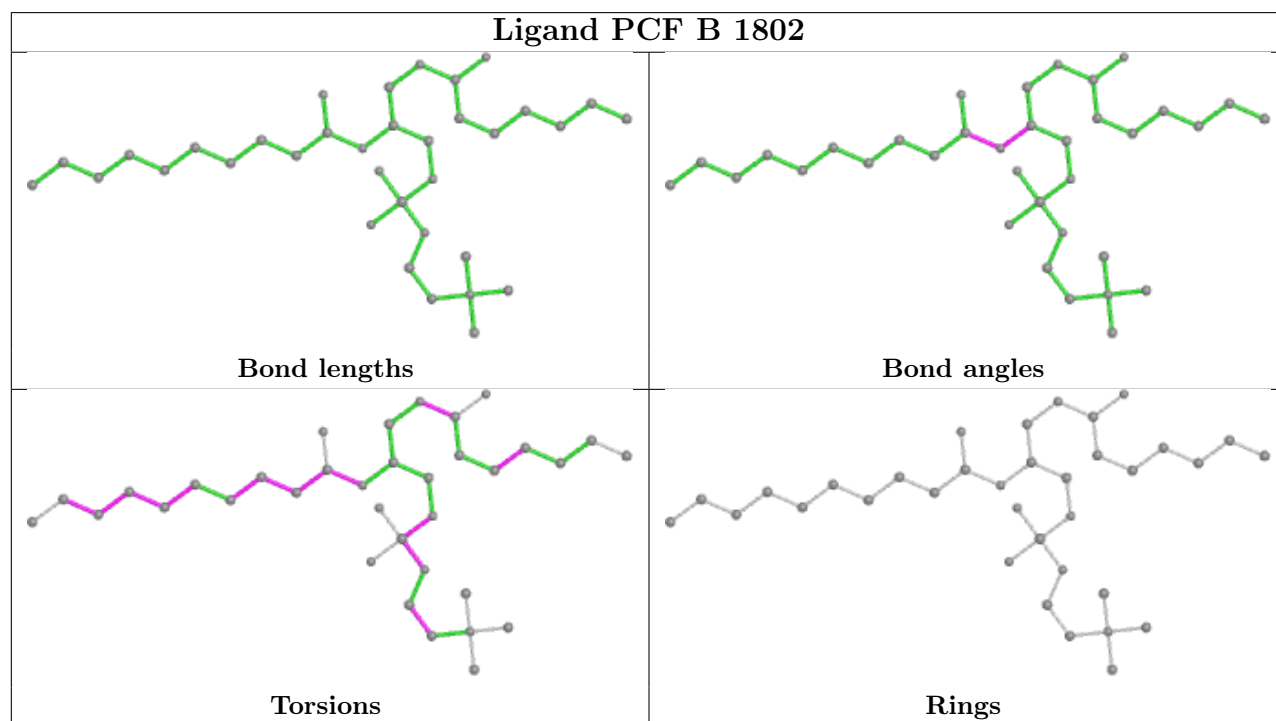
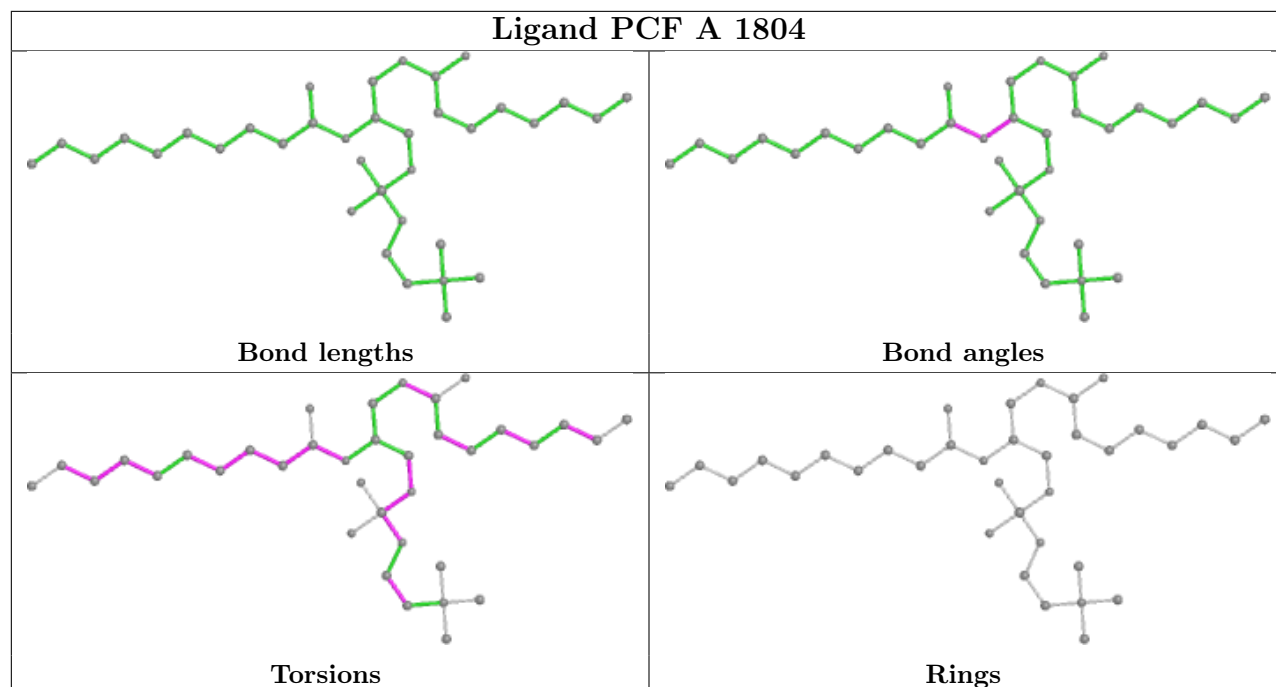


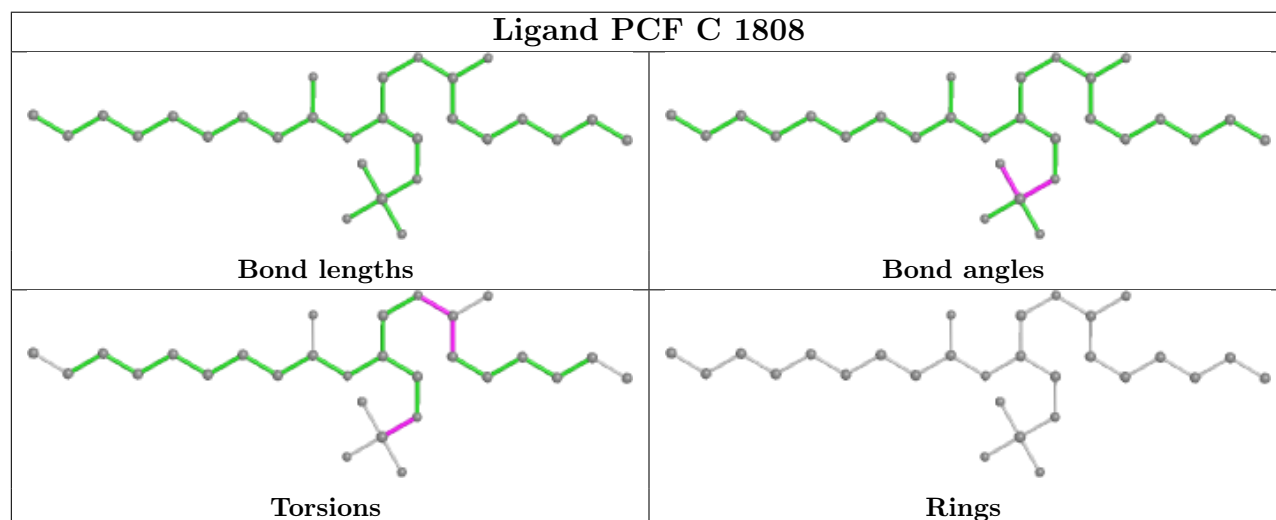
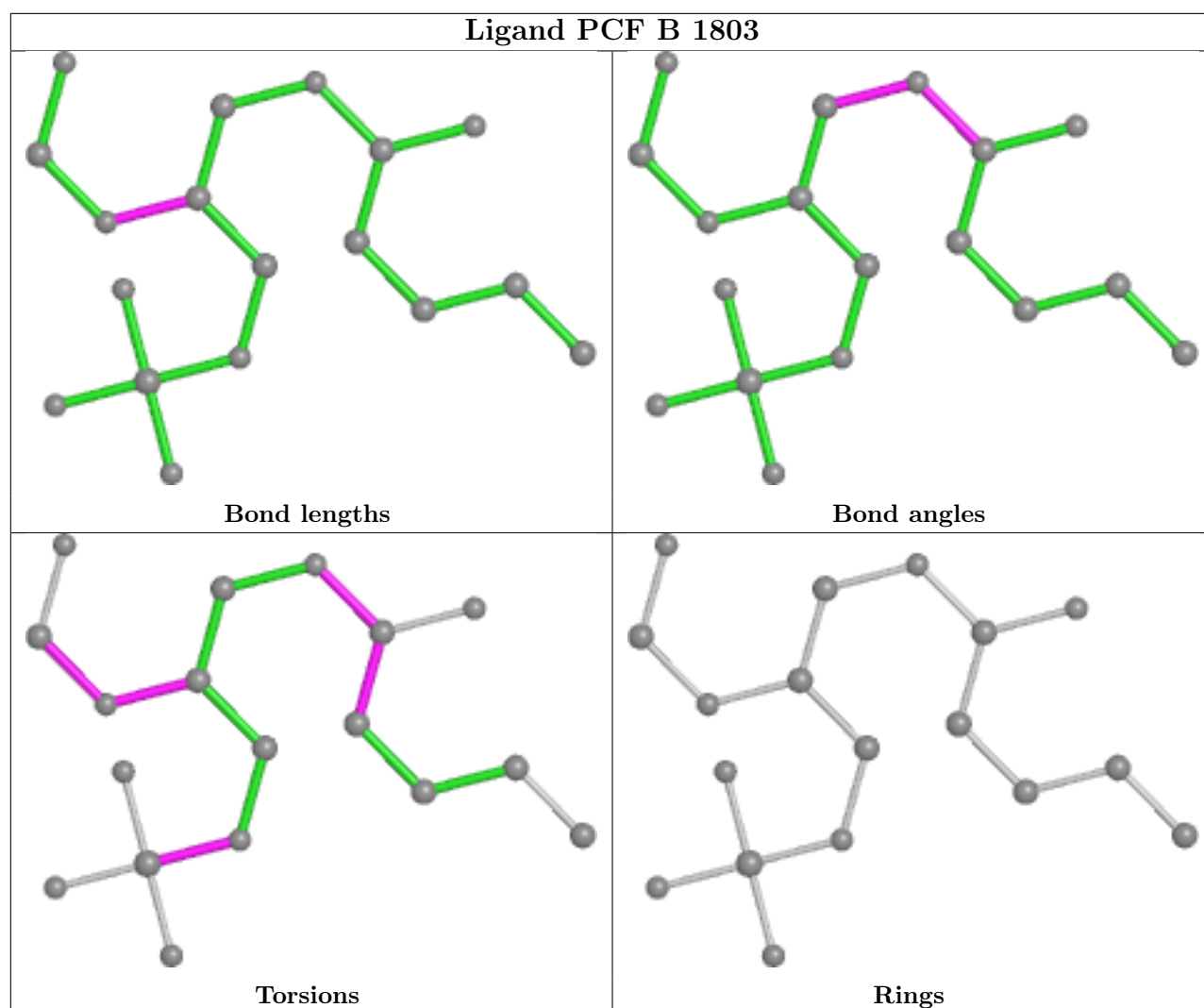


