Full wwPDB EM Validation Report ⓘ

Nov 2, 2026 – 06:59 pm GMT

PDB ID	:	9I4Y / pdb_00009i4y
EMDB ID	:	EMD-52622
Title	:	Toxoplasma gondii cytochrome c oxidase from the respiratory supercomplex III2-IV
Authors	:	Maclean, A.; Muhleip, A.
Deposited on	:	2025-01-27
Resolution	:	2.95 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

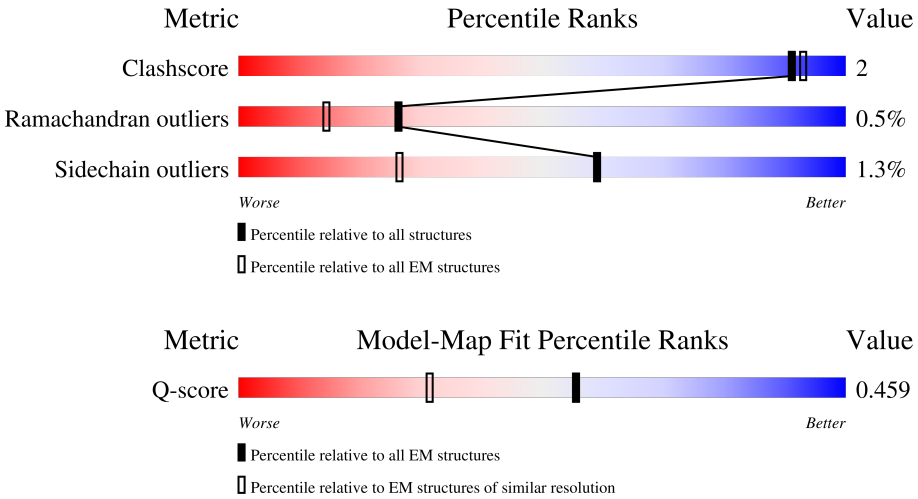
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.95 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.



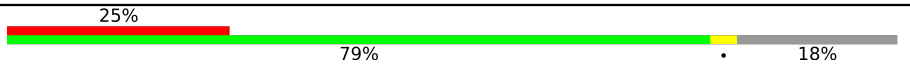
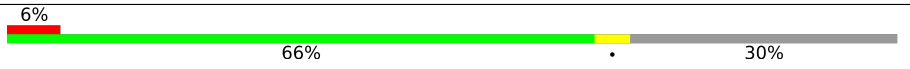
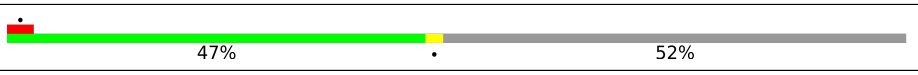
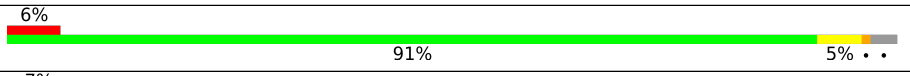
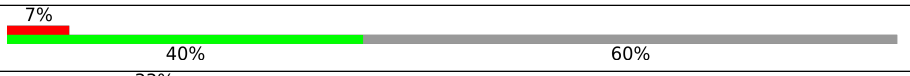
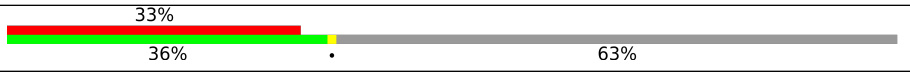
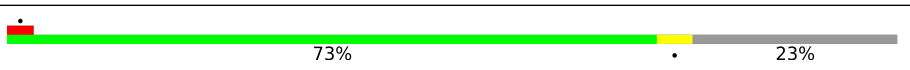
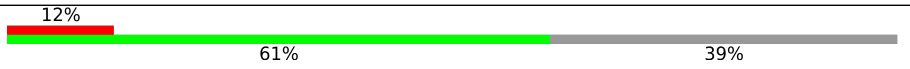
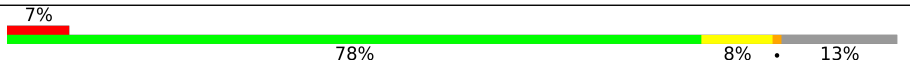
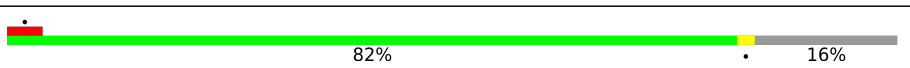
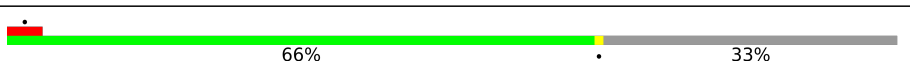
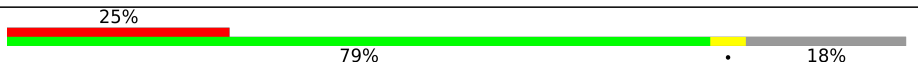
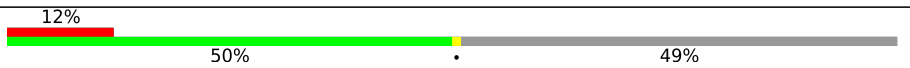
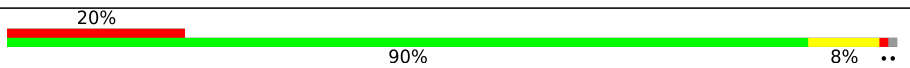
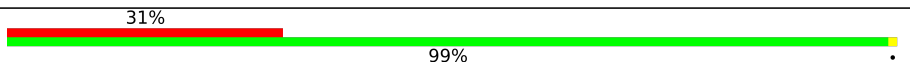
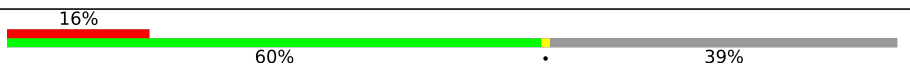
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13114 (2.45 - 3.45)

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

Mol	Chain	Length	Quality of chain
1	4B	299	5% 49% 49%
2	4C	191	65% 5% 30%
3	4D	108	5% 43% 55%
4	4E	244	85% 11%

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Mol	Chain	Length	Quality of chain
5	4F	204	
6	4G	310	
7	4H	220	
8	4I	191	
9	4J	307	
10	4K	119	
11	4L	165	
12	4M	152	
13	4N	220	
14	4O	266	
15	4P	218	
16	4Q	199	
17	4R	169	
18	4S	167	
19	4T	159	
20	4U	142	
21	4V	136	
22	4W	118	
23	4X	86	
24	4Y	67	
25	B	491	

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 60819 atoms, of which 30544 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 Putative cytochrome C oxidase subunit IIa.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	4B	151	2463	818	1204	213	219	9	0	0

- Molecule 2 is a protein called Cytochrome c oxidase polypeptide II.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	4C	134	2135	690	1064	180	196	5	0	0

- Molecule 3 is a protein called Cytochrome C family oxidase subunit II, transmembrane domain protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
3	4D	49	784	261	382	71	63	7	0	0

- Molecule 4 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	4E	238	3776	1247	1910	278	328	13	0	0

- Molecule 5 is a protein called Cg8 family protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
5	4F	167	2733	900	1338	248	243	4	0	0

- Molecule 6 is a protein called Putative cytochrome c oxidase subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
6	4G	229	3680	1204	1810	308	343	15	0	0

- Molecule 7 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	4H	155	Total	C	H	N	O	S	0	0
			2534	820	1269	217	220	8		

- Molecule 8 is a protein called Cytochrome c oxidase subunit 6B.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	4I	92	Total	C	H	N	O	S	0	0
			1493	480	717	141	146	9		

- Molecule 9 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	4J	222	Total	C	H	N	O	S	0	0
			3637	1218	1787	301	322	9		

- Molecule 10 is a protein called Membrane protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	4K	115	Total	C	H	N	O	S	0	0
			1869	625	913	166	160	5		

- Molecule 11 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	4L	66	Total	C	H	N	O	S	0	0
			1052	361	508	82	98	3		

- Molecule 12 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	4M	56	Total	C	H	N	O	S	0	0
			913	300	447	80	83	3		

- Molecule 13 is a protein called NADH-ubiquinone reductase complex 1 MLRQ subunit.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	4N	170	Total	C	H	N	O	S	0	0
			2799	936	1358	255	240	10		

- Molecule 14 is a protein called ApiCox30, TGGT1_297810.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	4O	163	Total	C	H	N	O	S	0	0
			2621	834	1304	217	261	5		

- Molecule 15 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	4P	189	Total	C	H	N	O	S	0	0
			3104	1028	1523	276	267	10		

- Molecule 16 is a protein called ApiCox22, TGGT1_312160.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	4Q	83	Total	C	H	N	O	S	0	0
			1322	426	654	113	124	5		

- Molecule 17 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	4R	80	Total	C	H	N	O	S	0	0
			1217	402	599	108	106	2		

- Molecule 18 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	4S	141	Total	C	H	N	O	S	0	0
			2296	759	1127	213	192	5		

- Molecule 19 is a protein called ApiCox18, TGGT1_221510.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	4T	107	Total	C	H	N	O	S	0	0
			1726	559	851	146	165	5		

- Molecule 20 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	4U	117	Total	C	H	N	O	S	0	0
			1833	582	922	166	157	6		

- Molecule 21 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	4V	70	Total	C	H	N	O	0	0
			1130	372	555	99	104		

- Molecule 22 is a protein called Zinc finger CDGSH-type domain-containing protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	4W	117	Total	C	H	N	O	S	0	0
			1788	591	874	156	156	11		

- Molecule 23 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	4X	86	Total	C	H	N	O	S	0	0
			1408	464	701	121	115	7		

- Molecule 24 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	4Y	41	Total	C	H	N	O	S	0	0
			673	225	343	56	47	2		

- Molecule 25 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	B	478	Total	C	H	N	O	S	0	0
			7449	2467	3742	561	642	37		

There are 13 discrepancies between the modelled and reference sequences:

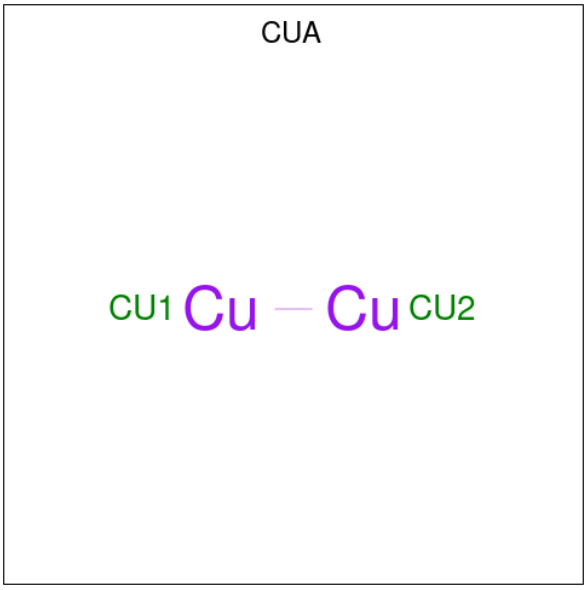
Chain	Residue	Modelled	Actual	Comment	Reference
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B	7	LEU	-	expression tag	UNP M1FK69
B	8	LYS	-	expression tag	UNP M1FK69
B	9	SER	-	expression tag	UNP M1FK69
B	10	ASN	-	expression tag	UNP M1FK69
B	11	THR	-	expression tag	UNP M1FK69
B	12	PHE	-	expression tag	UNP M1FK69
B	13	SER	-	expression tag	UNP M1FK69
B	14	CYS	-	expression tag	UNP M1FK69
B	15	LEU	-	expression tag	UNP M1FK69
B	16	LYS	-	expression tag	UNP M1FK69
B	17	GLN	-	expression tag	UNP M1FK69

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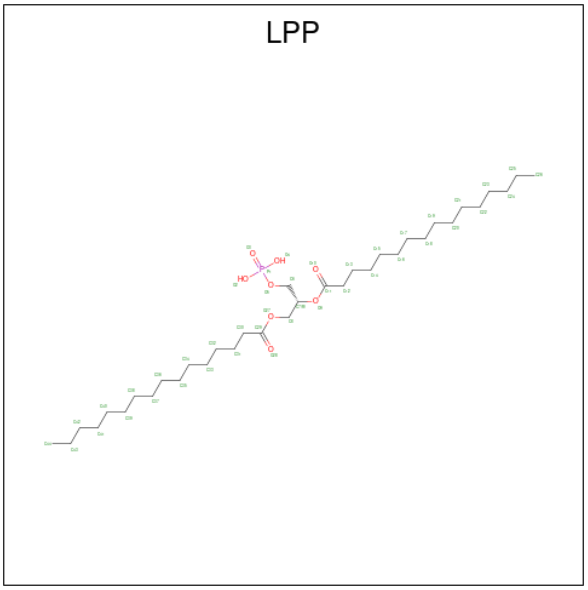
Chain	Residue	Modelled	Actual	Comment	Reference
B	18	SER	-	expression tag	UNP M1FK69

- Molecule 26 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu_2).



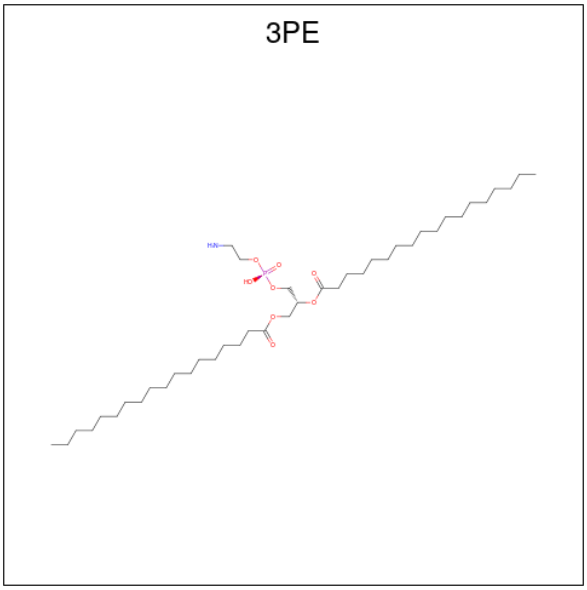
Mol	Chain	Residues	Atoms	AltConf
26	4C	1	Total Cu 2 2	0

- Molecule 27 is 2-(HEXADECANOYLOXY)-1-[(PHOSPHONOOXY)METHYL]ETHYL HEXADECANOATE (CCD ID: LPP) (formula: $C_{35}H_{69}O_8P$).



Mol	Chain	Residues	Atoms					AltConf
27	4D	1	Total	C	H	O	P	0
			111	35	67	8	1	
27	4H	1	Total	C	H	O	P	0
			111	35	67	8	1	

- Molecule 28 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



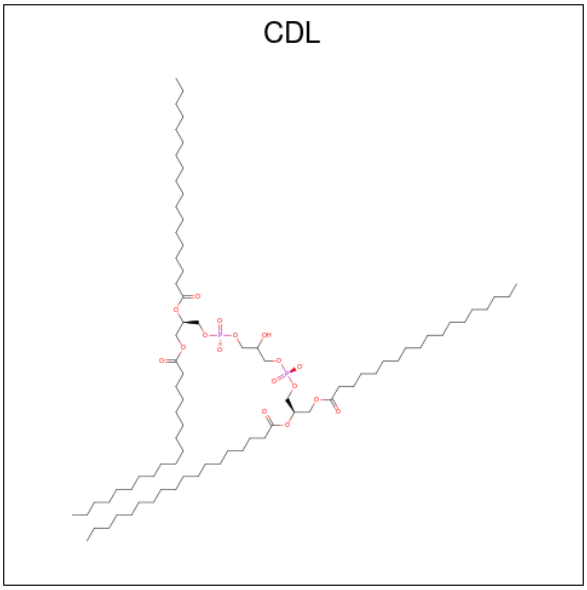
Mol	Chain	Residues	Atoms						AltConf
28	4D	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
28	4E	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
28	4E	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
28	4E	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
28	4E	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
28	4N	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
28	4R	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
28	4W	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	
28	B	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	

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Mol	Chain	Residues	Atoms						AltConf
28	B	1	Total	C	H	N	O	P	0
			133	41	82	1	8	1	

- Molecule 29 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).

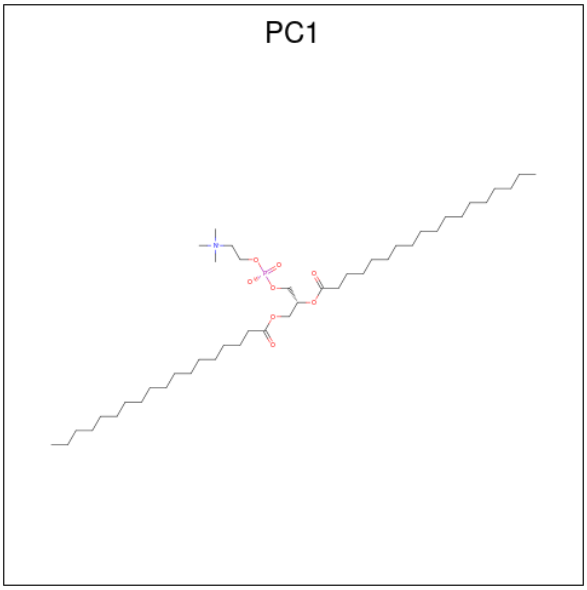


Mol	Chain	Residues	Atoms					AltConf
29	4E	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	4F	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	4F	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	4H	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	4L	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	4N	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	4U	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	4V	1	Total	C	H	O	P	0
			256	81	156	17	2	
29	B	1	Total	C	H	O	P	0
			256	81	156	17	2	

- Molecule 30 is ZINC ION (CCD ID: ZN) (formula: Zn).