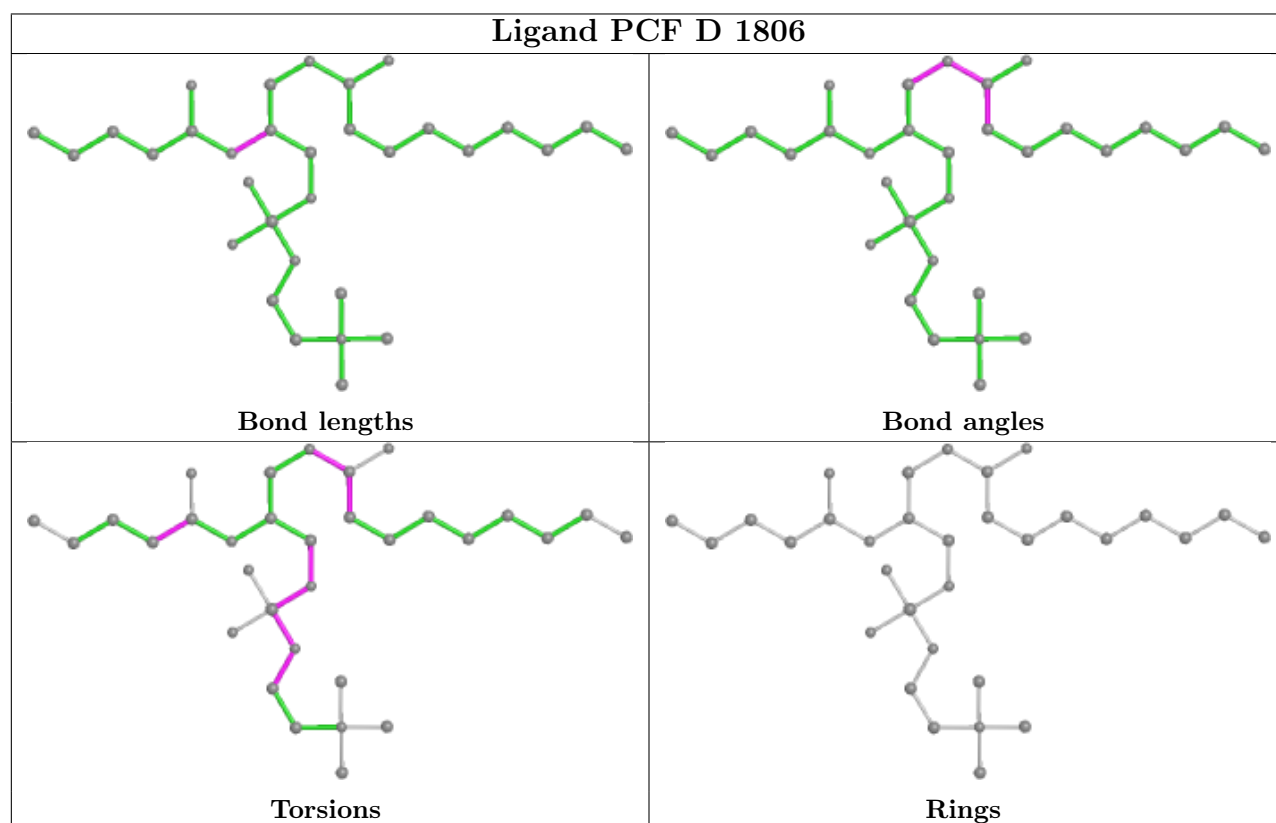
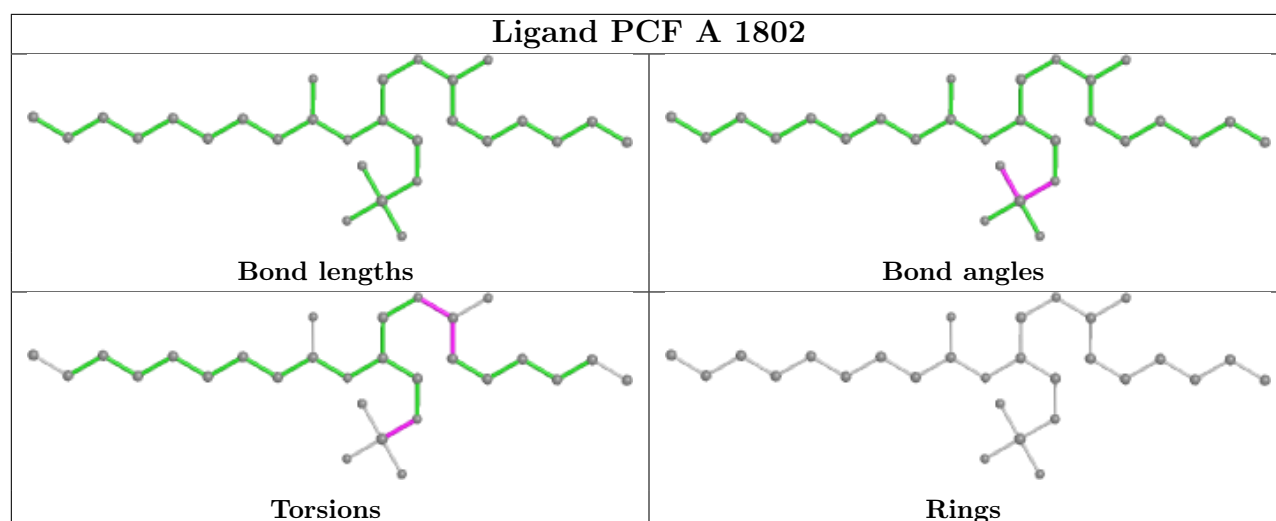




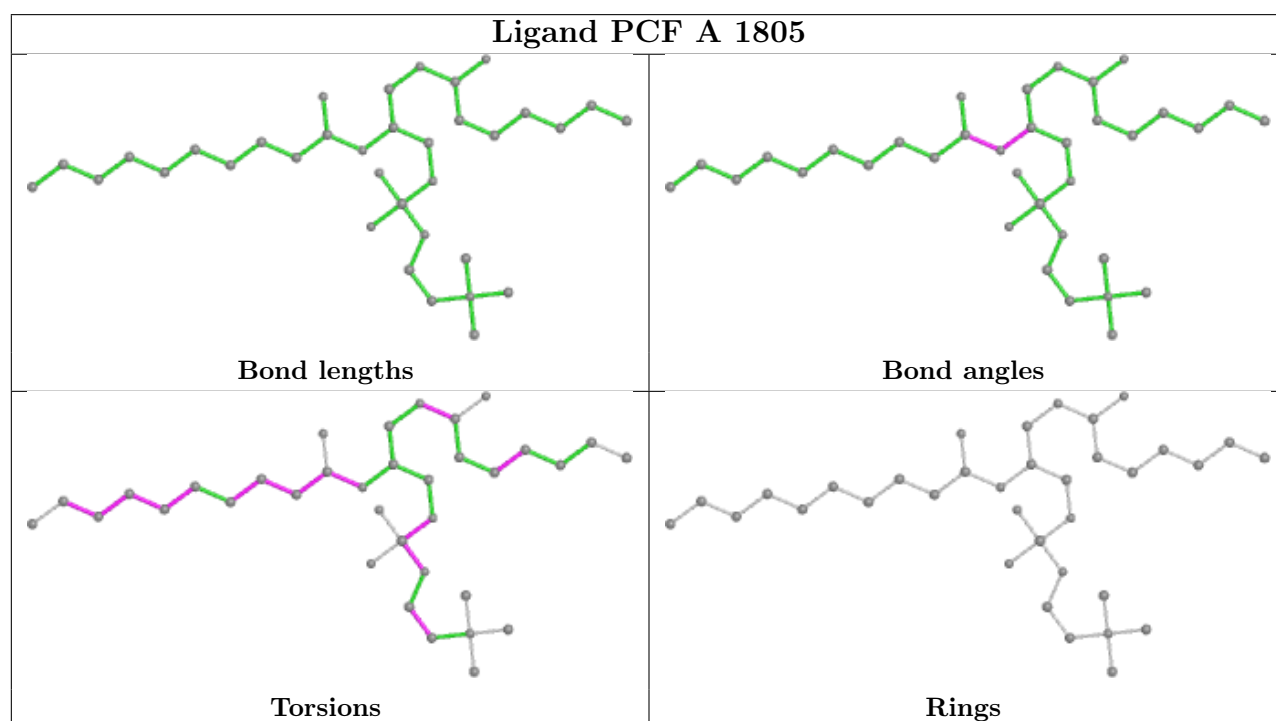
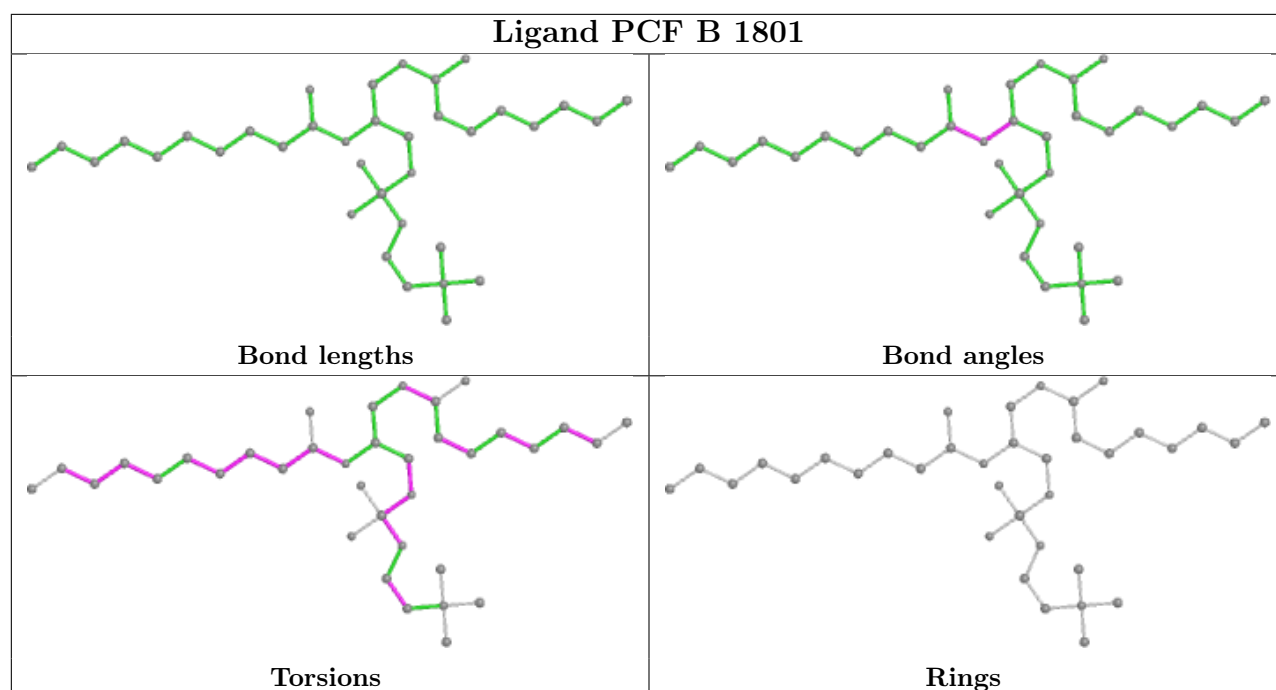