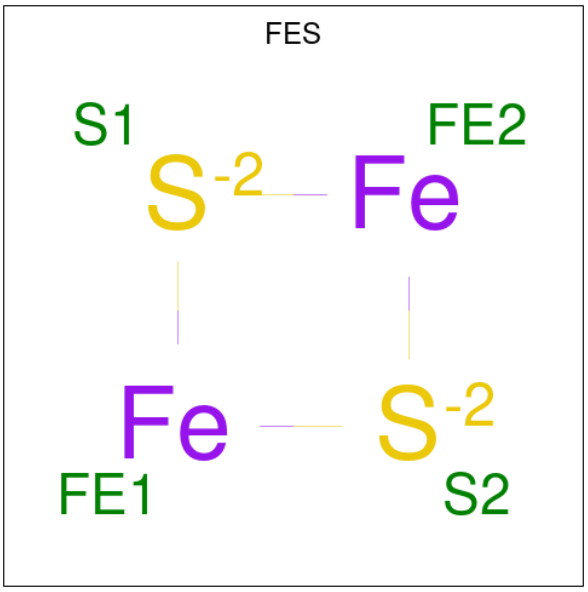
Mol	Chain	Residues	Atoms		AltConf
30	4G	1	Total	Zn	0
			1	1	

- Molecule 31 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



Mol	Chain	Residues	Atoms						AltConf
31	4L	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	
31	4Y	1	Total	C	H	N	O	P	0
			142	44	88	1	8	1	

- Molecule 32 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms	AltConf
32	4W	1	Total Fe S 4 2 2	0
32	4W	1	Total Fe S 4 2 2	0

- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
33	B	1	Total Mg 1 1	0

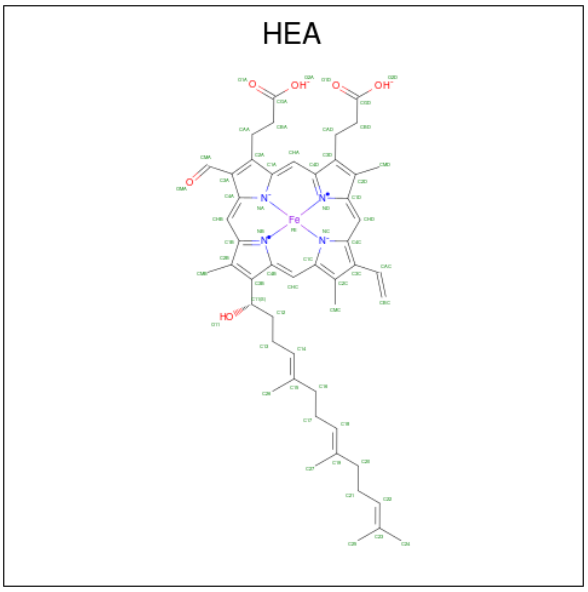
- Molecule 34 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
34	B	1	Total Ca 1 1	0

- Molecule 35 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

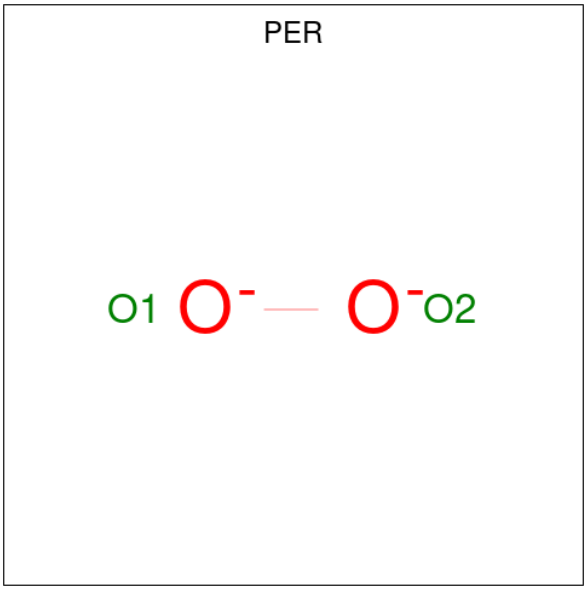
Mol	Chain	Residues	Atoms	AltConf
35	B	1	Total Cu 1 1	0

- Molecule 36 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms						AltConf
36	B	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	
36	B	1	Total	C	Fe	H	N	O	0
			114	49	1	54	4	6	

- Molecule 37 is PEROXIDE ION (CCD ID: PER) (formula: O_2).

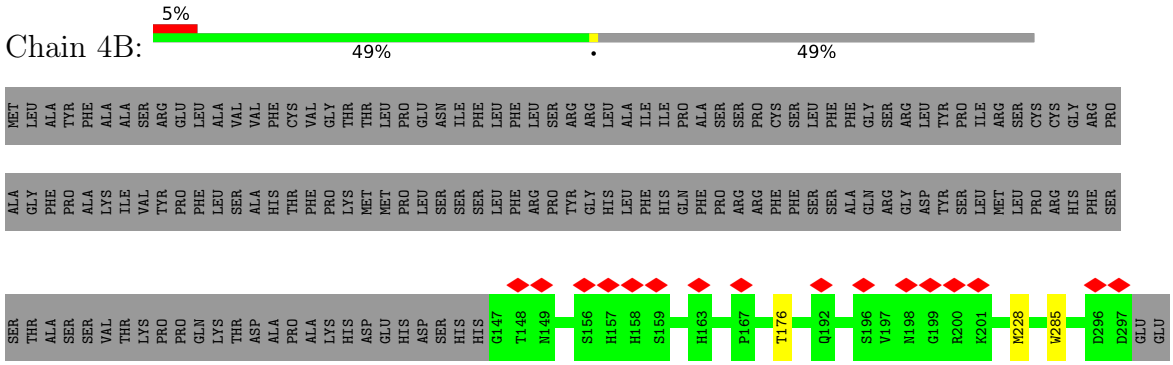


Mol	Chain	Residues	Atoms		AltConf
37	B	1	Total	O	0
			2	2	

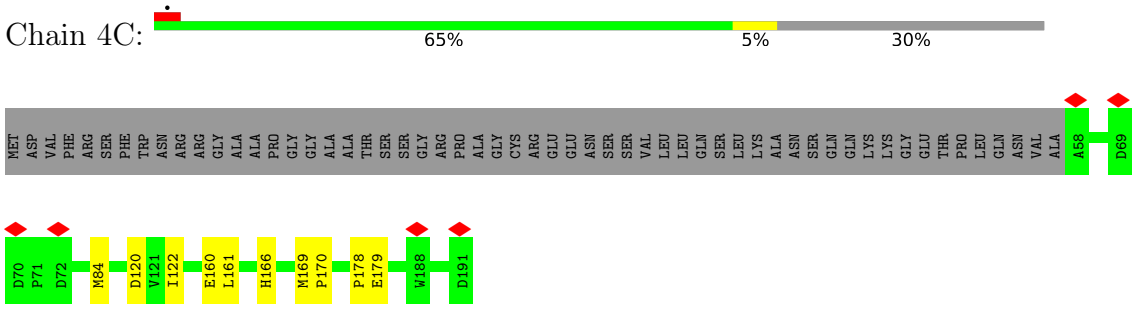
3 Residue-property plots (i)

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

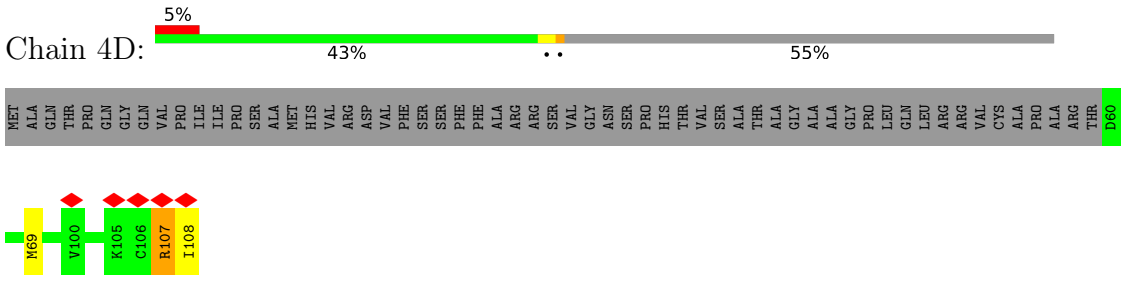
• Molecule 1: Putative cytochrome C oxidase subunit IIa



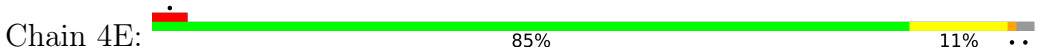
• Molecule 2: Cytochrome c oxidase polypeptide II

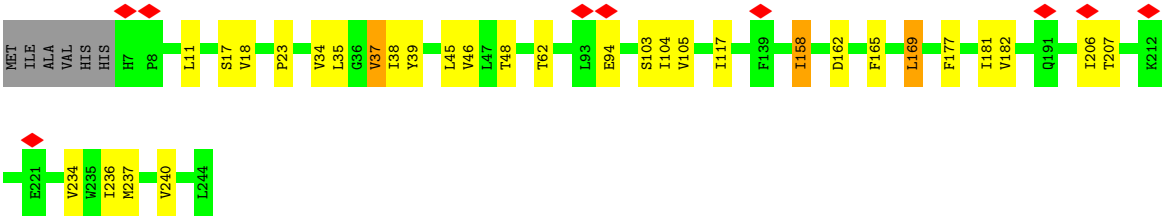


• Molecule 3: Cytochrome C family oxidase subunit II, transmembrane domain protein



• Molecule 4: Cytochrome c oxidase subunit 3

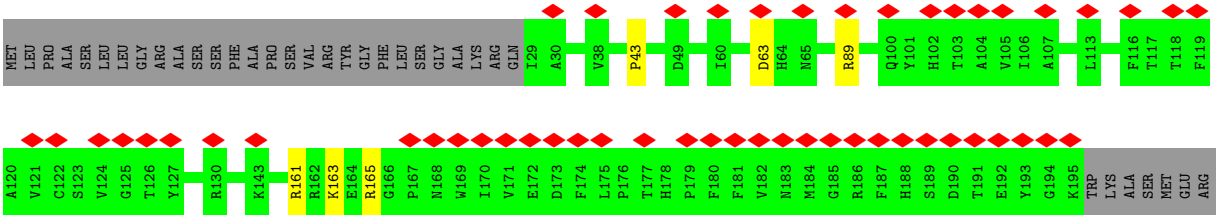




• Molecule 5: Cg8 family protein

Chain 4F:

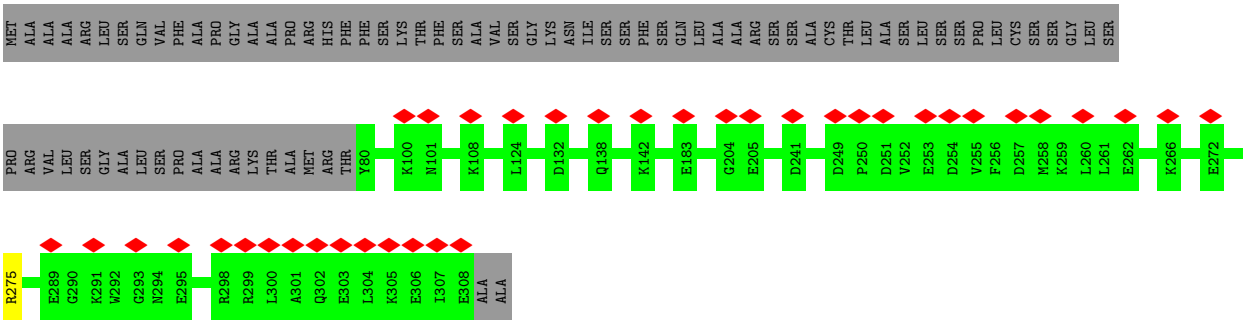




• Molecule 6: Putative cytochrome c oxidase subunit

Chain 4G:

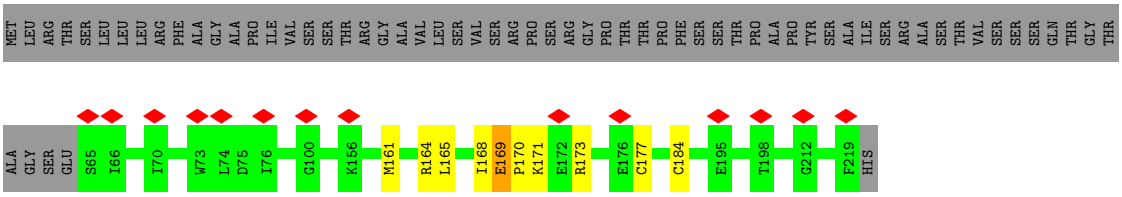




• Molecule 7: Transmembrane protein

Chain 4H:



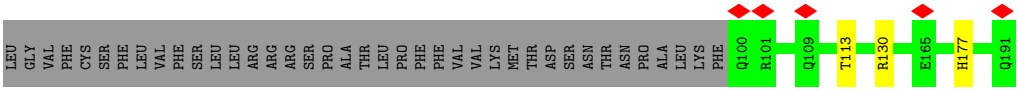


• Molecule 8: Cytochrome c oxidase subunit 6B

Chain 4I:





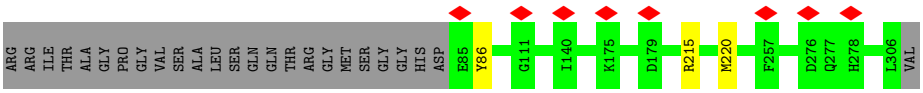


• Molecule 9: Transmembrane protein

Chain 4J:

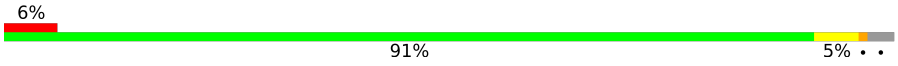






• Molecule 10: Membrane protein

Chain 4K:



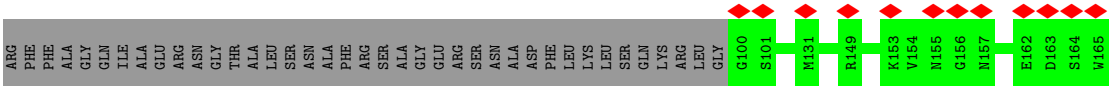


• Molecule 11: Transmembrane protein

Chain 4L:





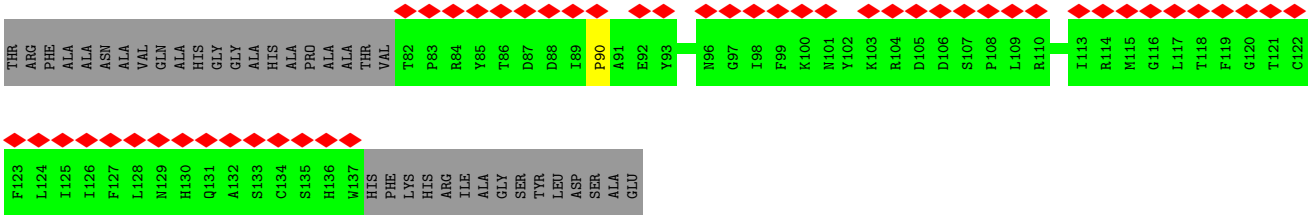


• Molecule 12: Transmembrane protein

Chain 4M:



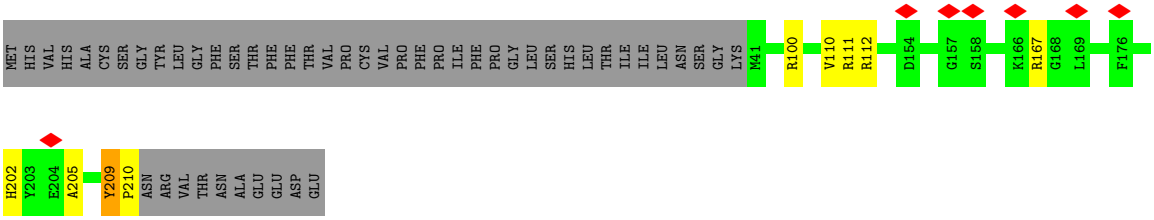




• Molecule 13: NADH-ubiquinone reductase complex 1 MLRQ subunit

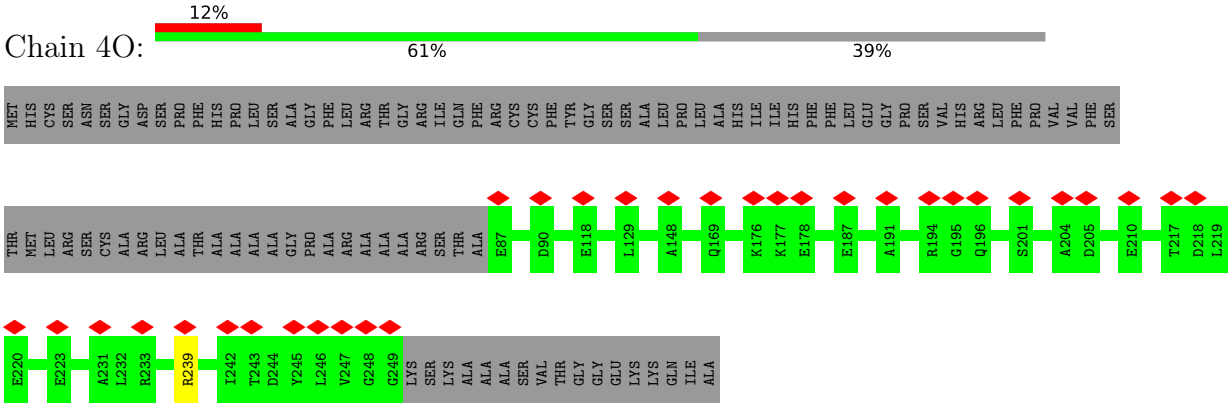
Chain 4N:





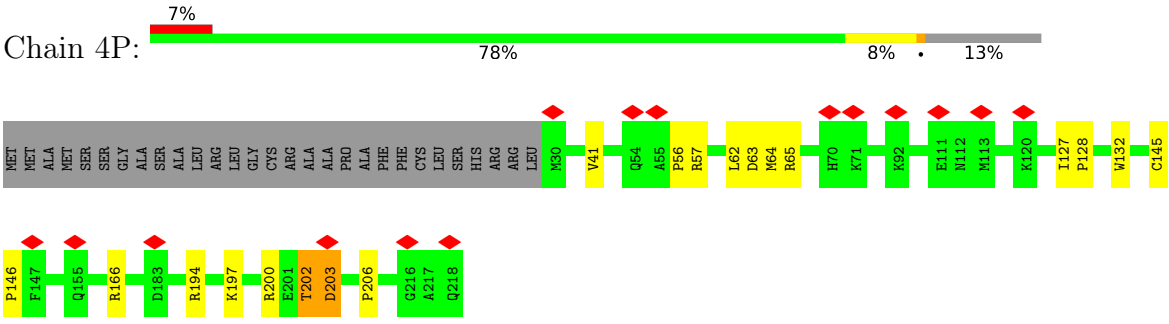
• Molecule 14: ApiCox30, TGGT1_297810

Chain 4O:



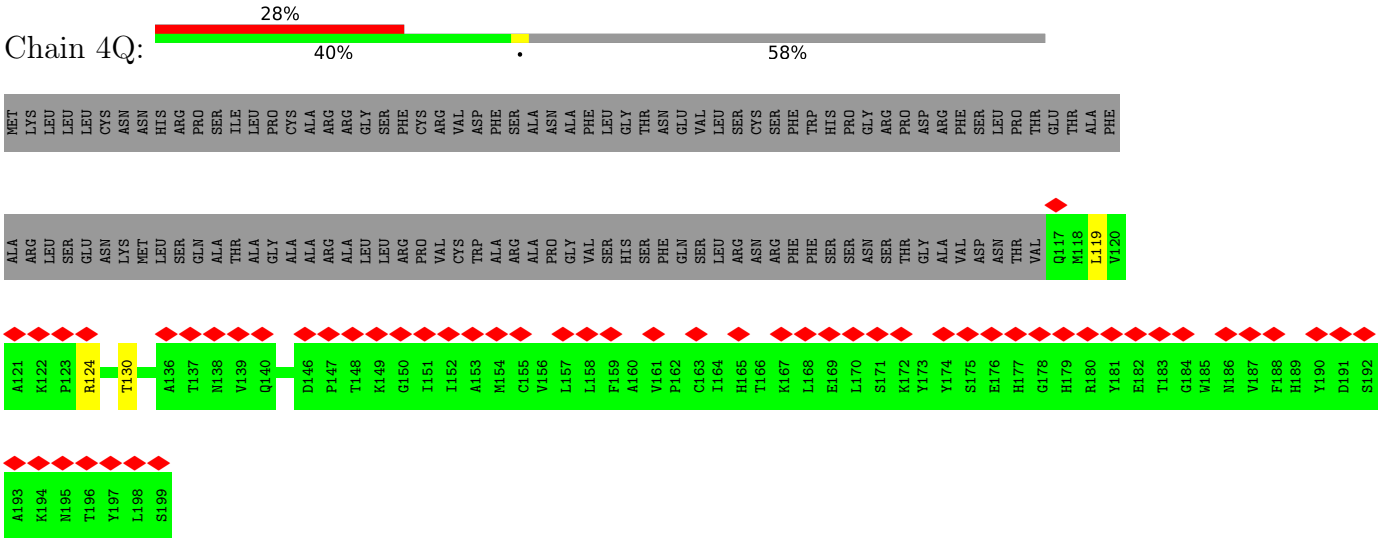
• Molecule 15: Transmembrane protein

Chain 4P:



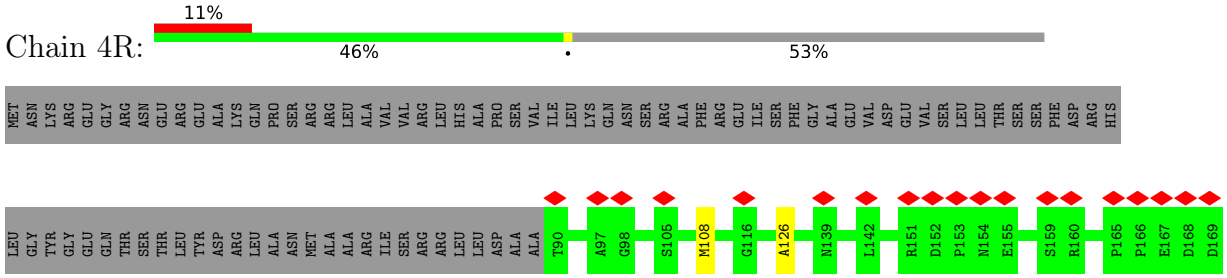
• Molecule 16: ApiCox22, TGGT1_312160

Chain 4Q:



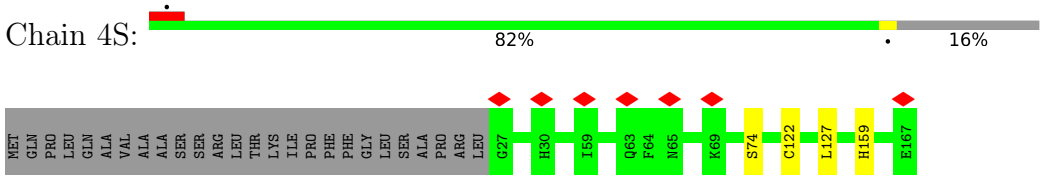
• Molecule 17: Transmembrane protein

Chain 4R:



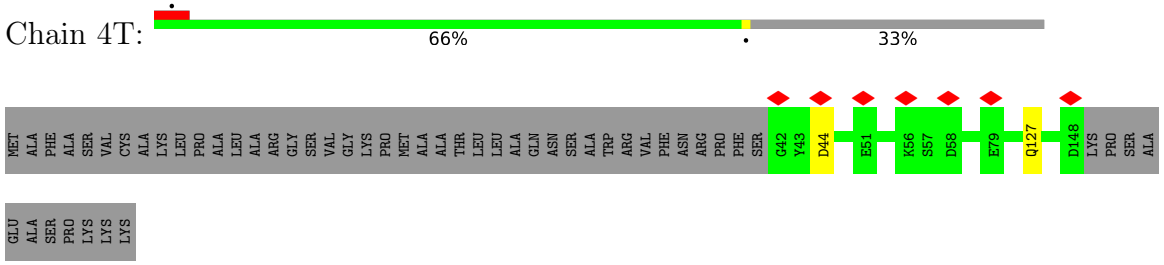
• Molecule 18: Transmembrane protein

Chain 4S:



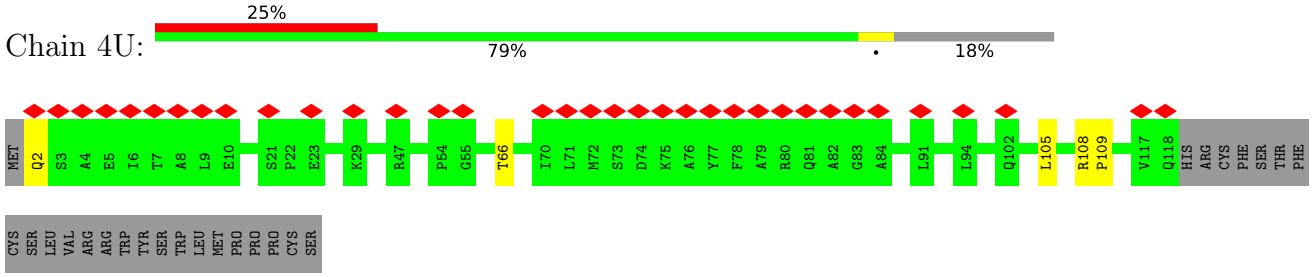
• Molecule 19: ApiCox18, TGGT1_221510

Chain 4T:



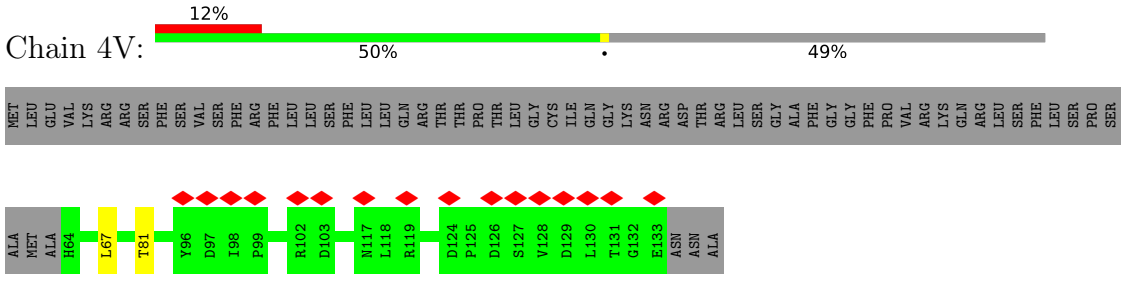
• Molecule 20: Transmembrane protein

Chain 4U:



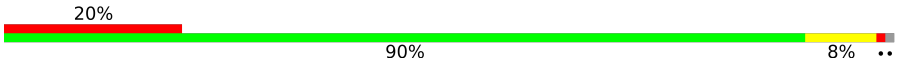
• Molecule 21: Transmembrane protein

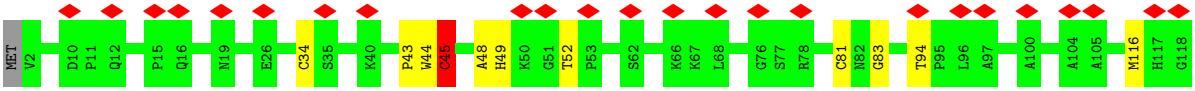
Chain 4V:



• Molecule 22: Zinc finger CDGSH-type domain-containing protein

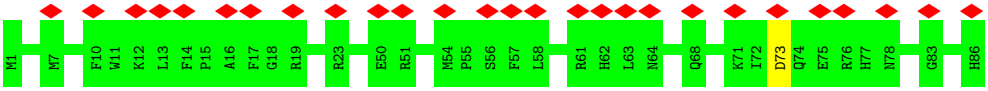
Chain 4W:





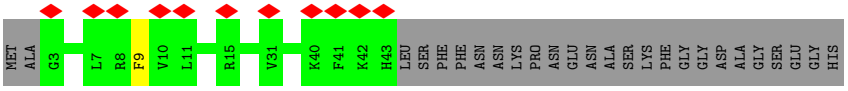
• Molecule 23: Transmembrane protein



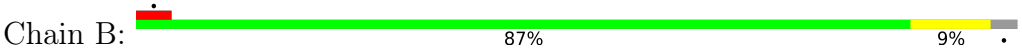


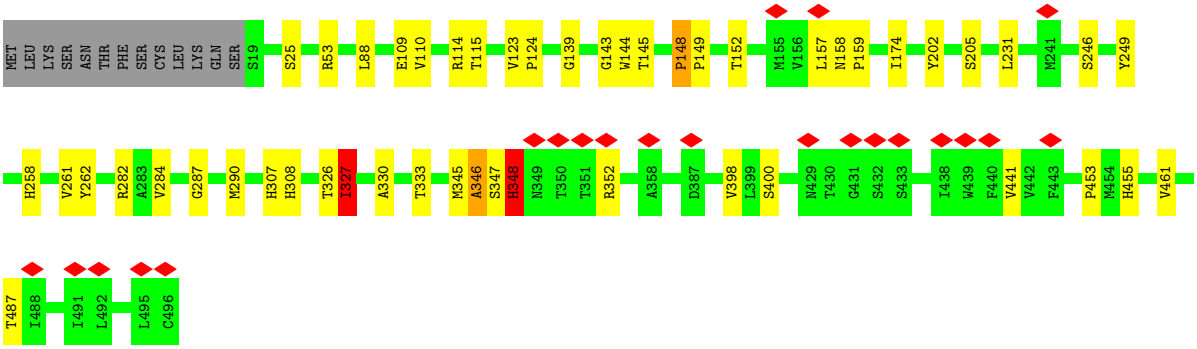
• Molecule 24: Transmembrane protein





• Molecule 25: Cytochrome c oxidase subunit 1





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	432000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	36	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	2.424	Depositor
Minimum map value	-1.690	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.076	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	507.84003, 507.84003, 507.84003	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8464, 0.8464, 0.8464	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MG, HEA, PC1, 3PE, CDL, CUA, FES, ZN, PER, LPP, CU

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	4B	0.79	0/1304	0.89	0/1779
2	4C	0.80	0/1099	0.97	0/1496
3	4D	0.72	0/418	0.99	2/568 (0.4%)
4	4E	0.68	0/1915	0.97	2/2611 (0.1%)
5	4F	0.75	0/1445	0.89	1/1969 (0.1%)
6	4G	0.74	0/1924	0.89	0/2606
7	4H	0.69	0/1302	0.88	0/1756
8	4I	0.68	0/796	0.84	0/1072
9	4J	0.71	0/1918	0.87	0/2609
10	4K	0.71	0/991	0.84	0/1350
11	4L	0.73	0/565	0.83	0/774
12	4M	0.77	0/480	0.89	0/650
13	4N	0.65	0/1495	0.87	0/2031
14	4O	0.72	0/1340	0.84	0/1818
15	4P	0.71	0/1639	0.97	3/2223 (0.1%)
16	4Q	0.73	0/686	0.83	0/931
17	4R	0.73	0/646	0.86	0/885
18	4S	0.69	0/1212	0.90	2/1638 (0.1%)
19	4T	0.77	0/899	0.93	0/1225
20	4U	0.74	0/935	0.83	0/1267
21	4V	0.70	0/591	0.82	0/801
22	4W	1.12	6/951 (0.6%)	1.08	5/1302 (0.4%)
23	4X	0.68	0/729	0.83	0/978
24	4Y	0.74	0/343	0.80	0/466
25	B	0.76	3/3812 (0.1%)	1.08	11/5198 (0.2%)
All	All	0.74	9/29435 (0.0%)	0.92	26/40003 (0.1%)

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
5	4F	0	2
6	4G	0	1
7	4H	0	2
8	4I	0	1
9	4J	0	1
10	4K	0	1
13	4N	0	3
15	4P	0	3
16	4Q	0	1
22	4W	1	1
25	B	0	6
All	All	1	22

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	4W	45	CYS	CA-CB	-16.50	1.25	1.53
22	4W	45	CYS	CB-SG	10.77	2.16	1.81
22	4W	45	CYS	C-N	8.60	1.46	1.33
22	4W	45	CYS	N-CA	-8.07	1.35	1.46
25	B	159	PRO	N-CD	-6.95	1.38	1.47
25	B	327	ILE	C-O	6.49	1.31	1.24
22	4W	44	TRP	C-O	-6.08	1.17	1.24
25	B	327	ILE	CA-C	-5.82	1.44	1.52
22	4W	49	HIS	CA-CB	-5.20	1.44	1.53

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	B	148	PRO	N-CA-C	12.90	126.44	110.70
25	B	348	HIS	CA-CB-CG	12.69	126.48	113.80
22	4W	45	CYS	N-CA-CB	11.74	130.33	110.49
25	B	148	PRO	CB-CA-C	-8.47	100.59	110.92
22	4W	44	TRP	CA-C-N	8.23	137.25	121.54
22	4W	44	TRP	C-N-CA	8.23	137.25	121.54
3	4D	107	ARG	N-CA-C	-7.91	99.88	110.55
25	B	455	HIS	N-CA-C	-6.80	103.88	111.71
25	B	453	PRO	N-CA-C	6.59	122.20	113.57
22	4W	45	CYS	O-C-N	-6.40	114.07	122.59
25	B	25	SER	N-CA-C	6.32	118.51	110.61
4	4E	169	LEU	CA-C-O	-6.28	114.23	120.82
18	4S	159	HIS	CA-CB-CG	6.26	120.06	113.80
15	4P	197	LYS	N-CA-C	-6.25	105.94	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	4E	165	PHE	N-CA-C	-6.21	105.36	113.12
25	B	143	GLY	N-CA-C	-6.03	105.19	112.48
15	4P	65	ARG	N-CA-C	-5.85	105.80	113.17
18	4S	74	SER	N-CA-C	-5.70	102.08	110.52
25	B	139	GLY	CA-C-O	-5.64	116.92	121.77
15	4P	203	ASP	CB-CA-C	5.56	115.34	109.83
25	B	327	ILE	O-C-N	5.51	127.71	122.20
22	4W	45	CYS	CB-CA-C	5.45	121.25	110.42
25	B	115	THR	N-CA-C	-5.20	107.10	113.50
5	4F	43	PRO	N-CA-C	5.12	120.00	114.68
25	B	157	LEU	N-CA-C	5.12	117.59	111.71
3	4D	107	ARG	CA-C-O	-5.08	115.82	121.81

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	4W	45	CYS	CA

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	4F	161	ARG	Sidechain
5	4F	89	ARG	Sidechain
6	4G	275	ARG	Sidechain
7	4H	164	ARG	Sidechain
7	4H	169	GLU	Peptide
8	4I	130	ARG	Sidechain
9	4J	215	ARG	Sidechain
10	4K	100	ARG	Sidechain
13	4N	100	ARG	Sidechain
13	4N	111	ARG	Sidechain
13	4N	112	ARG	Sidechain
15	4P	166	ARG	Sidechain
15	4P	200	ARG	Sidechain
15	4P	57	ARG	Sidechain
16	4Q	124	ARG	Sidechain
22	4W	45	CYS	Mainchain
25	B	114	ARG	Sidechain
25	B	282	ARG	Sidechain
25	B	326	THR	Mainchain
25	B	327	ILE	Mainchain
25	B	352	ARG	Sidechain

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Mol	Chain	Res	Type	Group
25	B	53	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	4B	1259	1204	1203	2	0
2	4C	1071	1064	1063	5	0
3	4D	402	382	381	2	0
4	4E	1866	1910	1909	20	0
5	4F	1395	1338	1337	1	0
6	4G	1870	1810	1806	0	0
7	4H	1265	1269	1268	5	0
8	4I	776	717	716	1	0
9	4J	1850	1787	1786	0	0
10	4K	956	913	912	2	0
11	4L	544	508	507	0	0
12	4M	466	447	446	0	0
13	4N	1441	1358	1357	4	0
14	4O	1317	1304	1303	1	0
15	4P	1581	1523	1522	6	0
16	4Q	668	654	653	0	0
17	4R	618	599	598	3	0
18	4S	1169	1127	1126	2	0
19	4T	875	851	850	0	0
20	4U	911	922	921	2	0
21	4V	575	555	554	2	0
22	4W	914	874	874	5	0
23	4X	707	701	701	0	0
24	4Y	330	343	342	1	0
25	B	3707	3742	3741	31	0
26	4C	2	0	0	0	0
27	4D	44	67	67	0	0
27	4H	44	67	67	0	0
28	4D	51	82	82	3	0
28	4E	204	328	328	10	0
28	4N	51	82	82	2	0
28	4R	51	82	82	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	4W	51	82	82	2	0
28	B	102	164	164	3	0
29	4E	100	156	156	1	0
29	4F	200	312	312	2	0
29	4H	100	156	156	1	0
29	4L	100	156	156	1	0
29	4N	100	156	156	0	0
29	4U	100	156	156	1	0
29	4V	100	156	156	5	0
29	B	100	156	156	1	0
30	4G	1	0	0	0	0
31	4L	54	88	88	0	0
31	4Y	54	88	88	4	0
32	4W	8	0	0	1	0
33	B	1	0	0	0	0
34	B	1	0	0	0	0
35	B	1	0	0	0	0
36	B	120	108	108	8	0
37	B	2	0	0	0	0
All	All	30275	30544	30518	100	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 2.