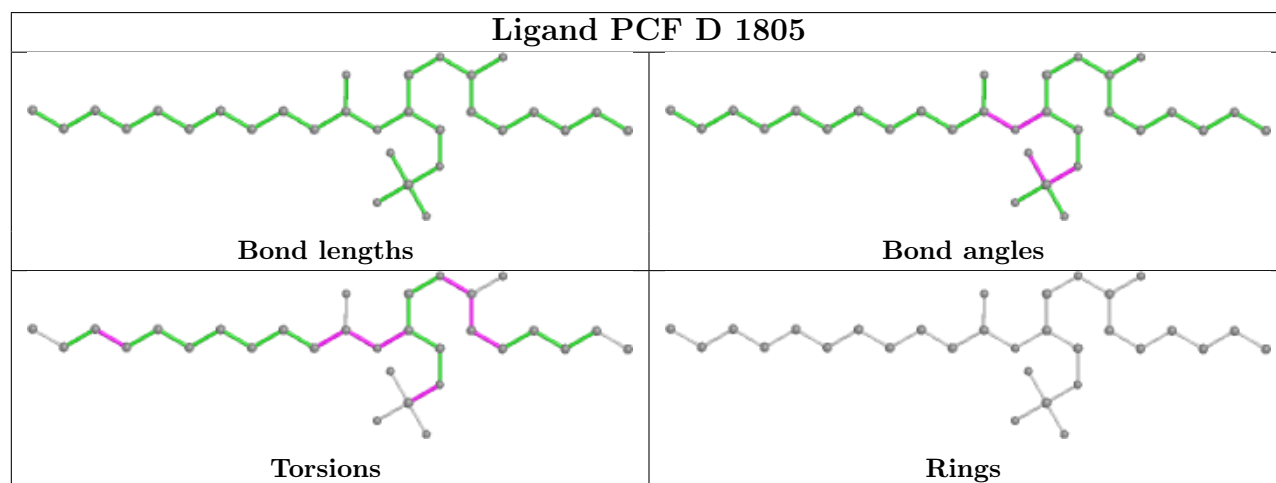
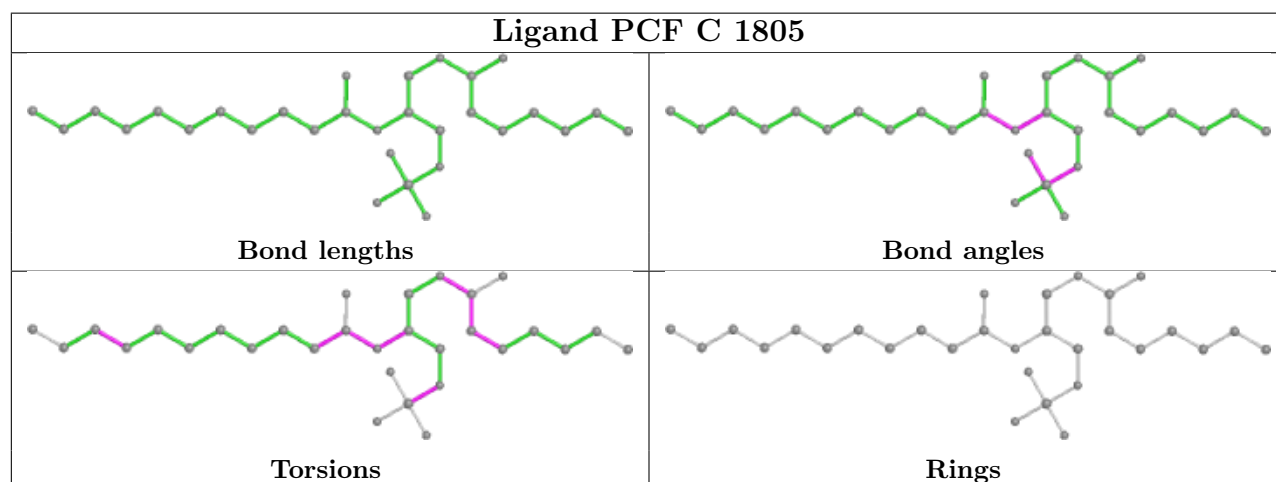
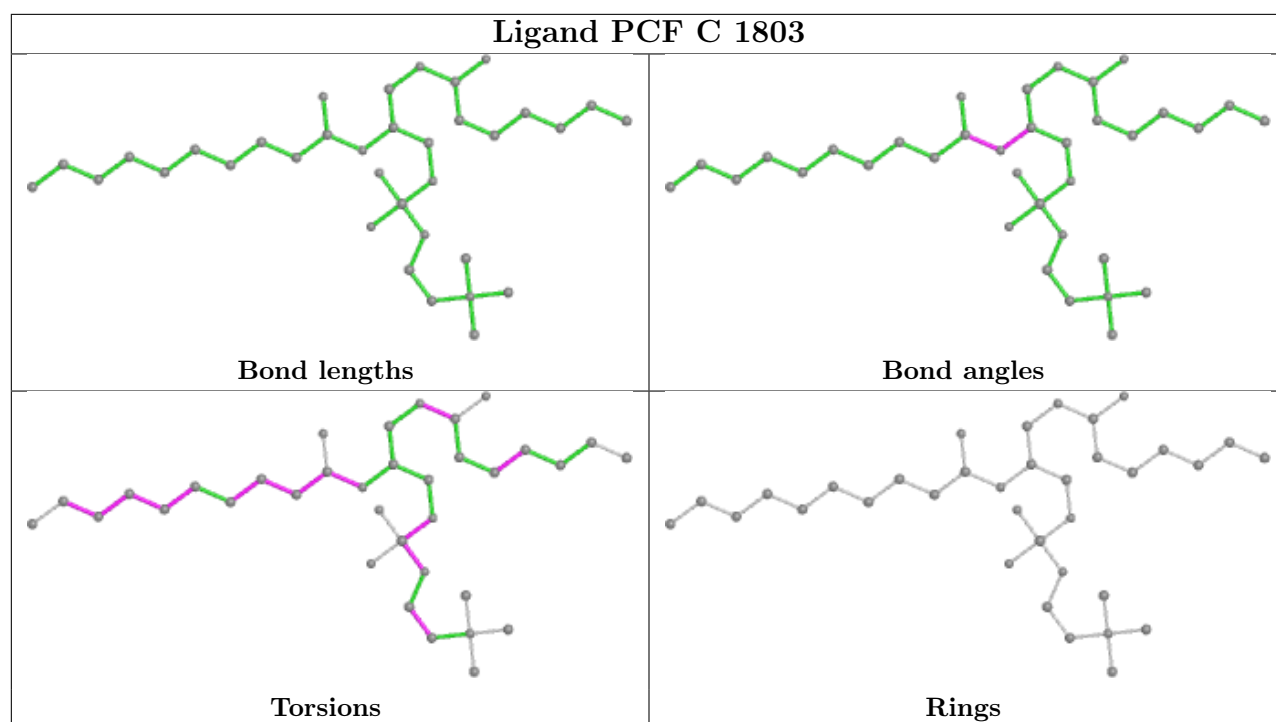


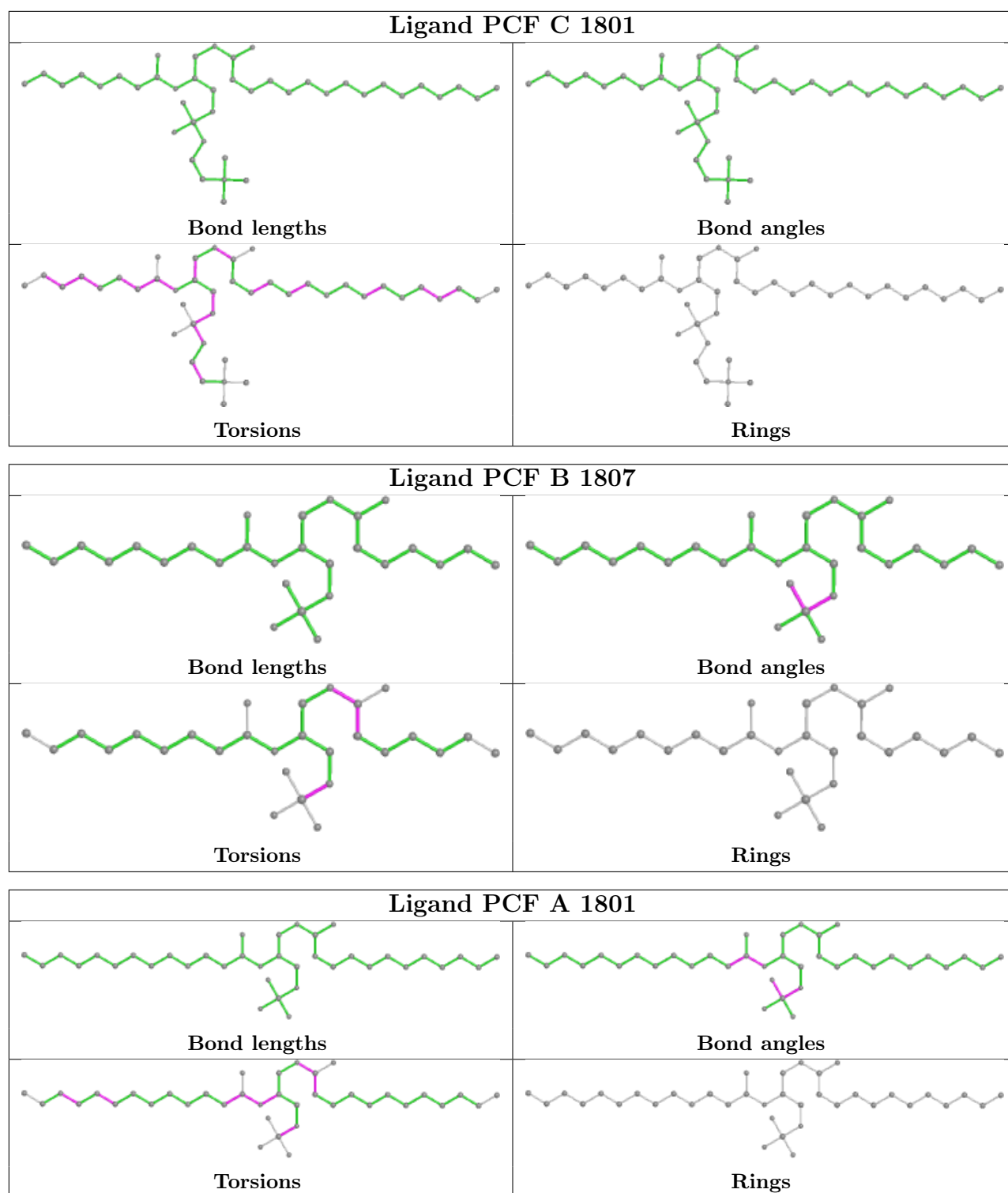


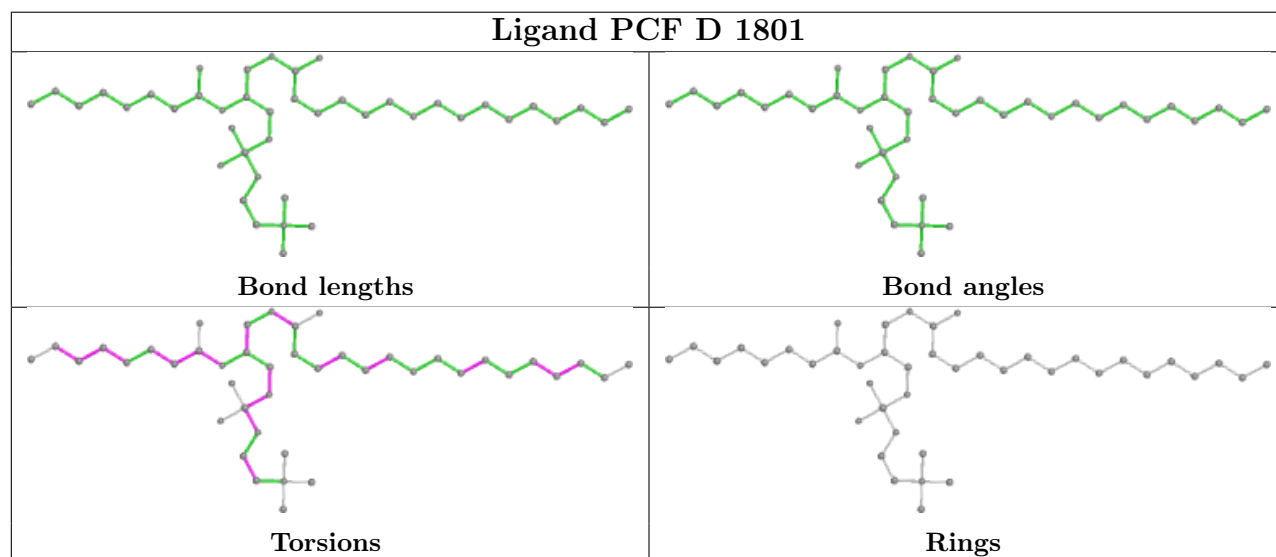
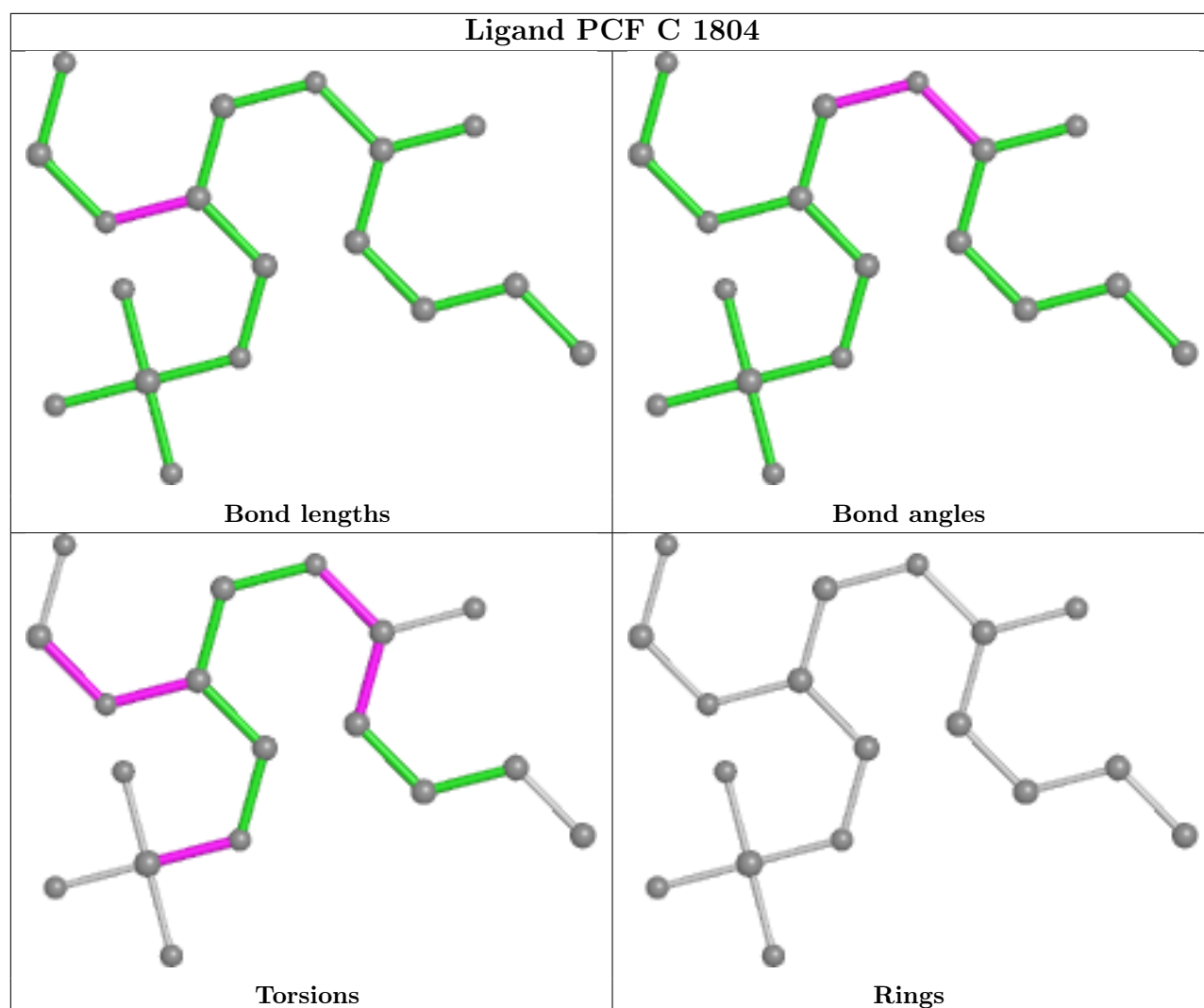


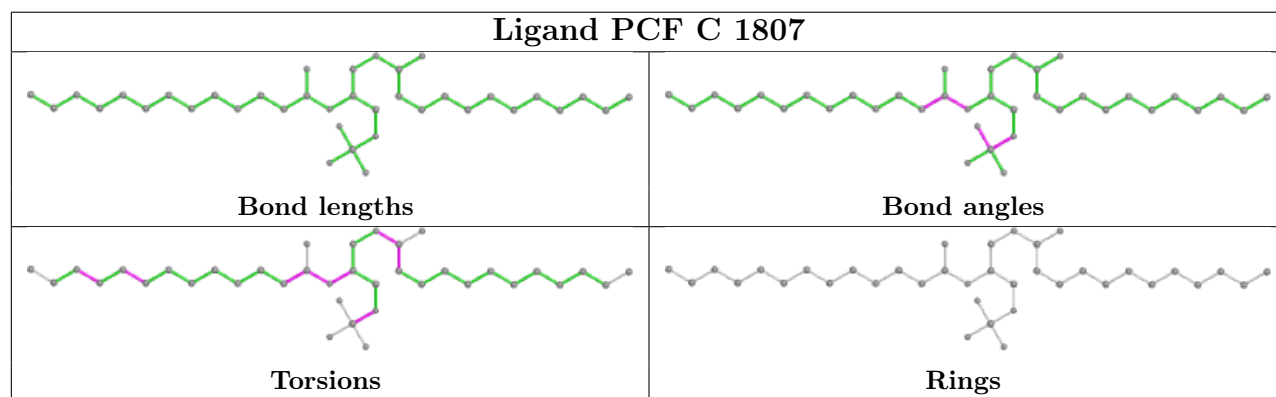
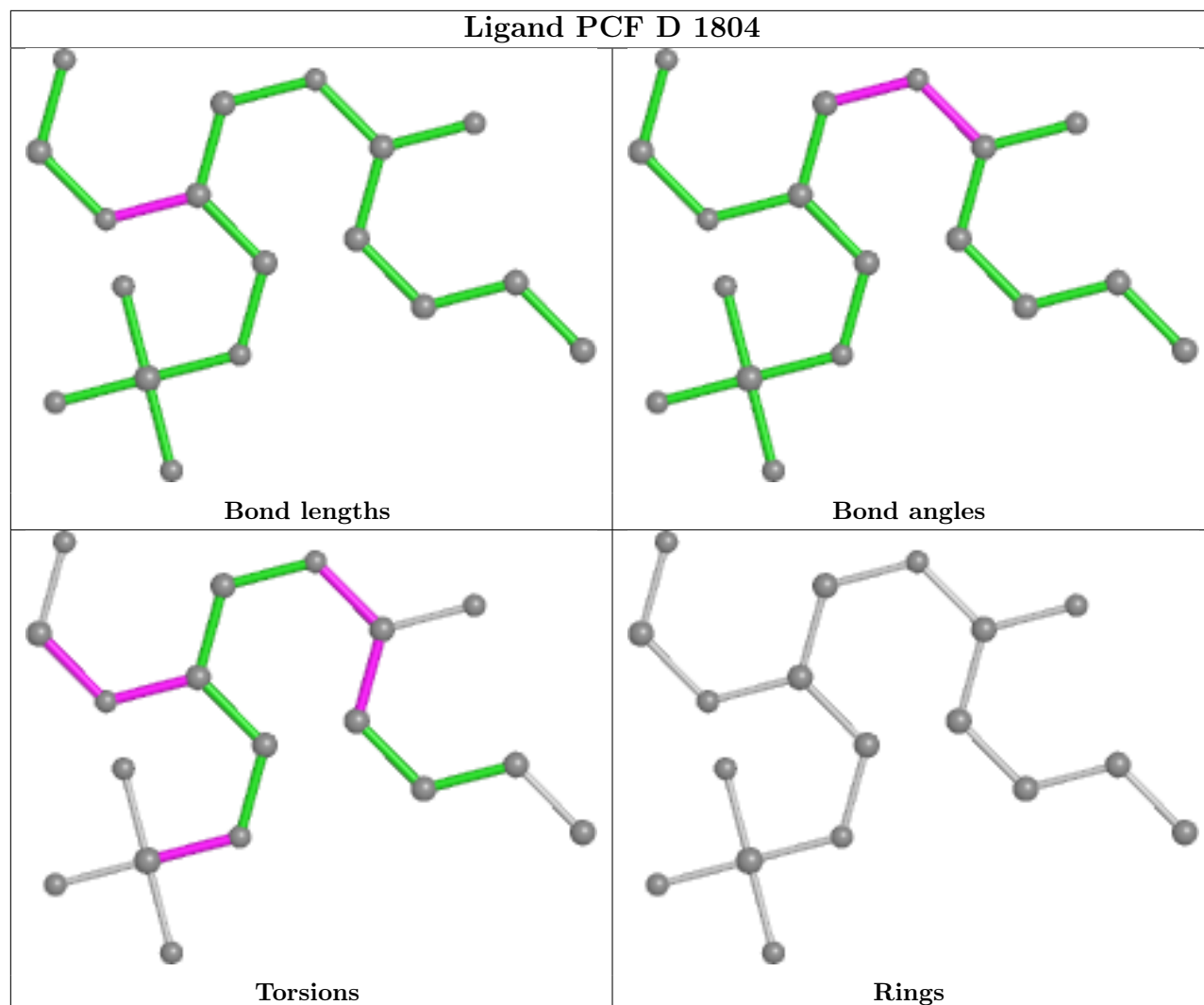


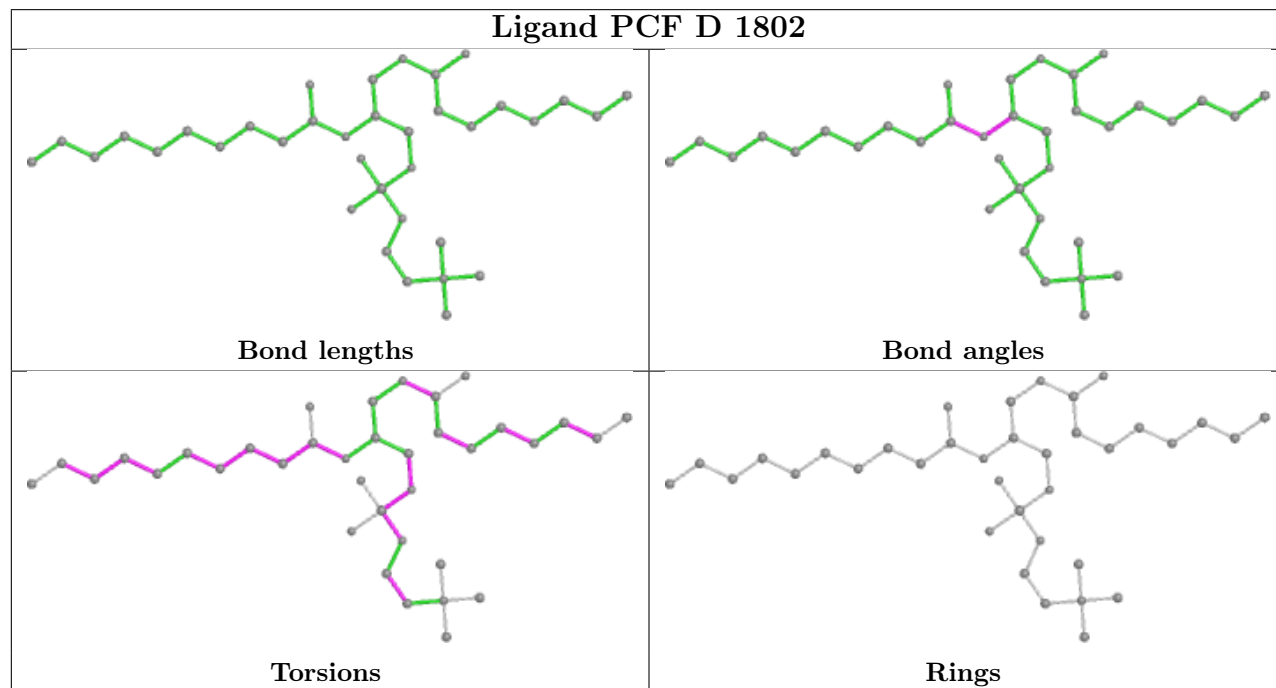
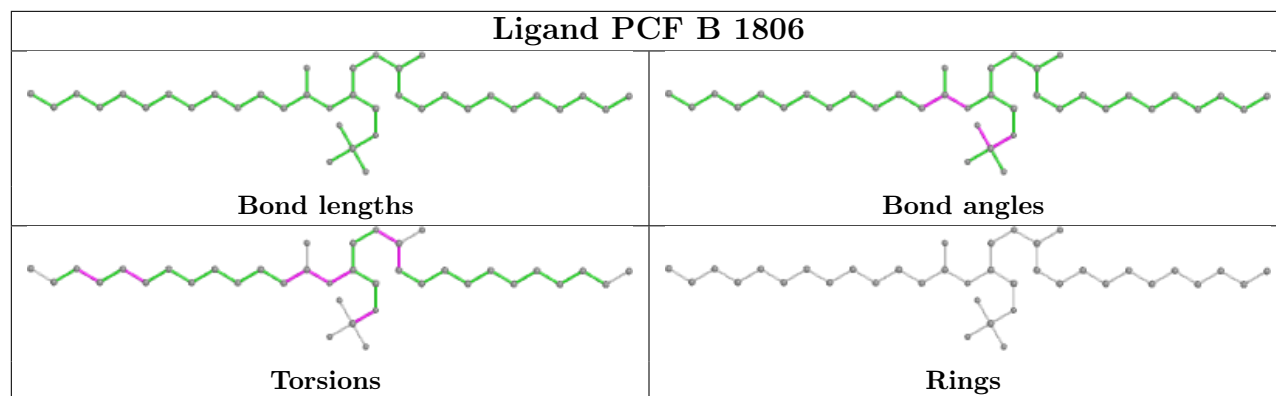