All (100) 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)
22:4W:45:CYS:CB	22:4W:45:CYS:SG	2.16	1.31
25:B:258:HIS:O	25:B:261:VAL:HG22	1.63	0.98
3:4D:107:ARG:O	3:4D:108:ILE:C	2.25	0.79
22:4W:45:CYS:SG	22:4W:45:CYS:C	2.68	0.76
22:4W:45:CYS:SG	22:4W:45:CYS:CA	2.75	0.74
25:B:109:GLU:HG3	25:B:110:VAL:H	1.57	0.69
25:B:109:GLU:HG3	25:B:110:VAL:N	2.10	0.67
24:4Y:9:PHE:CE2	31:4Y:301:PC1:H152	2.34	0.63
15:4P:202:THR:O	15:4P:203:ASP:HB2	1.98	0.63
36:B:505:HEA:HBC1	36:B:505:HEA:HHD	1.81	0.62
4:4E:38:ILE:HD13	29:4E:301:CDL:H401	1.83	0.60
25:B:123:VAL:HB	25:B:124:PRO:HD3	1.85	0.59
2:4C:122:ILE:HG13	25:B:149:PRO:HG2	1.84	0.58
7:4H:177:CYS:CB	7:4H:184:CYS:HG	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:4E:303:3PE:H222	29:4H:301:CDL:H781	1.88	0.56
2:4C:122:ILE:HG22	2:4C:160:GLU:HG2	1.90	0.54
25:B:174:ILE:HG22	25:B:174:ILE:O	2.07	0.53
25:B:152:THR:HA	25:B:231:LEU:HD21	1.91	0.52
36:B:506:HEA:HMC1	36:B:506:HEA:HBC1	1.91	0.52
36:B:505:HEA:HHC	36:B:505:HEA:H121	1.92	0.52
17:4R:108:MET:HE2	25:B:348:HIS:HB2	1.92	0.52
2:4C:160:GLU:O	2:4C:161:LEU:C	2.53	0.52
25:B:202:TYR:O	25:B:205:SER:OG	2.23	0.52
28:4E:303:3PE:H3H1	28:B:509:3PE:H3B2	1.92	0.51
22:4W:48:ALA:HB3	32:4W:602:FES:S1	2.50	0.51
4:4E:17:SER:O	4:4E:18:VAL:C	2.54	0.50
17:4R:108:MET:HG3	25:B:348:HIS:CD2	2.46	0.50
7:4H:169:GLU:HA	7:4H:170:PRO:C	2.36	0.50
4:4E:37:VAL:HG11	10:4K:85:MET:SD	2.52	0.50
4:4E:158:ILE:HD11	4:4E:169:LEU:HD23	1.93	0.49
25:B:148:PRO:HG2	25:B:249:TYR:CB	2.43	0.49
13:4N:110:VAL:HG21	28:4N:301:3PE:H32	1.95	0.48
4:4E:18:VAL:HG11	4:4E:23:PRO:HB3	1.96	0.48
13:4N:202:HIS:O	13:4N:205:ALA:HB3	2.14	0.48
15:4P:145:CYS:HB2	15:4P:146:PRO:HD3	1.94	0.48
2:4C:84:MET:HE3	2:4C:170:PRO:HD3	1.95	0.48
25:B:330:ALA:HB1	36:B:506:HEA:H242	1.96	0.48
28:4W:603:3PE:H321	28:4W:603:3PE:H361	1.96	0.48
25:B:149:PRO:HG3	25:B:246:SER:HB3	1.96	0.48
4:4E:182:VAL:HG11	28:4E:304:3PE:H392	1.95	0.47
13:4N:209:TYR:HB2	13:4N:210:PRO:HD3	1.96	0.47
25:B:148:PRO:HG2	25:B:249:TYR:HB3	1.95	0.47
28:4D:202:3PE:C33	28:4D:202:3PE:H31	2.44	0.46
4:4E:46:VAL:CG2	15:4P:132:TRP:CG	2.99	0.46
7:4H:170:PRO:HD2	7:4H:173:ARG:HB3	1.98	0.46
4:4E:94:GLU:HG3	8:4I:177:HIS:HB3	1.98	0.46
7:4H:177:CYS:HB3	7:4H:184:CYS:HG	1.80	0.46
1:4B:285:TRP:HA	2:4C:169:MET:SD	2.56	0.46
7:4H:165:LEU:HD12	7:4H:168:ILE:HD12	1.98	0.46
4:4E:237:MET:HE2	28:4E:305:3PE:H2C2	1.97	0.45
4:4E:182:VAL:HG21	28:4E:303:3PE:H3I2	1.98	0.45
10:4K:99:GLU:HG2	20:4U:105:LEU:HD13	1.98	0.45
4:4E:236:ILE:HG12	28:4E:302:3PE:H2I2	1.98	0.45
29:4F:301:CDL:H751	25:B:441:VAL:HG22	1.97	0.45
1:4B:228:MET:SD	25:B:348:HIS:NE2	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:B:109:GLU:CG	25:B:110:VAL:H	2.26	0.45
5:4F:163:LYS:C	5:4F:165:ARG:H	2.25	0.44
28:4D:202:3PE:H3I2	29:B:502:CDL:H351	1.99	0.44
4:4E:237:MET:HA	4:4E:240:VAL:HG22	1.99	0.44
28:4E:303:3PE:H3I3	28:4E:304:3PE:H3A1	1.99	0.44
4:4E:104:ILE:O	4:4E:105:VAL:C	2.61	0.44
25:B:109:GLU:CG	25:B:110:VAL:N	2.79	0.44
25:B:149:PRO:HG3	25:B:246:SER:CB	2.47	0.44
4:4E:45:LEU:HA	4:4E:48:THR:HG22	1.99	0.44
25:B:345:MET:O	25:B:346:ALA:HB3	2.17	0.44
4:4E:207:THR:HG21	14:4O:239:ARG:HD3	1.99	0.44
28:4E:303:3PE:H2G1	28:B:509:3PE:H3B1	2.00	0.43
25:B:258:HIS:NE2	25:B:262:TYR:CE2	2.86	0.43
28:4E:303:3PE:H31	28:4E:303:3PE:H321	1.72	0.43
29:4U:201:CDL:H832	36:B:505:HEA:H273	2.01	0.43
25:B:307:HIS:CD2	25:B:308:HIS:CD2	3.07	0.43
25:B:148:PRO:HG3	25:B:249:TYR:CG	2.53	0.43
15:4P:194:ARG:HG3	15:4P:206:PRO:HB2	2.01	0.42
17:4R:126:ALA:HB2	28:4W:603:3PE:H362	2.01	0.42
4:4E:37:VAL:HG21	4:4E:39:TYR:CE1	2.53	0.42
25:B:345:MET:O	25:B:346:ALA:CB	2.67	0.42
4:4E:117:ILE:HD11	18:4S:122:CYS:CB	2.50	0.42
28:4E:305:3PE:H2C1	29:4V:201:CDL:H452	2.02	0.42
31:4Y:301:PC1:H153	31:4Y:301:PC1:P	2.59	0.42
31:4Y:301:PC1:H153	31:4Y:301:PC1:O13	2.19	0.42
25:B:123:VAL:O	25:B:124:PRO:C	2.62	0.41
3:4D:69:MET:HE1	28:4D:202:3PE:H231	2.02	0.41
4:4E:177:PHE:CE1	4:4E:181:ILE:HD11	2.55	0.41
4:4E:234:VAL:HG22	29:4V:201:CDL:H392	2.03	0.41
21:4V:81:THR:HG21	29:4V:201:CDL:H251	2.02	0.41
13:4N:110:VAL:HG11	28:4N:301:3PE:C32	2.50	0.41
18:4S:127:LEU:HD11	31:4Y:301:PC1:H3H2	2.03	0.41
20:4U:108:ARG:HB2	20:4U:109:PRO:HD3	2.02	0.41
29:4V:201:CDL:H842	28:B:508:3PE:H2C1	2.03	0.41
25:B:88:LEU:HD12	36:B:505:HEA:HBC2	2.01	0.41
25:B:144:TRP:CD1	25:B:145:THR:HG23	2.55	0.41
25:B:398:VAL:HG11	36:B:506:HEA:C2C	2.50	0.41
29:4F:301:CDL:H391	22:4W:83:GLY:HA3	2.02	0.41
21:4V:67:LEU:H	29:4V:201:CDL:HB21	1.86	0.41
25:B:284:VAL:HG11	25:B:290:MET:CE	2.50	0.41
29:4L:201:CDL:H742	29:4L:201:CDL:H162	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:4P:127:ILE:N	15:4P:128:PRO:HD2	2.35	0.41
4:4E:46:VAL:HG22	15:4P:132:TRP:CD2	2.57	0.40
25:B:258:HIS:CD2	25:B:262:TYR:HE2	2.40	0.40
25:B:333:THR:HG21	36:B:506:HEA:H14	2.03	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	4B	149/299 (50%)	142 (95%)	7 (5%)	0	100 100
2	4C	132/191 (69%)	125 (95%)	7 (5%)	0	100 100
3	4D	47/108 (44%)	44 (94%)	3 (6%)	0	100 100
4	4E	236/244 (97%)	214 (91%)	19 (8%)	3 (1%)	9 26
5	4F	165/204 (81%)	156 (94%)	9 (6%)	0	100 100
6	4G	227/310 (73%)	220 (97%)	7 (3%)	0	100 100
7	4H	153/220 (70%)	141 (92%)	11 (7%)	1 (1%)	18 40
8	4I	90/191 (47%)	89 (99%)	1 (1%)	0	100 100
9	4J	220/307 (72%)	215 (98%)	4 (2%)	1 (0%)	24 49
10	4K	113/119 (95%)	108 (96%)	4 (4%)	1 (1%)	14 34
11	4L	64/165 (39%)	62 (97%)	2 (3%)	0	100 100
12	4M	54/152 (36%)	51 (94%)	2 (4%)	1 (2%)	6 17
13	4N	168/220 (76%)	162 (96%)	5 (3%)	1 (1%)	21 45
14	4O	161/266 (60%)	160 (99%)	1 (1%)	0	100 100
15	4P	187/218 (86%)	172 (92%)	12 (6%)	3 (2%)	7 21
16	4Q	81/199 (41%)	77 (95%)	4 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	4R	78/169 (46%)	74 (95%)	4 (5%)	0	100	100
18	4S	139/167 (83%)	136 (98%)	3 (2%)	0	100	100
19	4T	105/159 (66%)	102 (97%)	3 (3%)	0	100	100
20	4U	115/142 (81%)	111 (96%)	4 (4%)	0	100	100
21	4V	68/136 (50%)	66 (97%)	2 (3%)	0	100	100
22	4W	115/118 (98%)	105 (91%)	8 (7%)	2 (2%)	7	20
23	4X	84/86 (98%)	81 (96%)	3 (4%)	0	100	100
24	4Y	39/67 (58%)	38 (97%)	1 (3%)	0	100	100
25	B	476/491 (97%)	439 (92%)	34 (7%)	3 (1%)	21	45
All	All	3466/4948 (70%)	3290 (95%)	160 (5%)	16 (0%)	26	49

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	4E	37	VAL
7	4H	171	LYS
13	4N	209	TYR
25	B	346	ALA
15	4P	56	PRO
22	4W	45	CYS
4	4E	103	SER
15	4P	62	LEU
10	4K	9	GLY
22	4W	116	MET
9	4J	86	TYR
25	B	287	GLY
25	B	461	VAL
12	4M	90	PRO
15	4P	63	ASP
4	4E	34	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	4B	136/265 (51%)	135 (99%)	1 (1%)	76 87
2	4C	115/159 (72%)	111 (96%)	4 (4%)	32 57
3	4D	44/90 (49%)	44 (100%)	0	100 100
4	4E	213/218 (98%)	207 (97%)	6 (3%)	38 62
5	4F	150/179 (84%)	149 (99%)	1 (1%)	76 87
6	4G	202/262 (77%)	202 (100%)	0	100 100
7	4H	139/192 (72%)	138 (99%)	1 (1%)	76 87
8	4I	85/173 (49%)	84 (99%)	1 (1%)	63 79
9	4J	193/257 (75%)	192 (100%)	1 (0%)	81 90
10	4K	99/102 (97%)	95 (96%)	4 (4%)	28 53
11	4L	60/139 (43%)	60 (100%)	0	100 100
12	4M	51/118 (43%)	51 (100%)	0	100 100
13	4N	149/193 (77%)	148 (99%)	1 (1%)	76 87
14	4O	146/223 (66%)	146 (100%)	0	100 100
15	4P	167/188 (89%)	164 (98%)	3 (2%)	51 72
16	4Q	74/171 (43%)	72 (97%)	2 (3%)	39 64
17	4R	67/142 (47%)	67 (100%)	0	100 100
18	4S	118/139 (85%)	118 (100%)	0	100 100
19	4T	99/138 (72%)	97 (98%)	2 (2%)	48 71
20	4U	97/122 (80%)	95 (98%)	2 (2%)	47 69
21	4V	59/116 (51%)	59 (100%)	0	100 100
22	4W	100/101 (99%)	95 (95%)	5 (5%)	22 47
23	4X	73/73 (100%)	72 (99%)	1 (1%)	59 77
24	4Y	35/54 (65%)	35 (100%)	0	100 100
25	B	409/422 (97%)	403 (98%)	6 (2%)	57 76
All	All	3080/4236 (73%)	3039 (99%)	41 (1%)	59 78

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	4B	176	THR
2	4C	120	ASP
2	4C	166	HIS
2	4C	178	PRO

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Mol	Chain	Res	Type
2	4C	179	GLU
4	4E	11	LEU
4	4E	35	LEU
4	4E	62	THR
4	4E	158	ILE
4	4E	162	ASP
4	4E	206	ILE
5	4F	63	ASP
7	4H	161	MET
8	4I	113	THR
9	4J	220	MET
10	4K	67	ASP
10	4K	70	ASN
10	4K	99	GLU
10	4K	104	ASN
13	4N	167	ARG
15	4P	41	VAL
15	4P	64	MET
15	4P	202	THR
16	4Q	119	LEU
16	4Q	130	THR
19	4T	44	ASP
19	4T	127	GLN
20	4U	2	GLN
20	4U	66	THR
22	4W	34	CYS
22	4W	43	PRO
22	4W	52	THR
22	4W	81	CYS
22	4W	94	THR
23	4X	73	ASP
25	B	158	ASN
25	B	327	ILE
25	B	347	SER
25	B	348	HIS
25	B	400	SER
25	B	487	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	4B	166	ASN

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Mol	Chain	Res	Type
1	4B	193	GLN
1	4B	236	HIS
2	4C	111	HIS
2	4C	145	ASN
2	4C	157	GLN
4	4E	21	GLN
4	4E	190	ASN
5	4F	47	ASN
5	4F	59	GLN
6	4G	118	ASN
7	4H	205	ASN
8	4I	188	HIS
9	4J	150	GLN
9	4J	161	HIS
10	4K	18	ASN
14	4O	131	GLN
14	4O	149	GLN
15	4P	82	HIS
15	4P	155	GLN
18	4S	30	HIS
19	4T	89	HIS
19	4T	99	HIS
20	4U	25	ASN
21	4V	89	HIS
22	4W	49	HIS
22	4W	93	ASN
23	4X	74	GLN
23	4X	77	HIS
25	B	116	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 33 ligands modelled in this entry, 4 are monoatomic - leaving 29 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
28	3PE	4N	301	-	50,50,50	0.32	0	53,55,55	0.44	0
36	HEA	B	506	25	66,67,67	2.30	26 (39%)	78,103,103	2.43	28 (35%)
29	CDL	4F	301	-	99,99,99	0.55	0	105,111,111	0.51	0
28	3PE	B	509	-	50,50,50	0.33	0	53,55,55	0.52	0
37	PER	B	507	35	1,1,1	1.03	0	-		
29	CDL	4F	302	-	99,99,99	0.41	0	105,111,111	0.71	0
28	3PE	B	508	-	50,50,50	0.31	0	53,55,55	0.55	1 (1%)
32	FES	4W	601	22	0,4,4	-	-	-		
26	CUA	4C	201	2	0,1,1	-	-	-		
27	LPP	4H	302	-	43,43,43	0.57	0	47,48,48	0.60	0
28	3PE	4R	201	-	50,50,50	0.30	0	53,55,55	0.36	0
31	PC1	4Y	301	-	53,53,53	0.65	0	59,61,61	0.44	0
29	CDL	4N	302	-	99,99,99	0.63	0	105,111,111	0.47	0
29	CDL	4V	201	-	99,99,99	0.56	0	105,111,111	0.50	0
29	CDL	4H	301	-	99,99,99	0.60	0	105,111,111	0.48	0
32	FES	4W	602	22	0,4,4	-	-	-		
36	HEA	B	505	25	66,67,67	2.27	25 (37%)	78,103,103	2.42	28 (35%)
28	3PE	4W	603	-	50,50,50	0.31	0	53,55,55	0.41	0
28	3PE	4E	303	-	50,50,50	0.37	0	53,55,55	0.69	1 (1%)
31	PC1	4L	202	-	53,53,53	0.50	0	59,61,61	0.70	0
28	3PE	4E	305	-	50,50,50	0.31	0	53,55,55	0.40	0
29	CDL	4L	201	-	99,99,99	0.58	0	105,111,111	0.47	0
27	LPP	4D	201	-	43,43,43	0.58	0	47,48,48	0.58	0
28	3PE	4D	202	-	50,50,50	0.32	0	53,55,55	0.60	0
29	CDL	B	502	-	99,99,99	0.40	0	105,111,111	0.80	0
28	3PE	4E	304	-	50,50,50	0.32	0	53,55,55	0.57	0
29	CDL	4U	201	-	99,99,99	0.46	0	105,111,111	0.72	2 (1%)
28	3PE	4E	302	-	50,50,50	0.28	0	53,55,55	0.53	1 (1%)
29	CDL	4E	301	-	99,99,99	0.60	0	105,111,111	0.47	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
28	3PE	4N	301	-	-	16/54/54/54	-
36	HEA	B	506	25	-	8/36/76/76	-
29	CDL	4F	301	-	-	25/110/110/110	-
28	3PE	B	509	-	-	9/54/54/54	-
29	CDL	4F	302	-	-	7/110/110/110	-
28	3PE	B	508	-	-	14/54/54/54	-
32	FES	4W	601	22	-	-	0/1/1/1
27	LPP	4H	302	-	-	10/45/45/45	-
28	3PE	4R	201	-	-	16/54/54/54	-
31	PC1	4Y	301	-	-	11/57/57/57	-
29	CDL	4N	302	-	-	24/110/110/110	-
29	CDL	4V	201	-	-	35/110/110/110	-
29	CDL	4H	301	-	-	20/110/110/110	-
32	FES	4W	602	22	-	-	0/1/1/1
36	HEA	B	505	25	-	10/36/76/76	-
28	3PE	4W	603	-	-	13/54/54/54	-
28	3PE	4E	303	-	-	21/54/54/54	-
31	PC1	4L	202	-	-	10/57/57/57	-
28	3PE	4E	305	-	-	10/54/54/54	-
29	CDL	4L	201	-	-	17/110/110/110	-
27	LPP	4D	201	-	-	11/45/45/45	-
28	3PE	4D	202	-	-	21/54/54/54	-
29	CDL	B	502	-	-	21/110/110/110	-
28	3PE	4E	304	-	-	13/54/54/54	-
29	CDL	4U	201	-	-	20/110/110/110	-
28	3PE	4E	302	-	-	23/54/54/54	-
29	CDL	4E	301	-	-	30/110/110/110	-

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	B	505	HEA	C3B-C2B	5.49	1.47	1.34
36	B	505	HEA	FE-NB	5.11	2.10	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	B	506	HEA	FE-NB	5.11	2.10	1.94
36	B	506	HEA	FE-ND	5.07	2.10	1.94
36	B	505	HEA	FE-ND	4.94	2.10	1.94
36	B	506	HEA	C3A-C2A	4.79	1.47	1.36
36	B	506	HEA	C3B-C2B	4.75	1.45	1.34
36	B	506	HEA	C3D-C2D	4.46	1.46	1.36
36	B	506	HEA	FE-NC	4.43	2.10	1.95
36	B	505	HEA	FE-NC	4.30	2.09	1.95
36	B	505	HEA	C3A-C2A	4.05	1.45	1.36
36	B	505	HEA	C1A-NA	4.03	1.47	1.39
36	B	506	HEA	C1A-NA	4.02	1.47	1.39
36	B	505	HEA	CHC-C4B	4.00	1.46	1.38
36	B	505	HEA	C3D-C2D	3.95	1.45	1.36
36	B	505	HEA	C1D-ND	-3.94	1.33	1.40
36	B	505	HEA	C4A-NA	3.76	1.47	1.39
36	B	506	HEA	CHD-C1D	3.74	1.46	1.38
36	B	506	HEA	CHA-C1A	3.65	1.45	1.38
36	B	506	HEA	CHC-C4B	3.53	1.45	1.38
36	B	506	HEA	C4A-NA	3.51	1.46	1.39
36	B	505	HEA	CHB-C4A	3.44	1.45	1.38
36	B	506	HEA	C1D-ND	-3.37	1.34	1.40
36	B	506	HEA	C4B-NB	-3.25	1.34	1.40
36	B	505	HEA	CHA-C1A	3.25	1.44	1.38
36	B	505	HEA	CHC-C1C	3.05	1.46	1.39
36	B	506	HEA	CHB-C4A	3.04	1.44	1.38
36	B	506	HEA	CHD-C4C	3.02	1.46	1.39
36	B	505	HEA	C4B-C3B	3.02	1.49	1.44
36	B	506	HEA	CHA-C4D	2.97	1.46	1.39
36	B	506	HEA	CHC-C1C	2.96	1.46	1.39
36	B	505	HEA	C4B-NB	-2.87	1.35	1.40
36	B	505	HEA	CHD-C1D	2.81	1.44	1.38
36	B	505	HEA	C1C-NC	-2.80	1.34	1.39
36	B	505	HEA	CHB-C1B	2.75	1.45	1.39
36	B	506	HEA	C4B-C3B	2.74	1.49	1.44
36	B	506	HEA	C4C-NC	-2.66	1.34	1.39
36	B	506	HEA	C1C-NC	-2.60	1.34	1.39
36	B	505	HEA	CHD-C4C	2.53	1.45	1.39
36	B	505	HEA	C4C-NC	-2.46	1.35	1.39
36	B	505	HEA	C4D-ND	-2.34	1.34	1.38
36	B	506	HEA	C3C-C4C	2.27	1.48	1.42
36	B	505	HEA	C3C-C4C	2.26	1.48	1.42
36	B	505	HEA	CHA-C4D	2.26	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	B	506	HEA	C1B-NB	-2.25	1.34	1.38
36	B	506	HEA	C1A-C2A	2.20	1.49	1.45
36	B	505	HEA	C1B-NB	-2.17	1.34	1.38
36	B	506	HEA	CHB-C1B	2.07	1.43	1.39
36	B	505	HEA	O2D-CGD	-2.07	1.23	1.30
36	B	506	HEA	O2A-CGA	-2.03	1.23	1.30
36	B	506	HEA	C1C-C2C	2.02	1.48	1.43

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	B	505	HEA	C3C-C4C-NC	6.48	114.23	110.25
36	B	505	HEA	C3D-C4D-ND	6.44	116.59	110.36
36	B	506	HEA	C2B-C1B-NB	6.08	117.17	109.88
36	B	506	HEA	C3D-C4D-ND	6.03	116.19	110.36
36	B	506	HEA	C3C-C4C-NC	6.02	113.95	110.25
36	B	505	HEA	C2D-C1D-ND	5.69	116.58	109.84
36	B	506	HEA	C3C-C2C-C1C	-5.26	100.82	107.16
36	B	505	HEA	C2B-C1B-NB	5.25	116.17	109.88
36	B	505	HEA	C4A-NA-C1A	-5.11	100.34	105.35
36	B	506	HEA	C3B-C4B-NB	5.06	115.83	109.84
36	B	505	HEA	C3B-C4B-NB	4.96	115.72	109.84
36	B	505	HEA	C2A-C1A-NA	4.92	115.11	110.32
36	B	506	HEA	C4A-NA-C1A	-4.82	100.63	105.35
36	B	506	HEA	C2D-C1D-ND	4.63	115.33	109.84
36	B	505	HEA	C1D-C2D-C3D	-4.33	102.41	106.96
36	B	506	HEA	C2C-C1C-NC	4.32	116.65	110.08
36	B	505	HEA	C3C-C2C-C1C	-4.21	102.08	107.16
36	B	505	HEA	C3A-C2A-C1A	-4.01	103.24	107.08
36	B	506	HEA	C26-C15-C16	4.00	122.01	115.27
36	B	505	HEA	C2C-C1C-NC	3.71	115.73	110.08
36	B	506	HEA	C2A-C1A-NA	3.70	113.93	110.32
36	B	506	HEA	C1B-C2B-C3B	-3.70	102.37	106.80
36	B	506	HEA	C3A-C2A-C1A	-3.57	103.66	107.08
36	B	506	HEA	C4D-C3D-C2D	-3.44	101.88	106.90
36	B	505	HEA	C4B-C3B-C2B	-3.41	101.58	107.41
36	B	506	HEA	C1D-C2D-C3D	-3.36	103.43	106.96
36	B	506	HEA	CMB-C2B-C1B	3.19	129.90	125.04
36	B	505	HEA	C4D-C3D-C2D	-3.17	102.27	106.90
36	B	506	HEA	CHB-C1B-C2B	-2.96	120.36	124.98
28	4E	302	3PE	O13-C11-C12	2.95	120.11	109.10
36	B	505	HEA	CHA-C1A-C2A	-2.94	120.17	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	B	506	HEA	C4B-C3B-C2B	-2.91	102.45	107.41
36	B	505	HEA	CHB-C1B-C2B	-2.88	120.49	124.98
36	B	505	HEA	C1B-C2B-C3B	-2.86	103.38	106.80
36	B	505	HEA	C1D-ND-C4D	-2.85	102.13	105.07
36	B	505	HEA	CHC-C4B-NB	-2.84	120.88	124.37
36	B	506	HEA	C4B-NB-C1B	-2.82	102.16	105.07
36	B	506	HEA	CHC-C1C-C2C	-2.67	119.70	127.24
36	B	506	HEA	C27-C19-C20	2.66	119.74	115.27
36	B	505	HEA	CHA-C4D-C3D	-2.59	121.03	124.84
36	B	506	HEA	CAD-C3D-C4D	2.54	129.09	124.66
36	B	505	HEA	CHD-C1D-C2D	-2.52	119.73	126.73
36	B	506	HEA	CHA-C4D-C3D	-2.49	121.18	124.84
36	B	505	HEA	CHC-C1C-C2C	-2.46	120.29	127.24
29	4U	201	CDL	OA6-CA5-C11	2.46	116.80	111.50
28	B	508	3PE	O31-C3-C2	-2.41	101.42	108.43
29	4U	201	CDL	CA4-OA6-CA5	2.41	123.72	117.79
36	B	505	HEA	CAD-C3D-C4D	2.38	128.82	124.66
36	B	505	HEA	CMD-C2D-C1D	2.35	128.62	125.04
36	B	506	HEA	CHB-C4A-C3A	-2.31	121.31	125.26
36	B	506	HEA	C16-C15-C14	-2.30	116.46	121.12
36	B	506	HEA	CMD-C2D-C1D	2.27	128.50	125.04
36	B	506	HEA	OMA-CMA-C3A	-2.26	120.57	125.69
36	B	505	HEA	OMA-CMA-C3A	-2.24	120.63	125.69
36	B	506	HEA	CHC-C4B-NB	-2.19	121.67	124.37
36	B	505	HEA	CAA-C2A-C1A	2.15	128.94	124.89
36	B	505	HEA	C4A-C3A-C2A	2.13	108.50	106.75
36	B	505	HEA	CMC-C2C-C1C	2.09	128.56	125.37
36	B	506	HEA	CHD-C1D-C2D	-2.05	121.03	126.73
28	4E	303	3PE	O21-C2-C1	2.01	115.66	108.40
36	B	505	HEA	C13-C12-C11	-2.00	111.34	114.35

There are no chirality outliers.

All (415) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	4D	202	3PE	C11-O13-P-O12
28	4D	202	3PE	O11-C1-C2-O21
28	4D	202	3PE	O32-C31-O31-C3
28	4D	202	3PE	C32-C31-O31-C3
28	4D	202	3PE	O22-C21-O21-C2
28	4D	202	3PE	C22-C21-O21-C2
28	4E	302	3PE	C12-C11-O13-P

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Mol	Chain	Res	Type	Atoms
28	4E	303	3PE	O13-C11-C12-N
28	4E	303	3PE	O32-C31-O31-C3
28	4E	303	3PE	C32-C31-O31-C3
28	4E	304	3PE	C11-O13-P-O12
28	4E	304	3PE	O13-C11-C12-N
28	4E	304	3PE	O22-C21-O21-C2
28	4E	304	3PE	C22-C21-O21-C2
28	4E	305	3PE	O13-C11-C12-N
28	4N	301	3PE	C11-O13-P-O12
28	4N	301	3PE	C11-O13-P-O14
28	4N	301	3PE	O21-C2-C3-O31
28	4N	301	3PE	O32-C31-O31-C3
28	4N	301	3PE	C32-C31-O31-C3
28	B	508	3PE	O13-C11-C12-N
28	B	509	3PE	C1-O11-P-O12
28	B	509	3PE	C11-O13-P-O12
29	4E	301	CDL	CA2-OA2-PA1-OA3
29	4E	301	CDL	CA3-OA5-PA1-OA3
29	4F	301	CDL	O1-C1-CB2-OB2
29	4F	301	CDL	CA2-OA2-PA1-OA4
29	4F	301	CDL	C11-CA5-OA6-CA4
29	4F	301	CDL	OB7-CB5-OB6-CB4
29	4H	301	CDL	CB3-OB5-PB2-OB3
29	4N	302	CDL	CA2-OA2-PA1-OA3
29	4N	302	CDL	CA2-OA2-PA1-OA4
29	4N	302	CDL	CA2-OA2-PA1-OA5
29	4N	302	CDL	CB3-OB5-PB2-OB4
29	4U	201	CDL	C1-CA2-OA2-PA1
29	4U	201	CDL	OA7-CA5-OA6-CA4
29	4U	201	CDL	C11-CA5-OA6-CA4
29	4U	201	CDL	CB3-OB5-PB2-OB4
29	4U	201	CDL	CB4-CB3-OB5-PB2
29	4V	201	CDL	CB2-OB2-PB2-OB4
29	4V	201	CDL	CB3-OB5-PB2-OB3
29	B	502	CDL	CB3-OB5-PB2-OB3
31	4Y	301	PC1	C11-O13-P-O14
36	B	505	HEA	C12-C11-C3B-C2B
36	B	505	HEA	C12-C11-C3B-C4B
36	B	505	HEA	C11-C12-C13-C14
36	B	506	HEA	C14-C15-C16-C17
36	B	506	HEA	C26-C15-C16-C17
29	B	502	CDL	OB9-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
29	B	502	CDL	C71-CB7-OB8-CB6
29	4E	301	CDL	OB9-CB7-OB8-CB6
29	4F	301	CDL	OA7-CA5-OA6-CA4
29	4F	301	CDL	C51-CB5-OB6-CB4
29	4E	301	CDL	C71-CB7-OB8-CB6
29	B	502	CDL	OA7-CA5-OA6-CA4
31	4Y	301	PC1	C32-C31-O31-C3
29	B	502	CDL	C11-CA5-OA6-CA4
31	4Y	301	PC1	O32-C31-O31-C3
29	4N	302	CDL	C31-CA7-OA8-CA6
29	4V	201	CDL	C71-CB7-OB8-CB6
28	4E	302	3PE	C21-C22-C23-C24
28	B	509	3PE	C21-C22-C23-C24
29	4N	302	CDL	OA9-CA7-OA8-CA6
28	4E	303	3PE	C31-C32-C33-C34
28	4W	603	3PE	C31-C32-C33-C34
29	4V	201	CDL	OB9-CB7-OB8-CB6
29	B	502	CDL	OA9-CA7-OA8-CA6
28	4D	202	3PE	C11-O13-P-O11
28	4E	304	3PE	C11-O13-P-O11
28	4N	301	3PE	C11-O13-P-O11
28	4R	201	3PE	C1-O11-P-O13
28	4W	603	3PE	C11-O13-P-O11
28	B	508	3PE	C1-O11-P-O13
28	B	509	3PE	C1-O11-P-O13
28	B	509	3PE	C11-O13-P-O11
29	4E	301	CDL	CA2-OA2-PA1-OA5
29	4F	302	CDL	CA2-OA2-PA1-OA5
29	4N	302	CDL	CB3-OB5-PB2-OB2
29	4U	201	CDL	CB3-OB5-PB2-OB2
29	4V	201	CDL	CB2-OB2-PB2-OB5
29	B	502	CDL	CB2-OB2-PB2-OB5
29	4V	201	CDL	CA5-C11-C12-C13
29	B	502	CDL	C31-CA7-OA8-CA6
29	4F	301	CDL	CA2-C1-CB2-OB2
28	4E	304	3PE	C26-C27-C28-C29
29	4L	201	CDL	C11-CA5-OA6-CA4
31	4Y	301	PC1	C3D-C3E-C3F-C3G
29	4L	201	CDL	OA7-CA5-OA6-CA4
29	4H	301	CDL	C78-C79-C80-C81
28	4E	305	3PE	C33-C34-C35-C36
27	4H	302	LPP	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
28	4E	302	3PE	C34-C35-C36-C37
28	4E	302	3PE	C36-C37-C38-C39
29	4V	201	CDL	C54-C55-C56-C57
29	4E	301	CDL	C36-C37-C38-C39
29	4L	201	CDL	C51-C52-C53-C54
28	4E	303	3PE	C3C-C3D-C3E-C3F
27	4H	302	LPP	C16-C17-C18-C19
28	4E	302	3PE	C2B-C2C-C2D-C2E
28	4R	201	3PE	C21-C22-C23-C24
29	4H	301	CDL	CB5-C51-C52-C53
28	4N	301	3PE	C33-C34-C35-C36
28	B	508	3PE	C36-C37-C38-C39
29	4E	301	CDL	C31-C32-C33-C34
29	4H	301	CDL	C76-C77-C78-C79
29	4H	301	CDL	C72-C73-C74-C75
28	4E	302	3PE	C2E-C2F-C2G-C2H
28	4E	303	3PE	C2A-C2B-C2C-C2D
29	4L	201	CDL	C32-C33-C34-C35
28	4E	302	3PE	C38-C39-C3A-C3B
29	4L	201	CDL	C80-C81-C82-C83
29	4H	301	CDL	C41-C42-C43-C44
29	4N	302	CDL	C51-CB5-OB6-CB4
28	4W	603	3PE	C37-C38-C39-C3A
31	4L	202	PC1	C21-C22-C23-C24
29	4H	301	CDL	C60-C61-C62-C63
29	4V	201	CDL	C41-C42-C43-C44
29	4H	301	CDL	C83-C84-C85-C86
31	4Y	301	PC1	C31-C32-C33-C34
29	4F	301	CDL	C31-CA7-OA8-CA6
28	4E	304	3PE	C2A-C2B-C2C-C2D
28	4E	303	3PE	C22-C23-C24-C25
29	4N	302	CDL	C76-C77-C78-C79
29	4U	201	CDL	C58-C59-C60-C61
28	4E	303	3PE	C26-C27-C28-C29
28	B	509	3PE	C3A-C3B-C3C-C3D
29	4V	201	CDL	C75-C76-C77-C78
29	4N	302	CDL	OB7-CB5-OB6-CB4
29	4F	301	CDL	C36-C37-C38-C39
29	4V	201	CDL	C76-C77-C78-C79
29	4H	301	CDL	CB3-OB5-PB2-OB2
31	4Y	301	PC1	C11-O13-P-O11
29	4L	201	CDL	C1-CB2-OB2-PB2

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Mol	Chain	Res	Type	Atoms
28	4N	301	3PE	C27-C28-C29-C2A
27	4H	302	LPP	O5-C6-C7-C8
28	4E	302	3PE	O11-C1-C2-C3
29	4V	201	CDL	C51-C52-C53-C54
28	4W	603	3PE	C3C-C3D-C3E-C3F
28	4D	202	3PE	C26-C27-C28-C29
28	4E	305	3PE	C35-C36-C37-C38
27	4D	201	LPP	C6-C7-C8-O27
28	4E	302	3PE	C22-C23-C24-C25
28	4E	303	3PE	C1-C2-C3-O31
28	4N	301	3PE	C1-C2-C3-O31
28	4R	201	3PE	C1-C2-C3-O31
29	4F	301	CDL	CB3-CB4-CB6-OB8
28	4E	305	3PE	O31-C31-C32-C33
28	4N	301	3PE	C2A-C2B-C2C-C2D
28	4D	202	3PE	C29-C2A-C2B-C2C
28	4E	304	3PE	C36-C37-C38-C39
29	4F	301	CDL	OA9-CA7-OA8-CA6
27	4D	201	LPP	C30-C29-O27-C8
28	4E	302	3PE	C26-C27-C28-C29
28	4E	303	3PE	C1-C2-O21-C21
29	4V	201	CDL	C64-C65-C66-C67
28	4N	301	3PE	O11-C1-C2-O21
28	4W	603	3PE	O11-C1-C2-O21
29	4F	301	CDL	C72-C71-CB7-OB8
28	4N	301	3PE	C24-C25-C26-C27
28	4R	201	3PE	O21-C2-C3-O31
28	B	508	3PE	O21-C2-C3-O31
29	4E	301	CDL	C19-C20-C21-C22
29	4H	301	CDL	C62-C63-C64-C65
29	4N	302	CDL	C51-C52-C53-C54
28	4E	304	3PE	C3D-C3E-C3F-C3G
29	B	502	CDL	C11-C12-C13-C14
28	4E	302	3PE	C3D-C3E-C3F-C3G
28	4E	303	3PE	O11-C1-C2-C3
28	4N	301	3PE	O11-C1-C2-C3
28	4W	603	3PE	O11-C1-C2-C3
29	4E	301	CDL	OB5-CB3-CB4-CB6
29	4H	301	CDL	OB5-CB3-CB4-CB6
29	4U	201	CDL	OA5-CA3-CA4-CA6
29	4V	201	CDL	OA5-CA3-CA4-CA6
29	4V	201	CDL	OB5-CB3-CB4-CB6