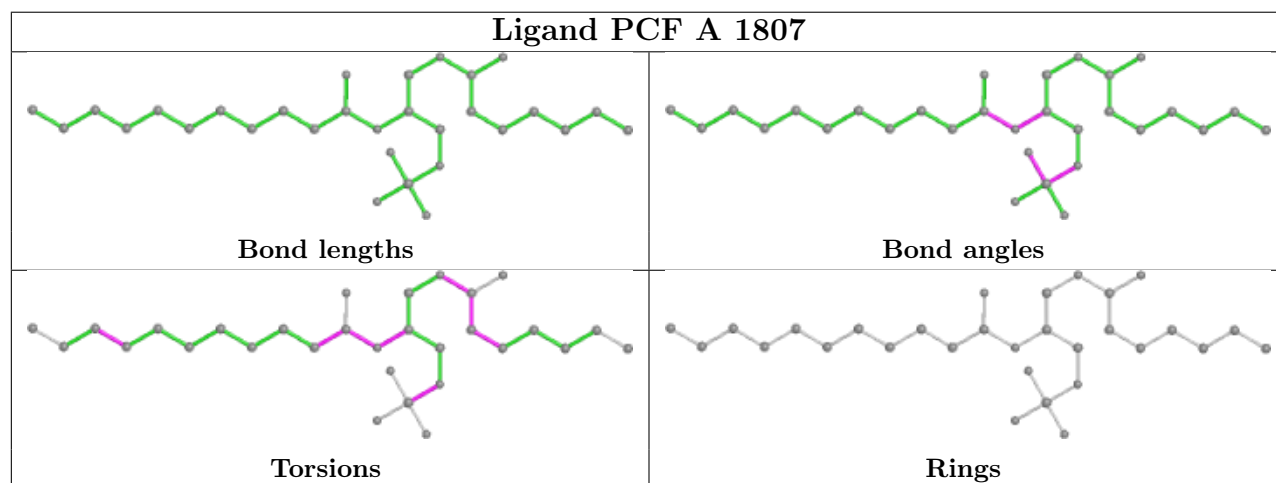
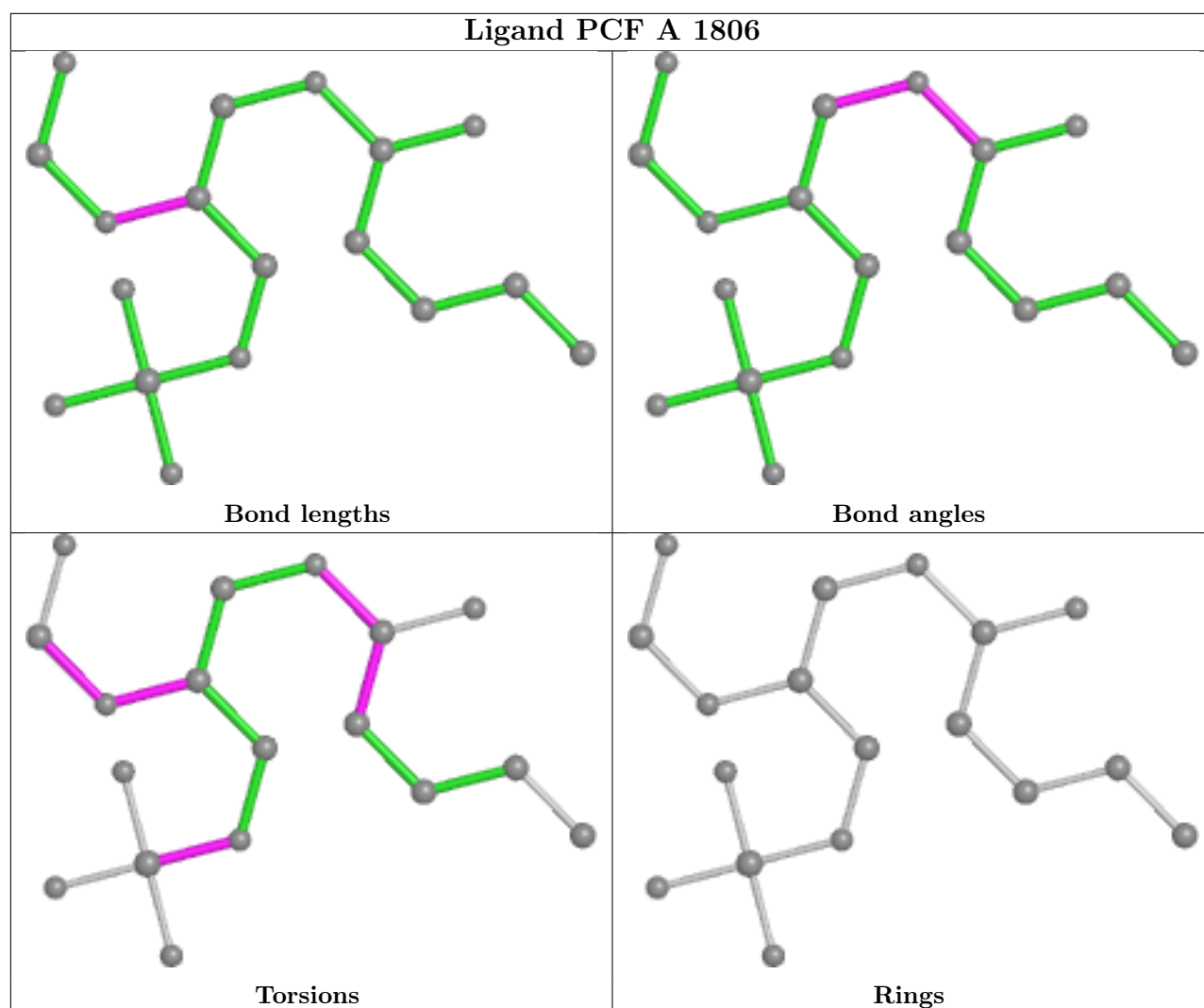


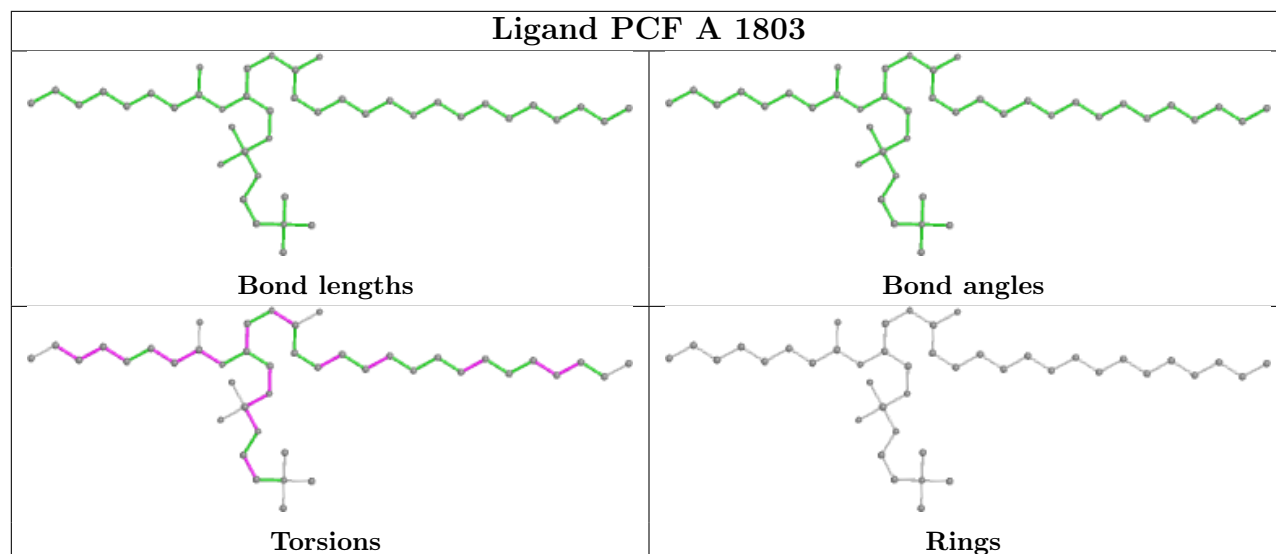












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



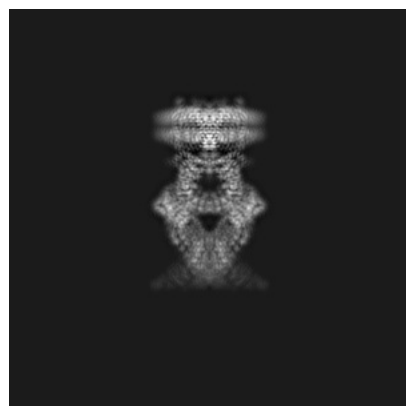
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8702. These allow visual inspection of the internal detail of the map and identification of artifacts.

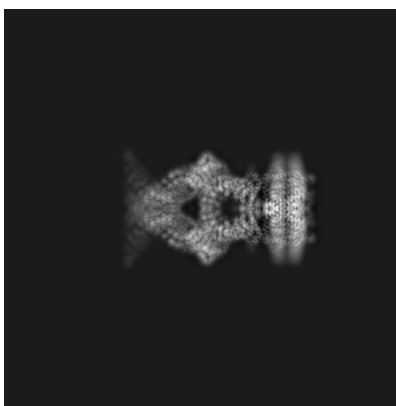
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

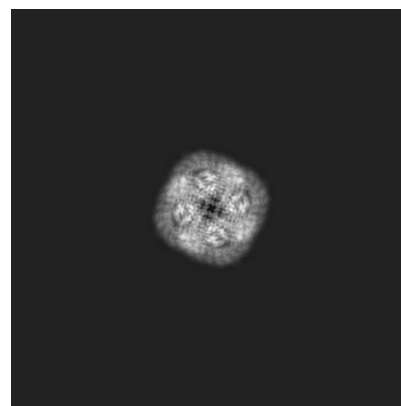
#### 6.1.1 Primary map



X

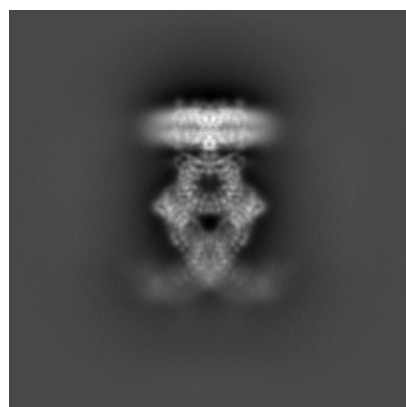


Y

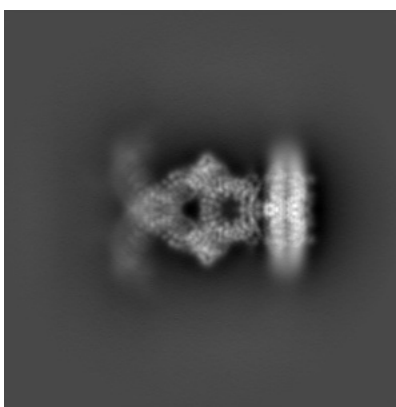


Z

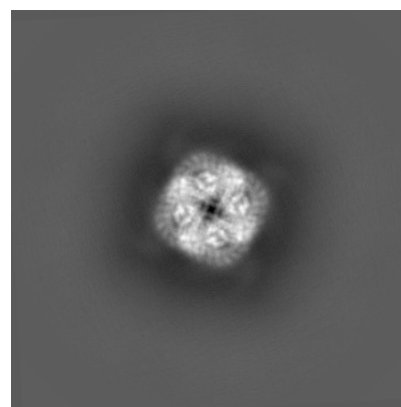
#### 6.1.2 Raw map



X



Y



Z

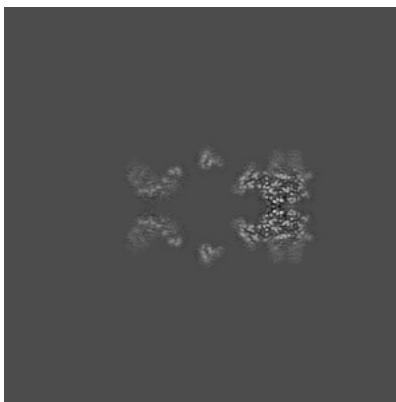
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

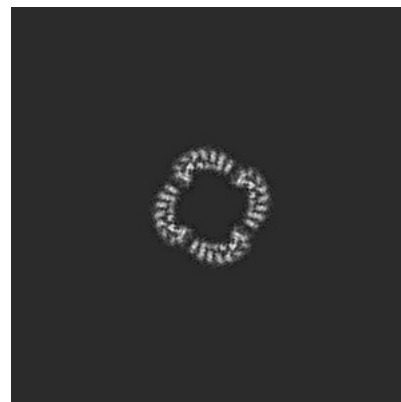
### 6.2.1 Primary map



X Index: 200

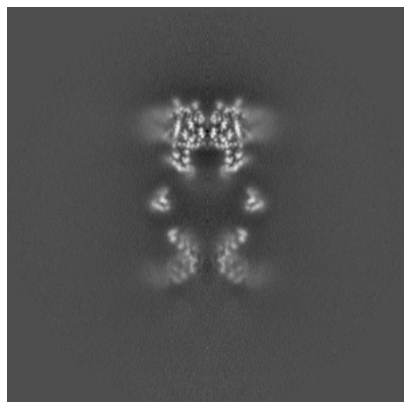


Y Index: 200

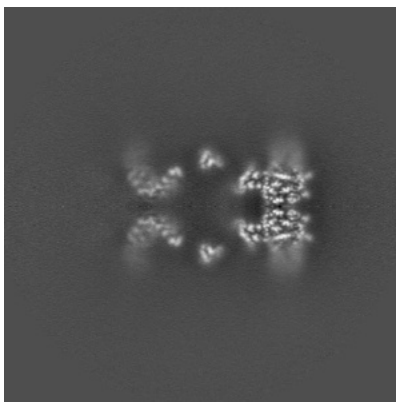


Z Index: 200

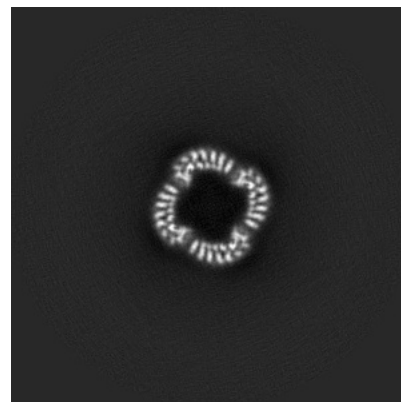
### 6.2.2 Raw map



X Index: 200



Y Index: 200

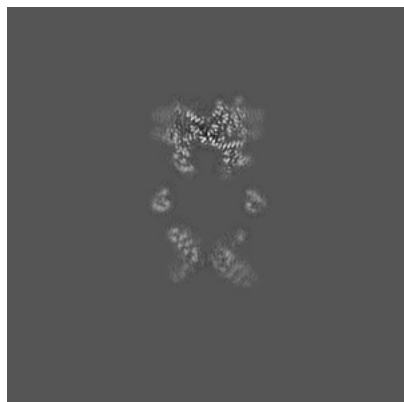


Z Index: 200

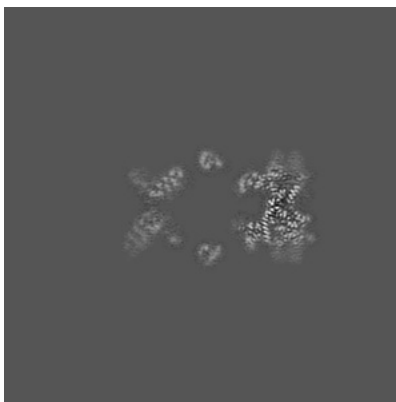
The images above show central slices of the map in three orthogonal directions.

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

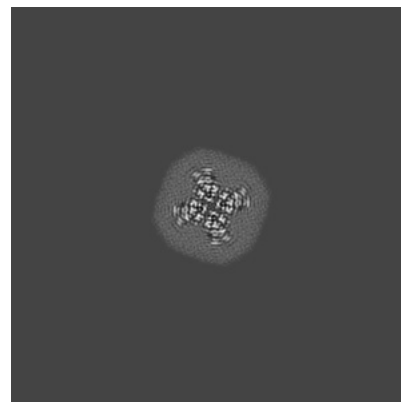
### 6.3.1 Primary map



X Index: 197

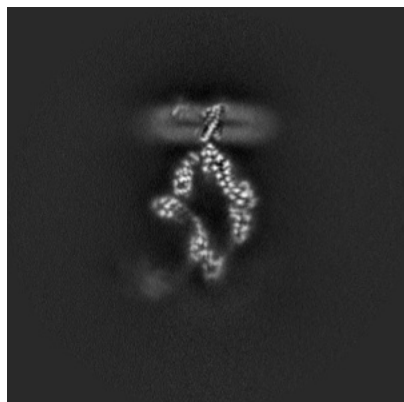


Y Index: 197

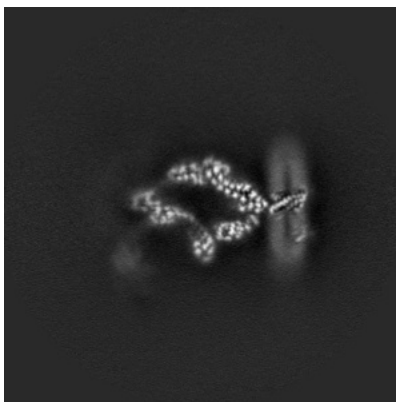


Z Index: 291

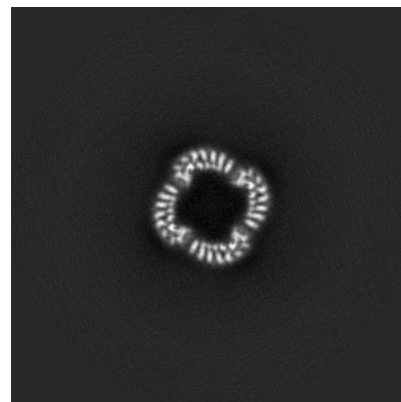
### 6.3.2 Raw map



X Index: 221



Y Index: 179

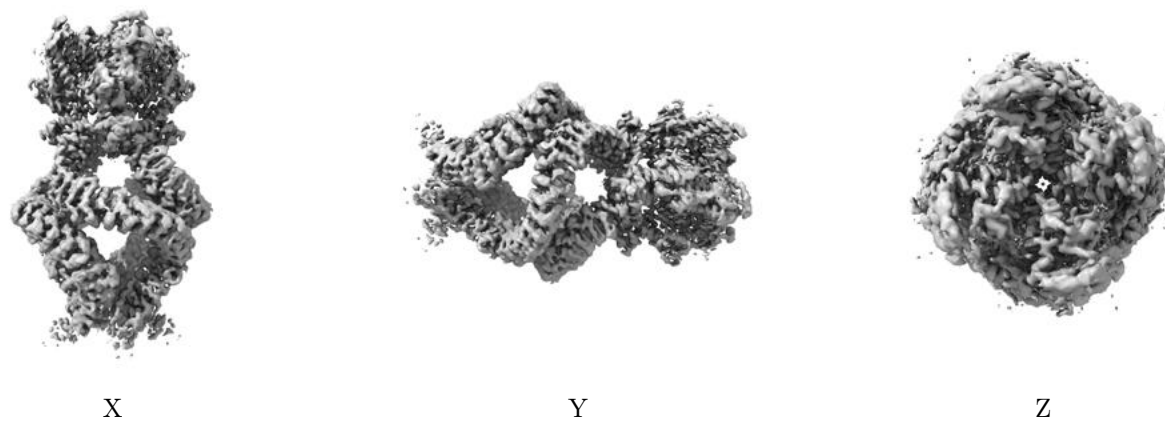


Z Index: 200

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

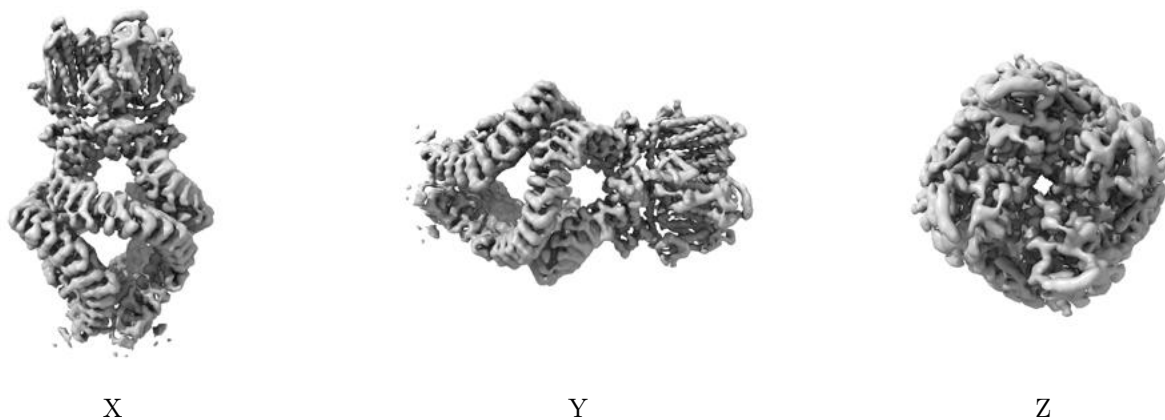
## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 10.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.4.2 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.