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Mol	Chain	Res	Type	Atoms
28	4E	303	3PE	C35-C36-C37-C38
29	4V	201	CDL	C77-C78-C79-C80
29	4H	301	CDL	C31-CA7-OA8-CA6
29	4L	201	CDL	C1-CA2-OA2-PA1
29	4N	302	CDL	C1-CA2-OA2-PA1
29	4V	201	CDL	CB4-CB3-OB5-PB2
27	4H	302	LPP	C19-C20-C21-C22
28	4W	603	3PE	C2F-C2G-C2H-C2I
29	B	502	CDL	C58-C59-C60-C61
28	4N	301	3PE	C26-C27-C28-C29
28	4E	304	3PE	C1-C2-C3-O31
28	B	508	3PE	C1-C2-C3-O31
29	B	502	CDL	CB3-CB4-CB6-OB8
27	4H	302	LPP	O9-C11-C12-C13
28	4E	303	3PE	C39-C3A-C3B-C3C
27	4H	302	LPP	O5-C6-C7-O9
29	4U	201	CDL	OA5-CA3-CA4-OA6
29	4V	201	CDL	OB5-CB3-CB4-OB6
29	4V	201	CDL	C52-C51-CB5-OB6
28	4W	603	3PE	C2B-C2C-C2D-C2E
27	4D	201	LPP	O28-C29-O27-C8
28	4E	302	3PE	O21-C2-C3-O31
28	4E	304	3PE	O21-C2-C3-O31
28	B	508	3PE	C25-C26-C27-C28
29	4V	201	CDL	C1-CB2-OB2-PB2
29	4F	301	CDL	C62-C63-C64-C65
29	4E	301	CDL	C72-C73-C74-C75
28	4D	202	3PE	O11-C1-C2-C3
28	B	509	3PE	C22-C23-C24-C25
29	4L	201	CDL	C31-CA7-OA8-CA6
28	4E	305	3PE	C23-C24-C25-C26
29	B	502	CDL	OB7-CB5-OB6-CB4
29	4V	201	CDL	C31-CA7-OA8-CA6
29	4N	302	CDL	C12-C13-C14-C15
31	4L	202	PC1	C39-C3A-C3B-C3C
29	4E	301	CDL	C1-CB2-OB2-PB2
29	4F	302	CDL	CA4-CA3-OA5-PA1
29	4N	302	CDL	CA4-CA3-OA5-PA1
29	4U	201	CDL	C1-CB2-OB2-PB2
29	4V	201	CDL	CB3-CB4-CB6-OB8
28	4E	302	3PE	O11-C1-C2-O21
28	4E	303	3PE	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
29	4V	201	CDL	OA5-CA3-CA4-OA6
29	4F	301	CDL	OB6-CB4-CB6-OB8
29	4U	201	CDL	OB6-CB4-CB6-OB8
29	4F	301	CDL	C77-C78-C79-C80
29	4H	301	CDL	OA9-CA7-OA8-CA6
28	4E	302	3PE	C33-C34-C35-C36
28	4E	305	3PE	C38-C39-C3A-C3B
28	4D	202	3PE	C31-C32-C33-C34
28	4E	305	3PE	C2C-C2D-C2E-C2F
29	4V	201	CDL	OB7-CB5-OB6-CB4
29	4V	201	CDL	C51-CB5-OB6-CB4
28	4W	603	3PE	C33-C34-C35-C36
28	4E	302	3PE	C1-O11-P-O13
29	B	502	CDL	CB3-OB5-PB2-OB2
27	4D	201	LPP	C7-C6-O5-P1
28	4W	603	3PE	C2-C1-O11-P
28	4R	201	3PE	C1-O11-P-O14
28	4W	603	3PE	C11-O13-P-O14
28	B	508	3PE	C1-O11-P-O14
28	B	509	3PE	C11-O13-P-O14
29	4F	302	CDL	CA2-OA2-PA1-OA3
29	4H	301	CDL	CB3-OB5-PB2-OB4
29	4U	201	CDL	CB3-OB5-PB2-OB3
29	B	502	CDL	CB2-OB2-PB2-OB3
29	B	502	CDL	CB2-OB2-PB2-OB4
29	4U	201	CDL	C72-C73-C74-C75
29	4V	201	CDL	OA9-CA7-OA8-CA6
28	4D	202	3PE	C12-C11-O13-P
28	4E	304	3PE	C12-C11-O13-P
31	4L	202	PC1	C12-C11-O13-P
36	B	506	HEA	C3B-C11-C12-C13
27	4D	201	LPP	C11-C12-C13-C14
28	4E	302	3PE	C24-C25-C26-C27
31	4Y	301	PC1	C3E-C3F-C3G-C3H
29	4E	301	CDL	OB5-CB3-CB4-OB6
29	4H	301	CDL	OB5-CB3-CB4-OB6
29	4F	302	CDL	C16-C17-C18-C19
28	4E	302	3PE	C37-C38-C39-C3A
28	4E	302	3PE	C2A-C2B-C2C-C2D
28	4E	302	3PE	C28-C29-C2A-C2B
31	4L	202	PC1	O13-C11-C12-N
29	4H	301	CDL	OA7-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
27	4D	201	LPP	O9-C7-C8-O27
28	4D	202	3PE	O21-C2-C3-O31
28	4E	303	3PE	O21-C2-C3-O31
29	4V	201	CDL	OB6-CB4-CB6-OB8
29	B	502	CDL	OB6-CB4-CB6-OB8
29	4L	201	CDL	C71-C72-C73-C74
28	4E	303	3PE	C2E-C2F-C2G-C2H
28	4E	303	3PE	C2-C1-O11-P
27	4H	302	LPP	C36-C37-C38-C39
29	4L	201	CDL	OA9-CA7-OA8-CA6
29	4H	301	CDL	C11-CA5-OA6-CA4
29	B	502	CDL	C51-CB5-OB6-CB4
29	4N	302	CDL	C13-C14-C15-C16
28	4D	202	3PE	C2-C1-O11-P
29	4N	302	CDL	OB5-CB3-CB4-OB6
28	4R	201	3PE	C27-C28-C29-C2A
29	4E	301	CDL	OA6-CA4-CA6-OA8
29	4L	201	CDL	OB6-CB4-CB6-OB8
28	4D	202	3PE	C1-O11-P-O13
28	4E	305	3PE	C11-O13-P-O11
28	4R	201	3PE	C11-O13-P-O11
29	4E	301	CDL	CA3-OA5-PA1-OA2
29	4E	301	CDL	CB2-OB2-PB2-OB5
29	4F	301	CDL	CB2-OB2-PB2-OB5
29	4L	201	CDL	CA3-OA5-PA1-OA2
31	4L	202	PC1	C11-O13-P-O11
31	4Y	301	PC1	C1-O11-P-O13
29	4E	301	CDL	C18-C19-C20-C21
29	4E	301	CDL	C38-C39-C40-C41
28	B	508	3PE	C29-C2A-C2B-C2C
28	4R	201	3PE	C2-C1-O11-P
29	B	502	CDL	C1-CA2-OA2-PA1
28	B	508	3PE	C32-C33-C34-C35
29	4V	201	CDL	C57-C58-C59-C60
29	4F	301	CDL	CA4-CA6-OA8-CA7
29	4N	302	CDL	CB2-C1-CA2-OA2
28	4R	201	3PE	C25-C26-C27-C28
28	4R	201	3PE	C26-C27-C28-C29
31	4Y	301	PC1	C39-C3A-C3B-C3C
28	4E	305	3PE	O32-C31-C32-C33
27	4D	201	LPP	C39-C40-C41-C42
28	4W	603	3PE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
29	4U	201	CDL	C76-C77-C78-C79
29	4N	302	CDL	O1-C1-CA2-OA2
29	4F	301	CDL	C81-C82-C83-C84
27	4H	302	LPP	C37-C38-C39-C40
29	4E	301	CDL	C59-C60-C61-C62
29	4E	301	CDL	C77-C78-C79-C80
28	4D	202	3PE	C3D-C3E-C3F-C3G
29	4L	201	CDL	CB2-C1-CA2-OA2
36	B	505	HEA	CAA-CBA-CGA-O1A
36	B	506	HEA	CAD-CBD-CGD-O2D
29	4F	301	CDL	C72-C71-CB7-OB9
36	B	506	HEA	CAD-CBD-CGD-O1D
29	4E	301	CDL	CA3-CA4-OA6-CA5
29	4E	301	CDL	CB3-CB4-OB6-CB5
29	4F	301	CDL	CA3-CA4-OA6-CA5
29	4F	301	CDL	CB6-CB4-OB6-CB5
29	4F	302	CDL	CA3-CA4-OA6-CA5
29	4N	302	CDL	CB6-CB4-OB6-CB5
27	4H	302	LPP	O10-C11-C12-C13
29	B	502	CDL	C59-C60-C61-C62
28	B	508	3PE	C39-C3A-C3B-C3C
28	4E	303	3PE	C33-C34-C35-C36
29	4E	301	CDL	OA7-CA5-OA6-CA4
29	4E	301	CDL	C15-C16-C17-C18
29	4U	201	CDL	CB7-C71-C72-C73
28	4D	202	3PE	C21-C22-C23-C24
27	4H	302	LPP	O9-C7-C8-O27
29	4H	301	CDL	OA6-CA4-CA6-OA8
29	4L	201	CDL	CB4-CB6-OB8-CB7
29	4N	302	CDL	CB4-CB6-OB8-CB7
29	4V	201	CDL	C21-C22-C23-C24
36	B	505	HEA	C15-C16-C17-C18
29	4F	301	CDL	C37-C38-C39-C40
29	4U	201	CDL	CB3-CB4-CB6-OB8
28	4R	201	3PE	C38-C39-C3A-C3B
28	4N	301	3PE	C34-C35-C36-C37
29	4E	301	CDL	C14-C15-C16-C17
29	4V	201	CDL	C62-C63-C64-C65
31	4L	202	PC1	C3F-C3G-C3H-C3I
28	4E	302	3PE	C29-C2A-C2B-C2C
31	4L	202	PC1	C2B-C2C-C2D-C2E
31	4L	202	PC1	C28-C29-C2A-C2B

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Mol	Chain	Res	Type	Atoms
36	B	505	HEA	CAA-CBA-CGA-O2A
36	B	506	HEA	CAA-CBA-CGA-O2A
29	4U	201	CDL	C32-C31-CA7-OA8
29	4H	301	CDL	C14-C15-C16-C17
36	B	506	HEA	CAA-CBA-CGA-O1A
29	4V	201	CDL	CB3-OB5-PB2-OB2
29	4E	301	CDL	C81-C82-C83-C84
29	4E	301	CDL	C20-C21-C22-C23
29	B	502	CDL	C40-C41-C42-C43
29	4V	201	CDL	C81-C82-C83-C84
28	4D	202	3PE	C3-C2-O21-C21
29	4H	301	CDL	CB3-CB4-OB6-CB5
27	4D	201	LPP	C29-C30-C31-C32
36	B	505	HEA	CAD-CBD-CGD-O2D
29	4N	302	CDL	C75-C76-C77-C78
27	4D	201	LPP	C17-C18-C19-C20
29	4E	301	CDL	C82-C83-C84-C85
31	4Y	301	PC1	C25-C26-C27-C28
28	4E	302	3PE	C1-C2-C3-O31
29	4F	302	CDL	C32-C31-CA7-OA8
29	4V	201	CDL	C52-C51-CB5-OB7
36	B	505	HEA	CAD-CBD-CGD-O1D
28	4R	201	3PE	C2-C3-O31-C31
28	4N	301	3PE	C2E-C2F-C2G-C2H
28	B	508	3PE	C2A-C2B-C2C-C2D
28	B	508	3PE	C23-C24-C25-C26
28	4R	201	3PE	O21-C21-C22-C23
29	4L	201	CDL	C57-C58-C59-C60
29	4V	201	CDL	C61-C62-C63-C64
28	4D	202	3PE	C3E-C3F-C3G-C3H
36	B	505	HEA	C16-C17-C18-C19
28	4E	303	3PE	O31-C31-C32-C33
29	4U	201	CDL	C32-C31-CA7-OA9
28	B	509	3PE	C32-C33-C34-C35
29	4N	302	CDL	C61-C62-C63-C64
29	4F	301	CDL	C64-C65-C66-C67
28	4D	202	3PE	C1-O11-P-O14
28	4E	302	3PE	C1-O11-P-O12
28	4E	305	3PE	C11-O13-P-O14
28	4R	201	3PE	C11-O13-P-O14
29	4E	301	CDL	CA2-OA2-PA1-OA4
29	4E	301	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
29	4F	301	CDL	CA2-OA2-PA1-OA3
29	4F	301	CDL	CB2-OB2-PB2-OB3
29	4L	201	CDL	CA3-OA5-PA1-OA3
29	4N	302	CDL	CA3-OA5-PA1-OA3
29	4U	201	CDL	CB2-OB2-PB2-OB3
29	B	502	CDL	CA3-OA5-PA1-OA3
31	4L	202	PC1	C11-O13-P-O14
31	4Y	301	PC1	C1-O11-P-O14
29	4L	201	CDL	C72-C73-C74-C75
28	4W	603	3PE	O13-C11-C12-N
36	B	506	HEA	O11-C11-C12-C13
28	B	508	3PE	O21-C21-C22-C23
29	4F	302	CDL	C32-C31-CA7-OA9
29	4U	201	CDL	C31-C32-C33-C34
29	4E	301	CDL	CB6-CB4-OB6-CB5
28	4E	303	3PE	C3B-C3C-C3D-C3E
27	4D	201	LPP	C31-C32-C33-C34
28	4E	303	3PE	O32-C31-C32-C33
27	4D	201	LPP	O27-C29-C30-C31
28	4D	202	3PE	O31-C31-C32-C33
29	4V	201	CDL	C12-C11-CA5-OA7
36	B	505	HEA	O11-C11-C3B-C2B
28	4R	201	3PE	O22-C21-C22-C23
28	4E	304	3PE	O21-C21-C22-C23
28	4R	201	3PE	C23-C24-C25-C26
31	4L	202	PC1	C27-C28-C29-C2A
28	B	508	3PE	C24-C25-C26-C27
29	4V	201	CDL	C12-C11-CA5-OA6
28	4E	302	3PE	C2F-C2G-C2H-C2I
29	4N	302	CDL	C12-C11-CA5-OA6

There are no ring outliers.

20 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	4N	301	3PE	2	0
36	B	506	HEA	4	0
29	4F	301	CDL	2	0
28	B	509	3PE	2	0
28	B	508	3PE	1	0
31	4Y	301	PC1	4	0
29	4V	201	CDL	5	0

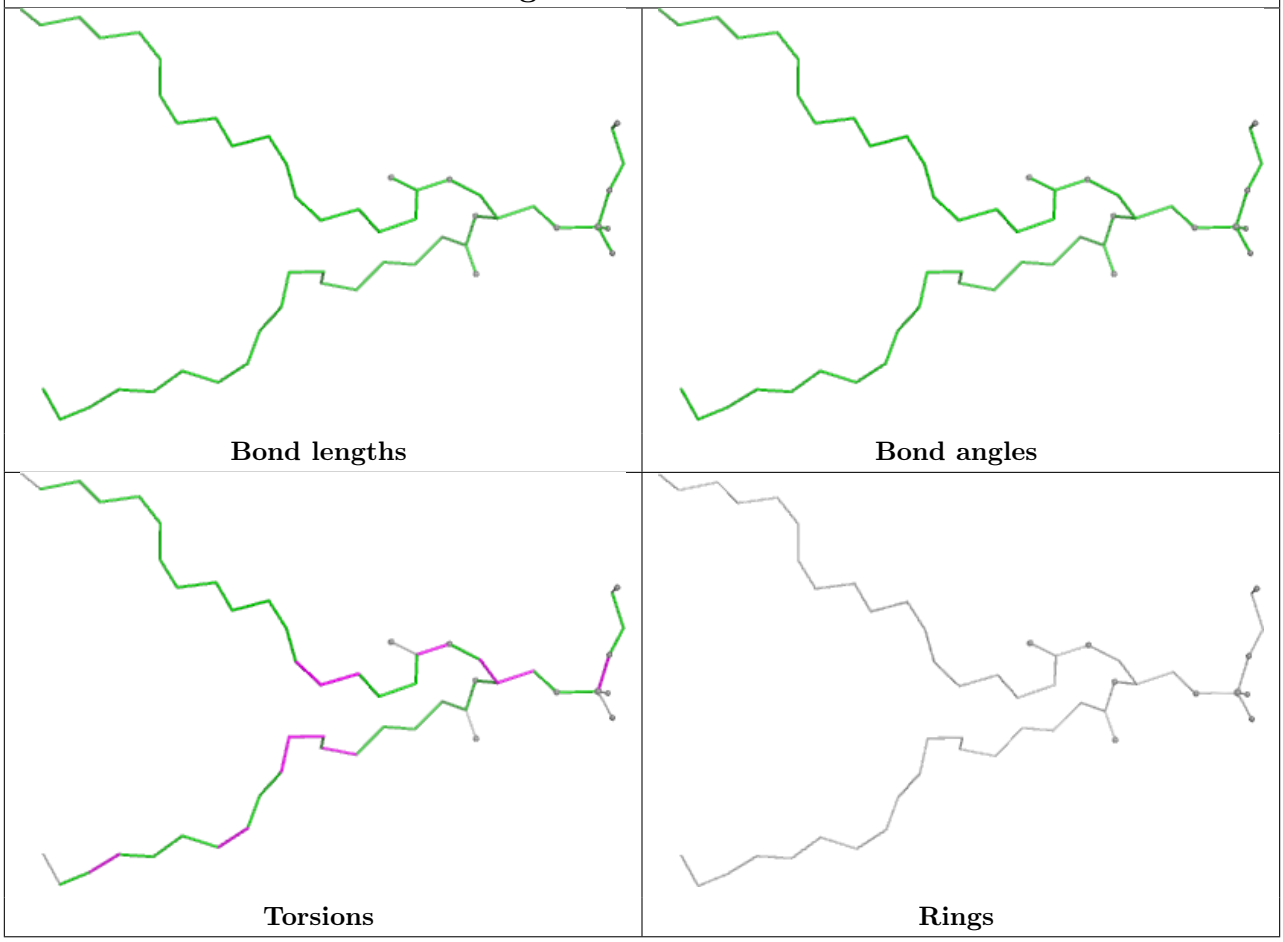
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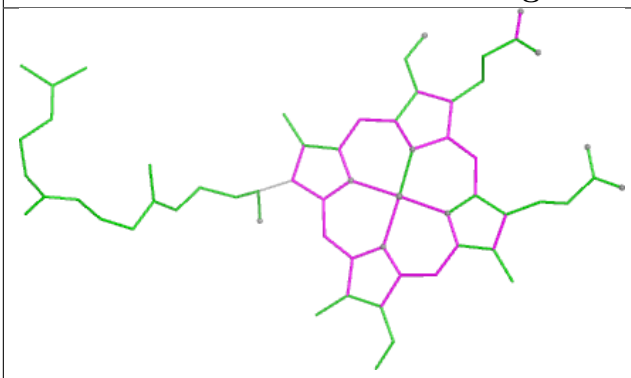
Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	4H	301	CDL	1	0
32	4W	602	FES	1	0
36	B	505	HEA	4	0
28	4W	603	3PE	2	0
28	4E	303	3PE	6	0
28	4E	305	3PE	2	0
29	4L	201	CDL	1	0
28	4D	202	3PE	3	0
29	B	502	CDL	1	0
28	4E	304	3PE	2	0
29	4U	201	CDL	1	0
28	4E	302	3PE	1	0
29	4E	301	CDL	1	0