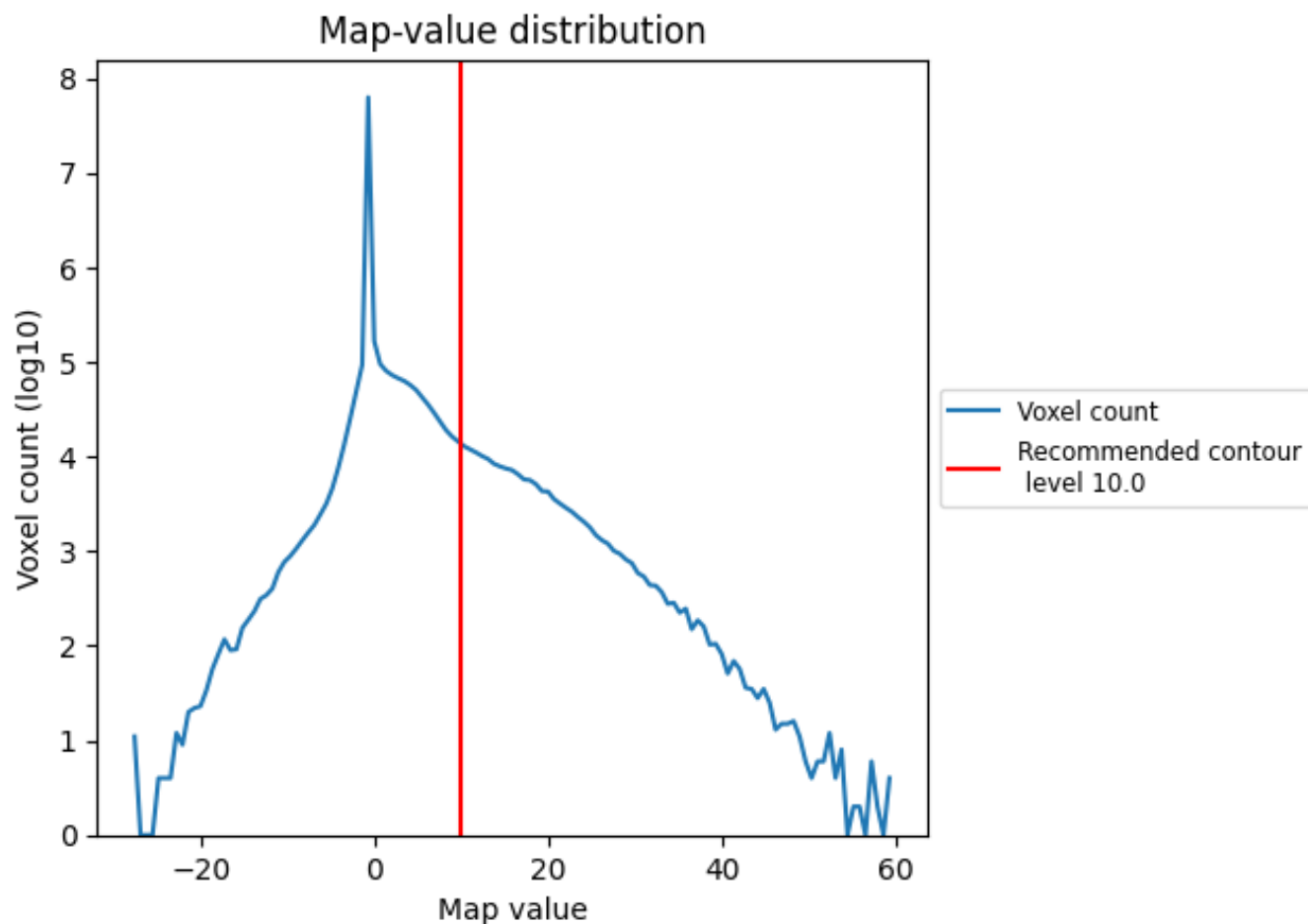
## 6.5 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

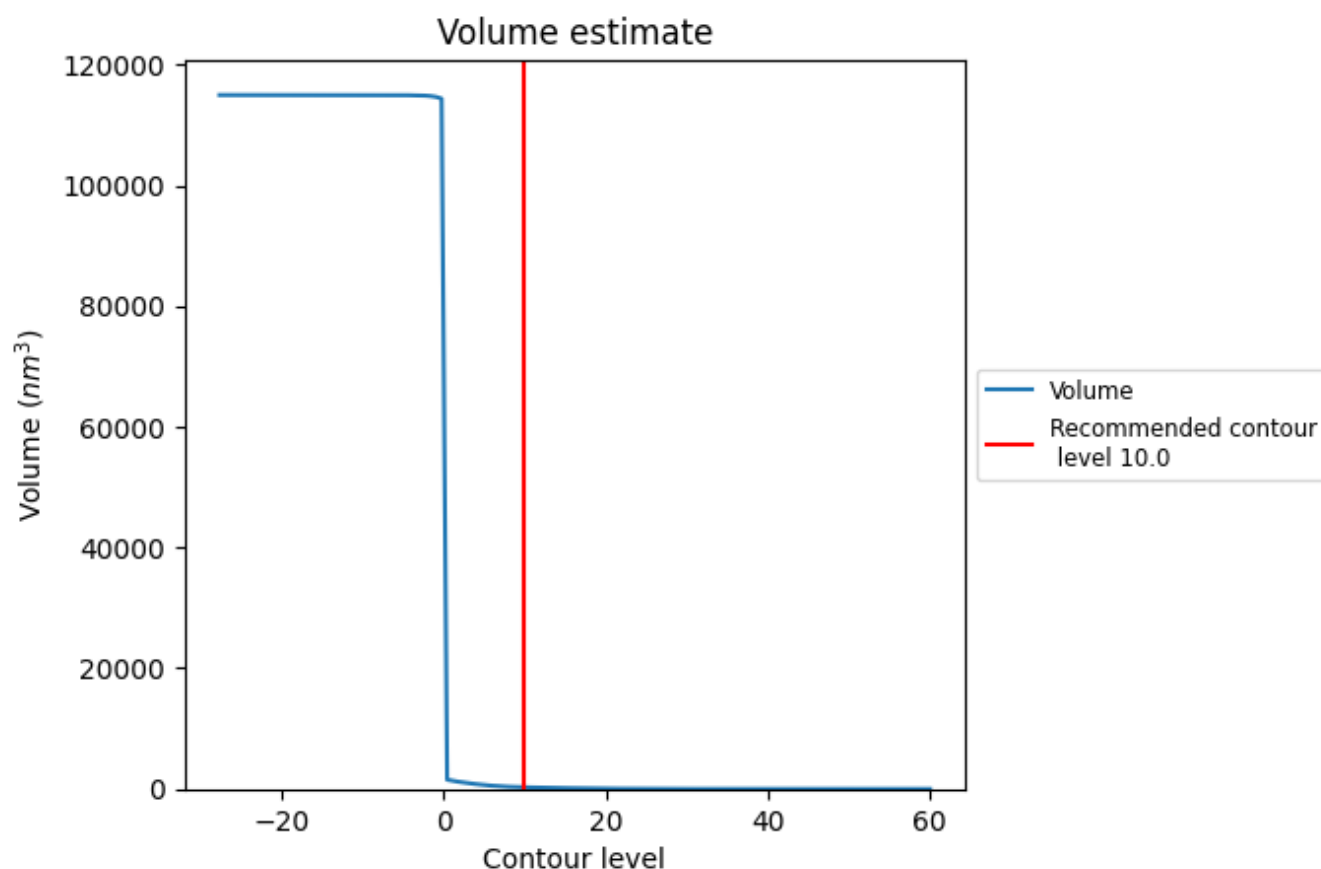
This section contains the results of statistical analysis of the map.

### 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.

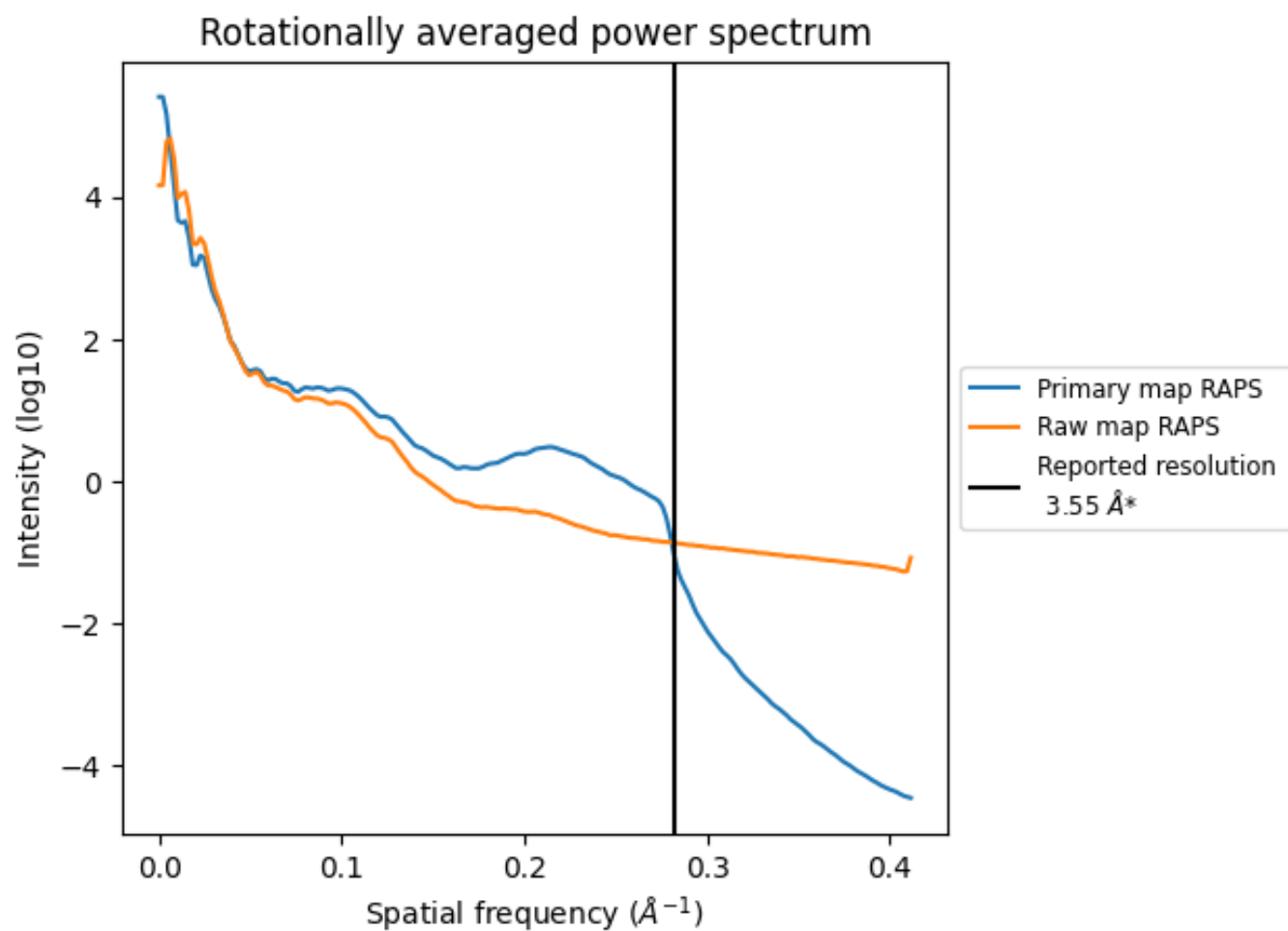
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 278  $\text{nm}^3$ ; this corresponds to an approximate mass of 251 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](#)