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

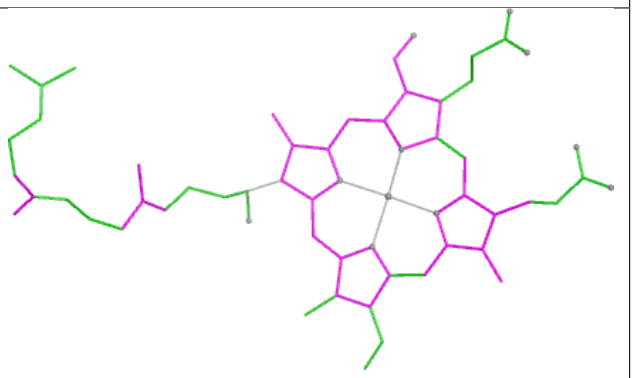
Ligand 3PE 4N 301



Ligand HEA B 506



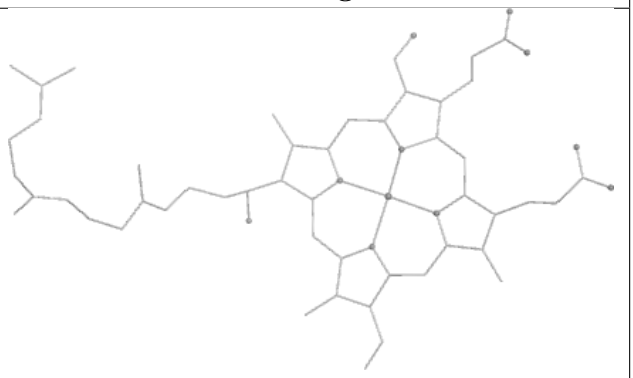
Bond lengths



Bond angles

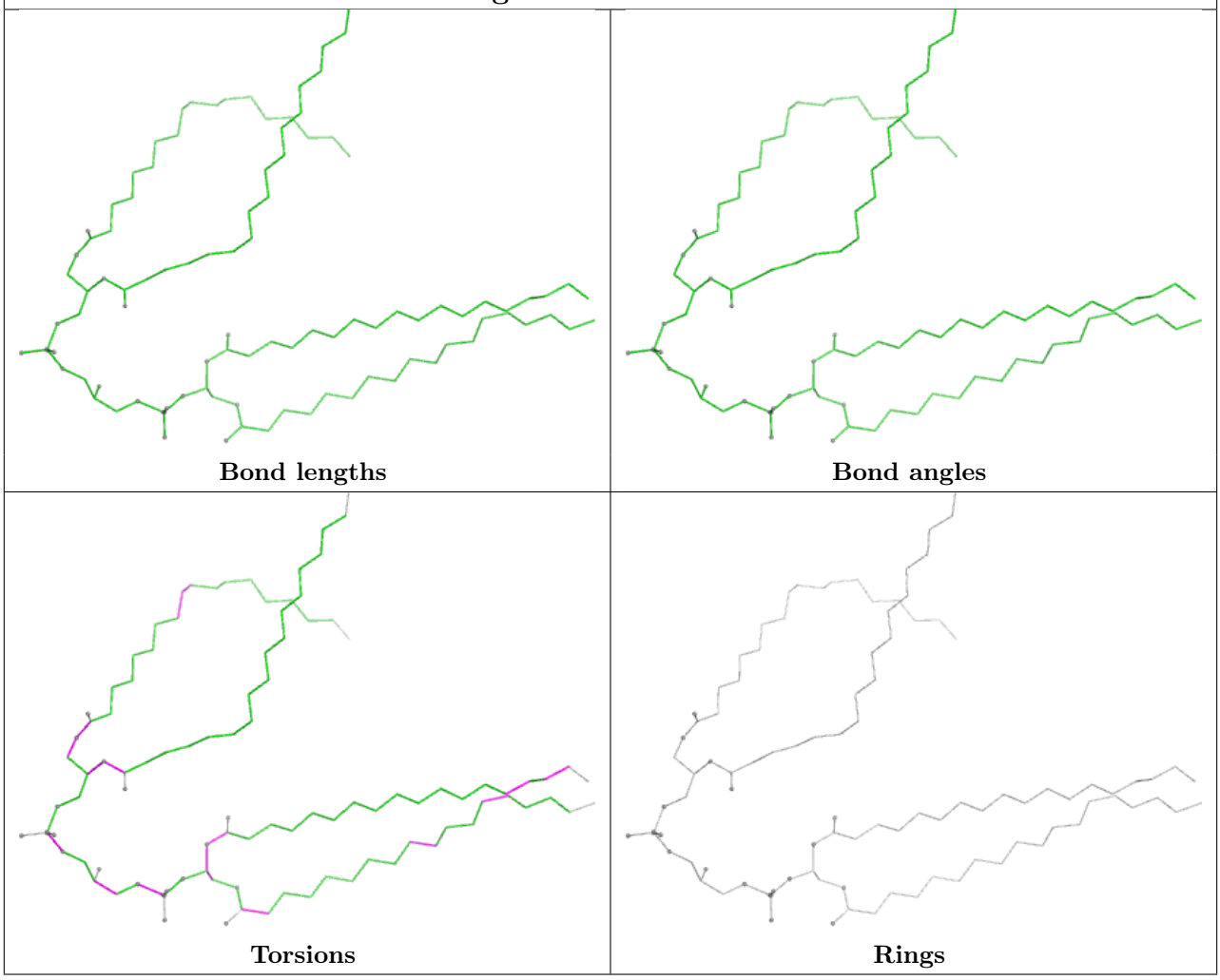


Torsions

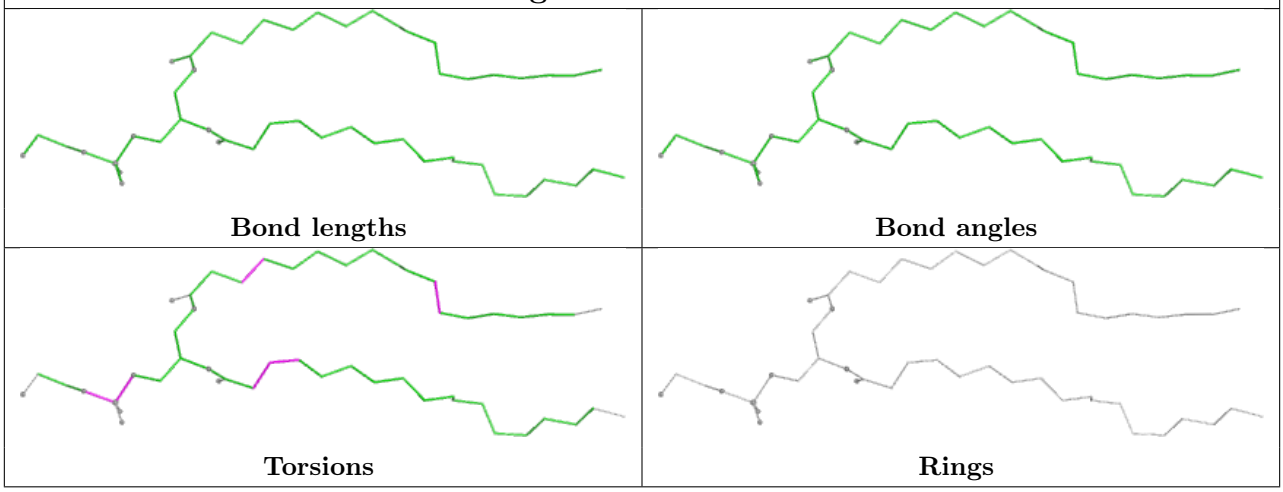


Rings

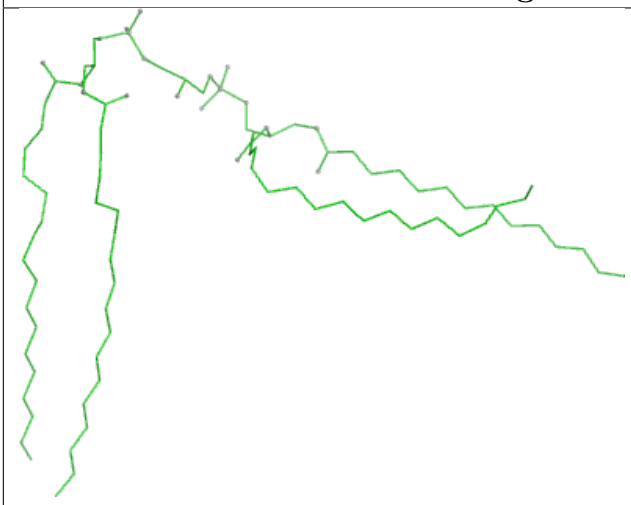
Ligand CDL 4F 301



Ligand 3PE B 509



Ligand CDL 4F 302



Bond lengths



Bond angles

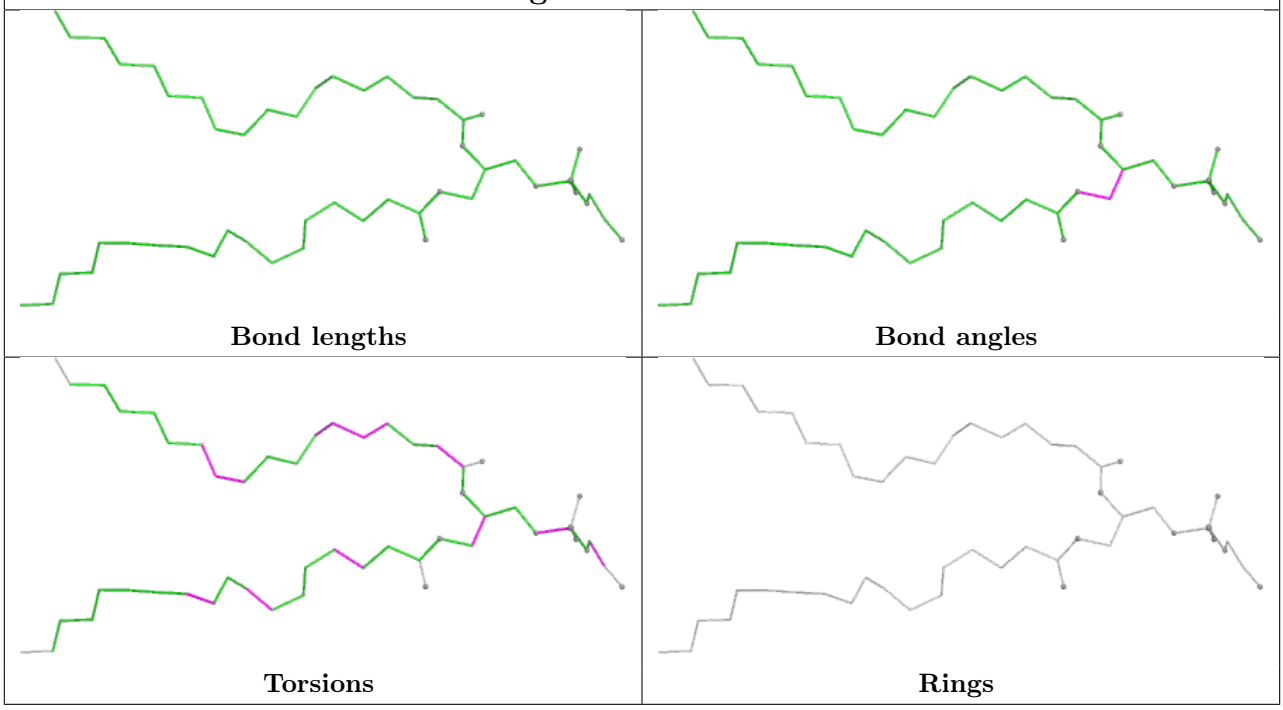


Torsions

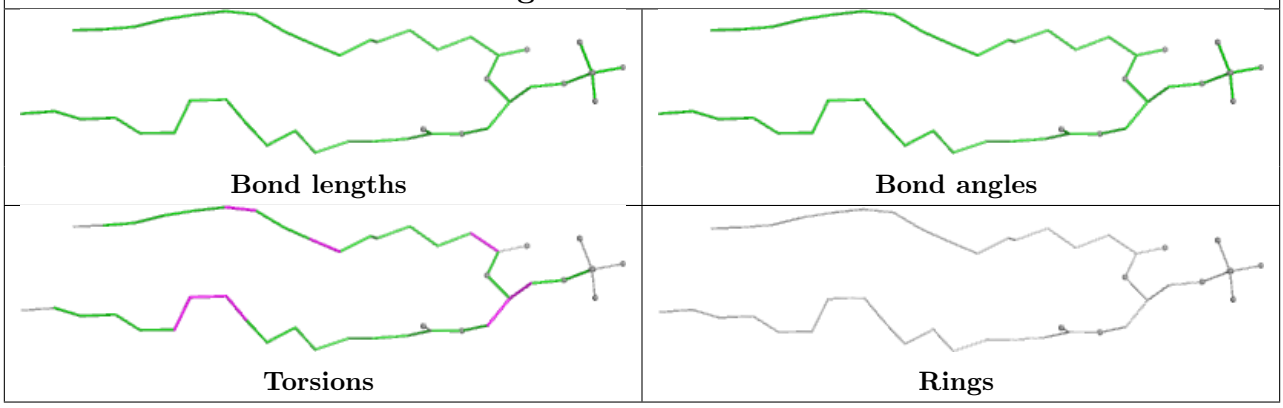


Rings

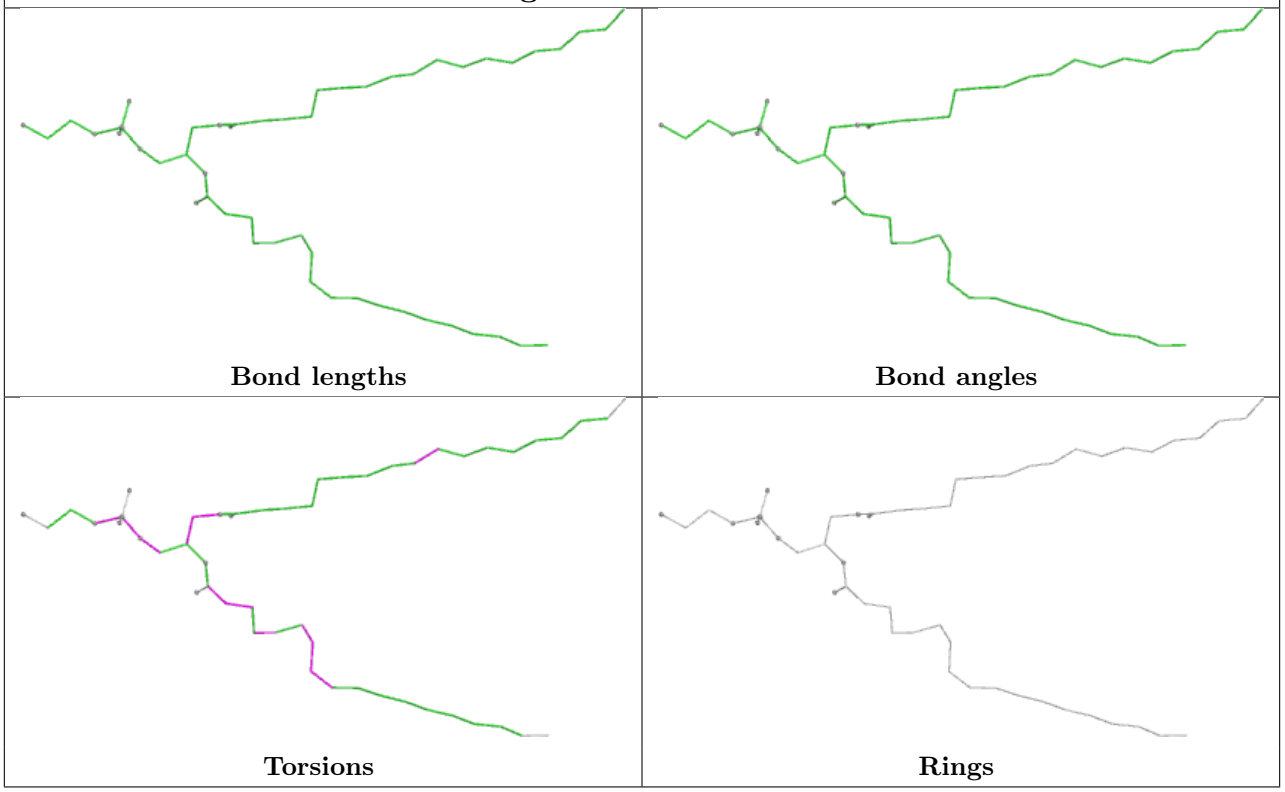
Ligand 3PE B 508



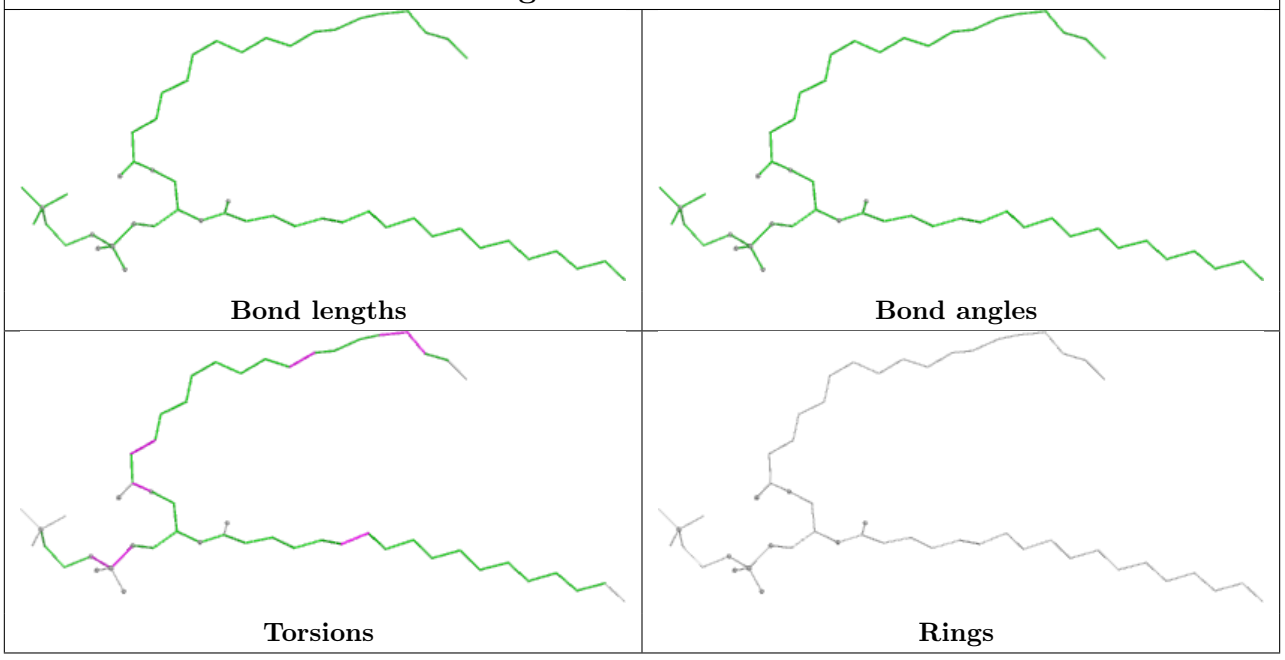