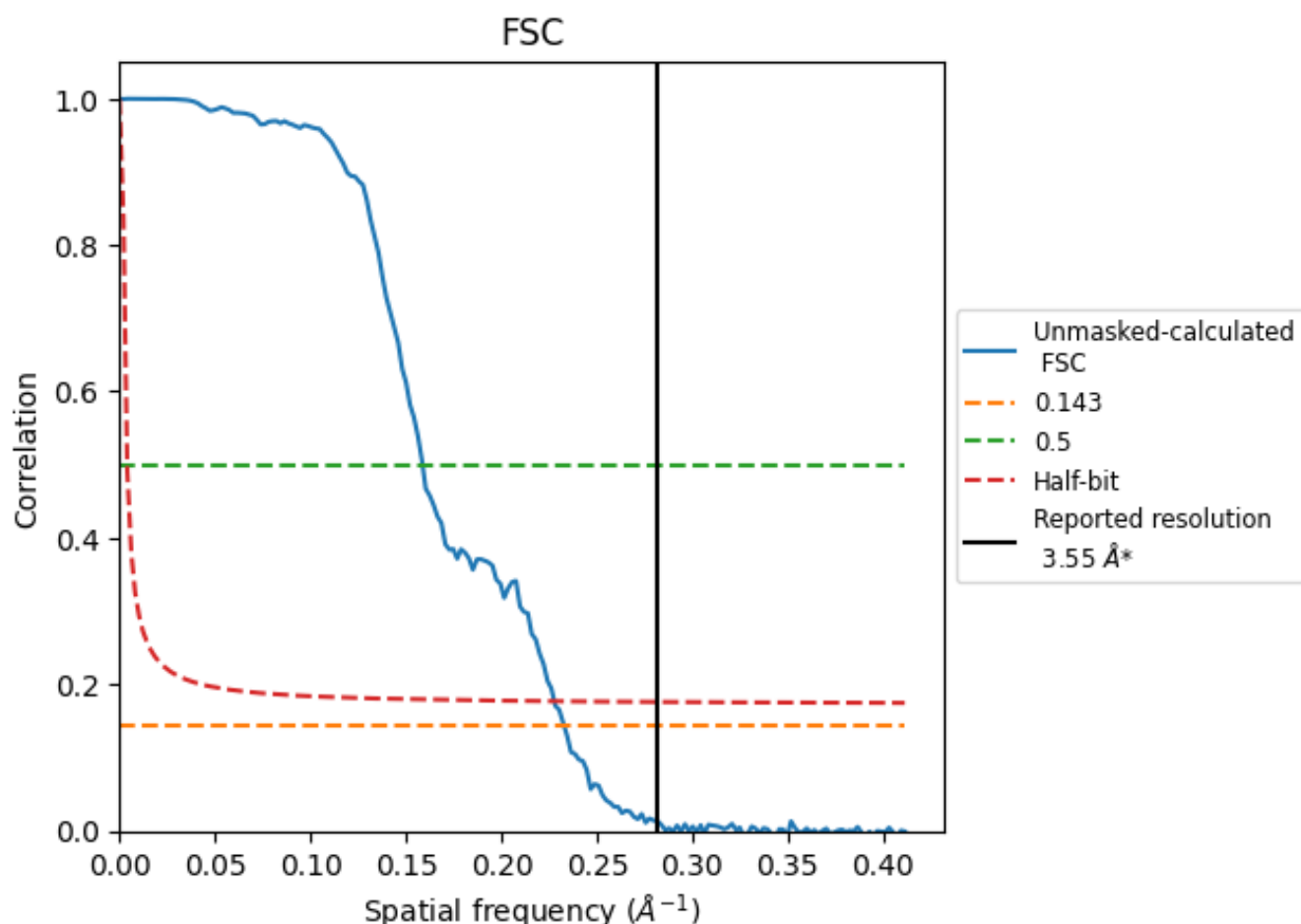


\*Reported resolution corresponds to spatial frequency of  $0.282 \text{ \AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.282  $\text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

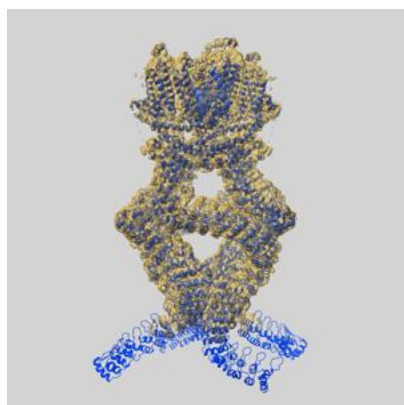
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.55	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.30	6.30	4.39

\*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 4.30 differs from the reported value 3.55 by more than 10 %

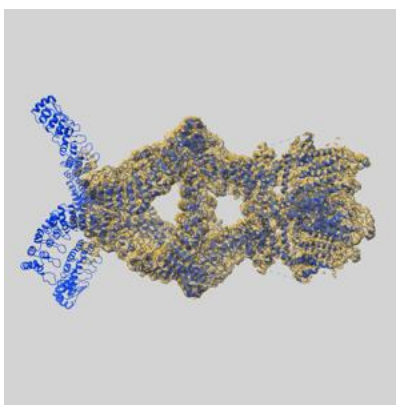
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8702 and PDB model 5VKQ. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

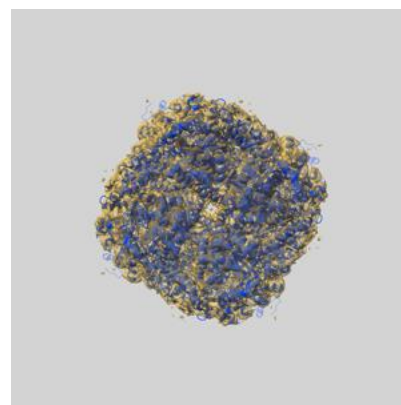
### 9.1 Map-model overlay [i](#)



X



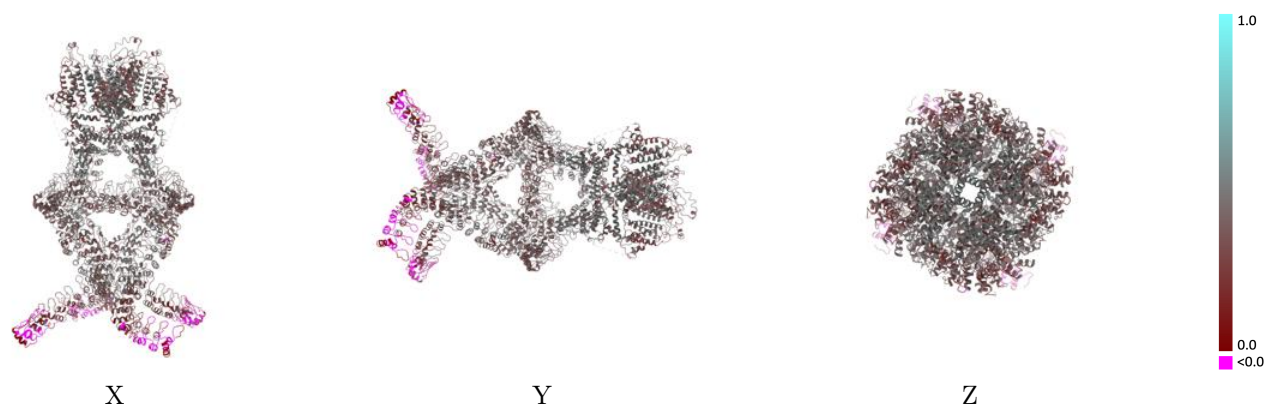
Y



Z

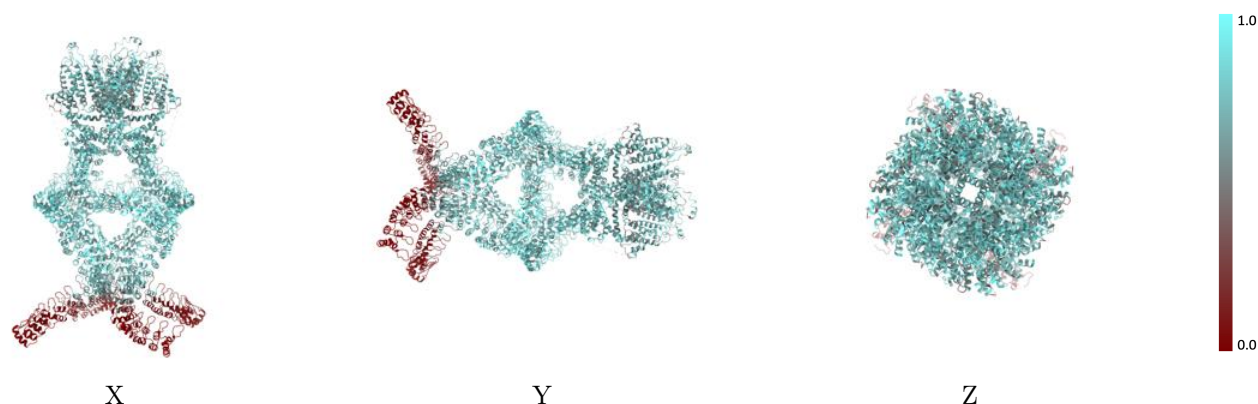
The images above show the 3D surface view of the map at the recommended contour level 10.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



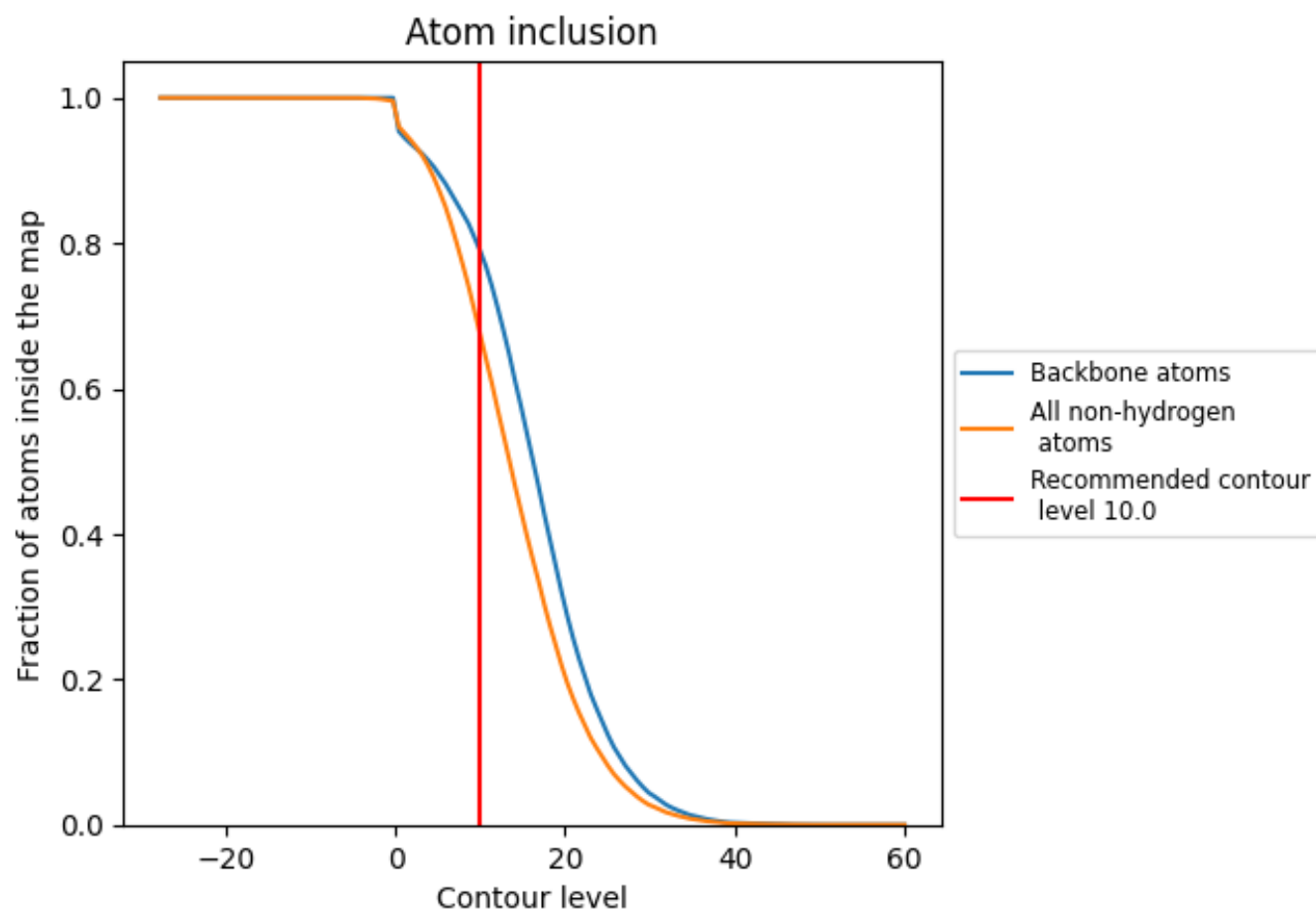
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (10.0).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 68% 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 (10.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6753	<div></div> 0.3780
A	<div></div> 0.6738	<div></div> 0.3770
B	<div></div> 0.6776	<div></div> 0.3840
C	<div></div> 0.6753	<div></div> 0.3760
D	<div></div> 0.6746	<div></div> 0.3760