Ligand LPP 4H 302



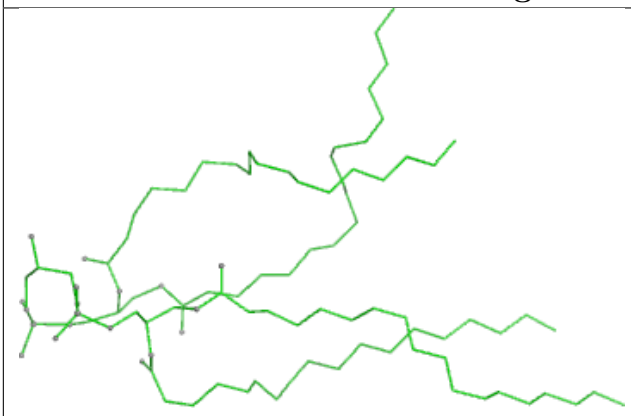
Ligand 3PE 4R 201



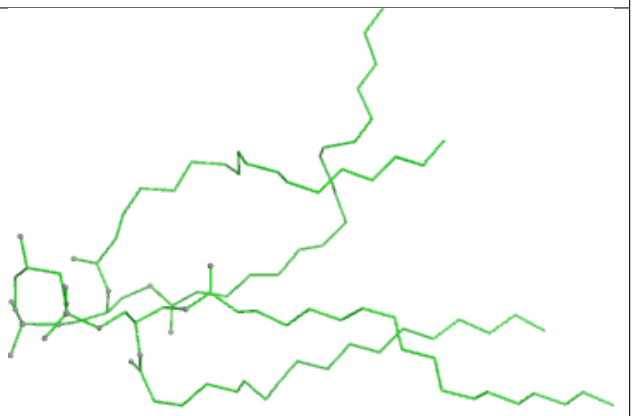
Ligand PC1 4Y 301



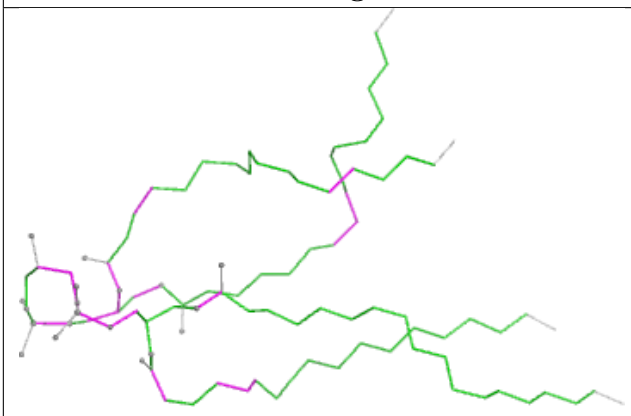
Ligand CDL 4N 302



Bond lengths



Bond angles

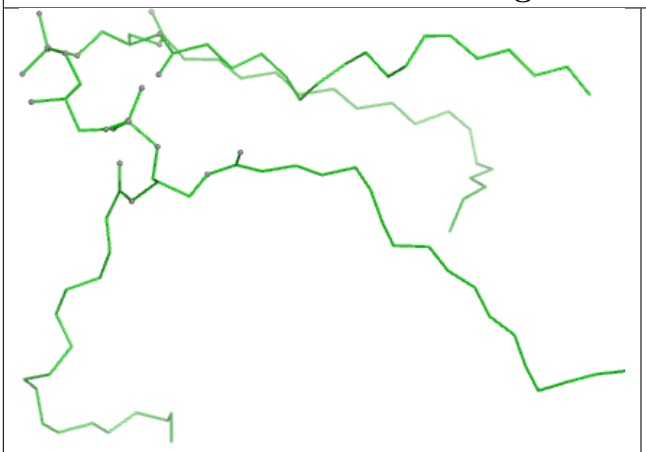


Torsions

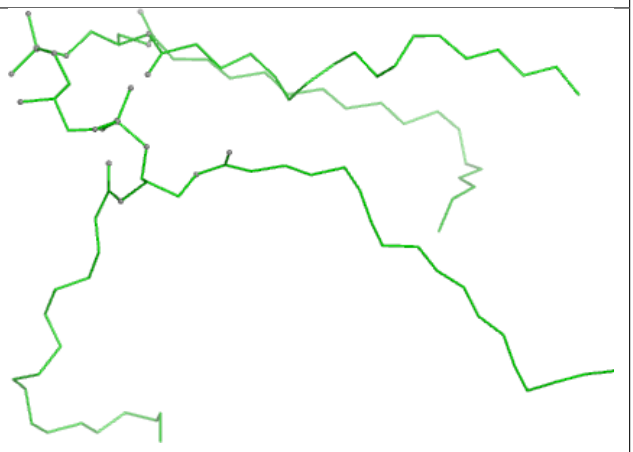


Rings

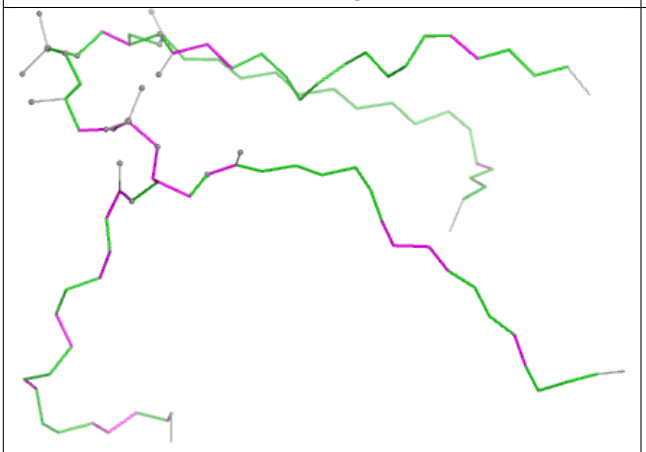
Ligand CDL 4V 201



Bond lengths



Bond angles

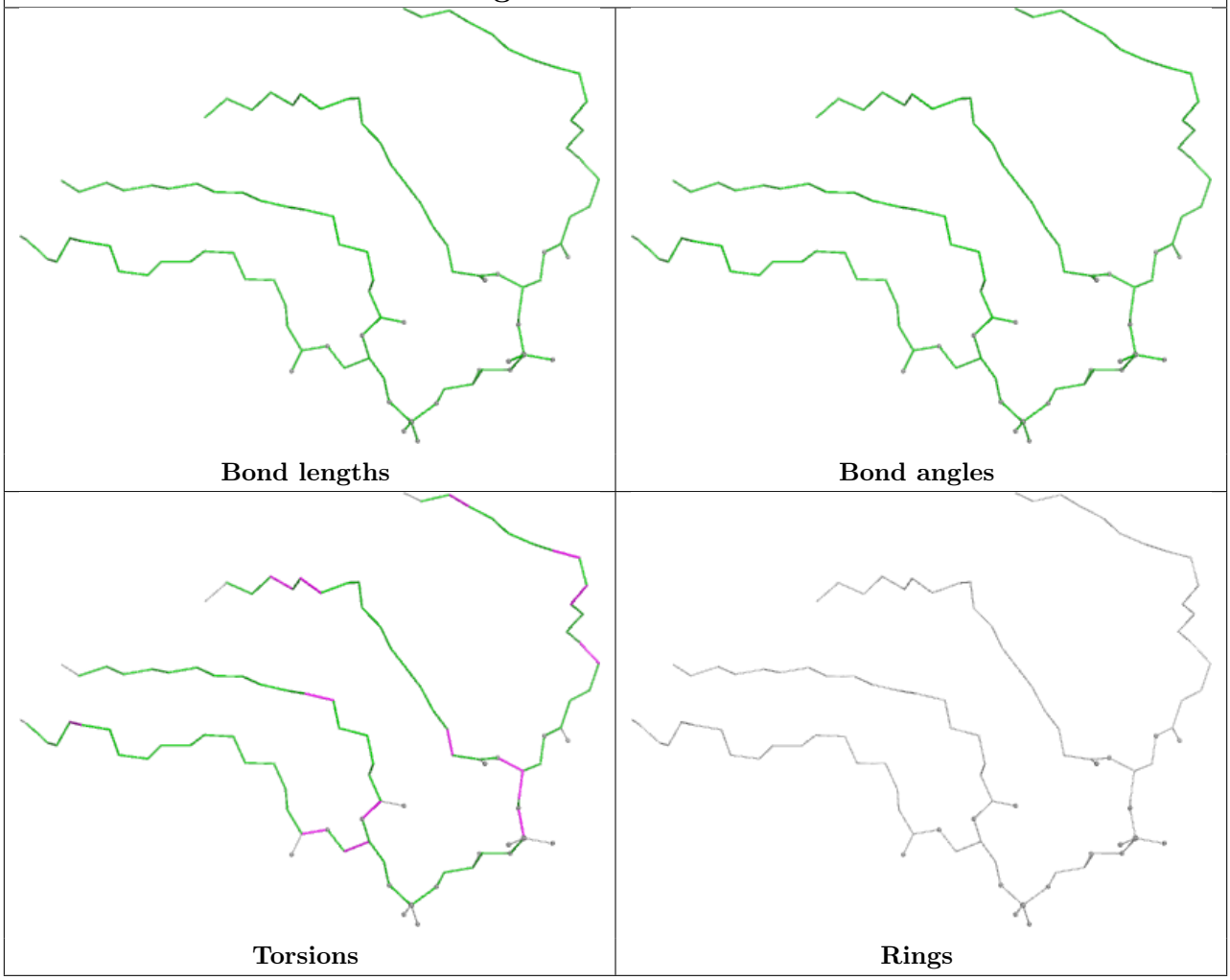


Torsions

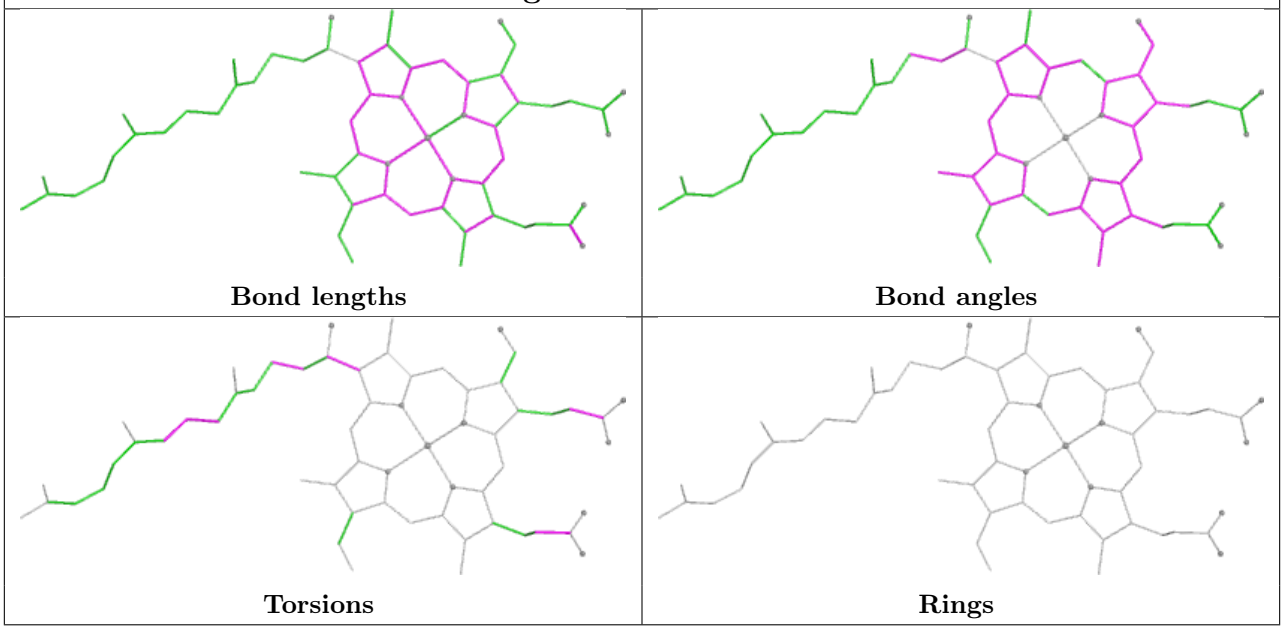


Rings

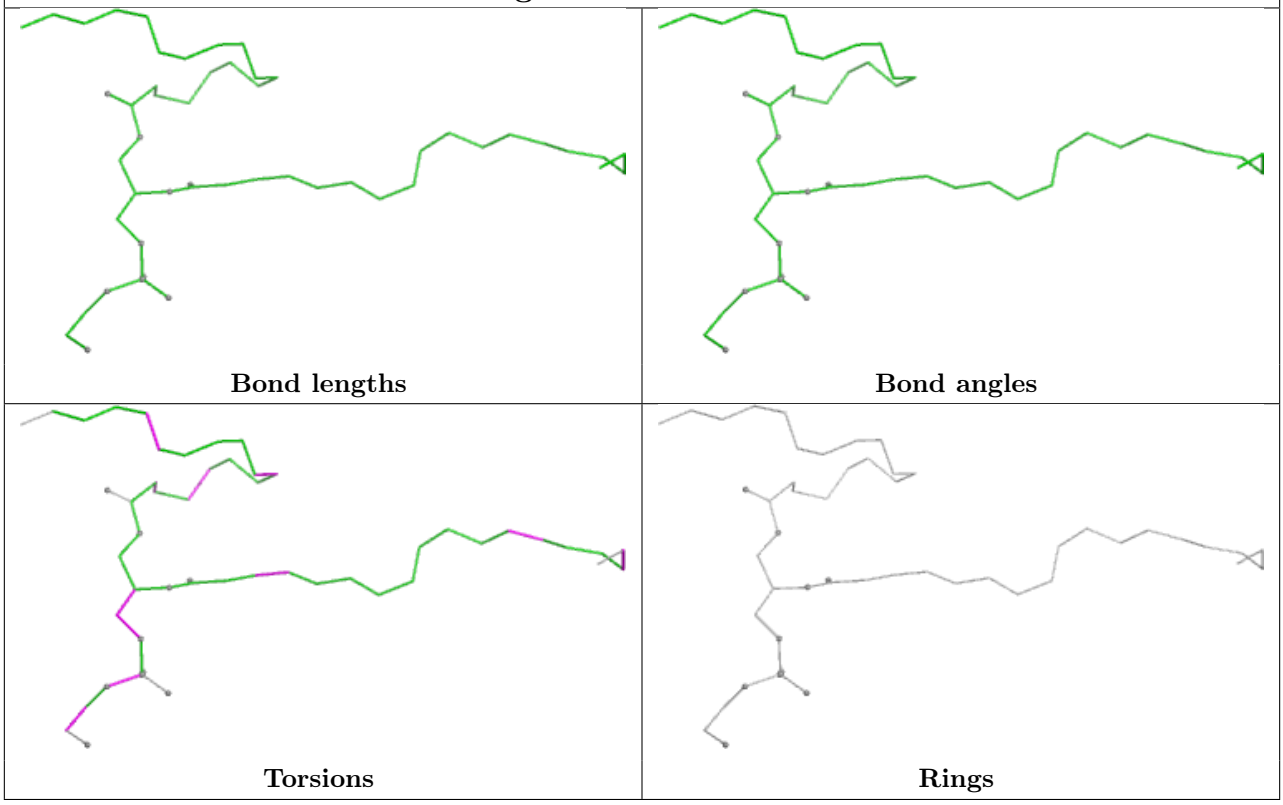
Ligand CDL 4H 301



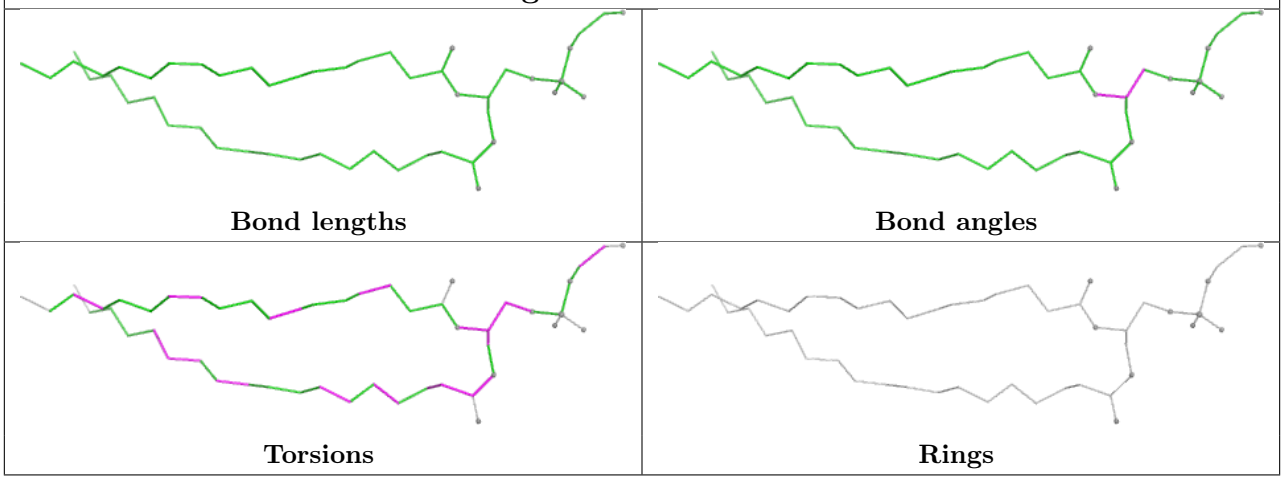
Ligand HEA B 505



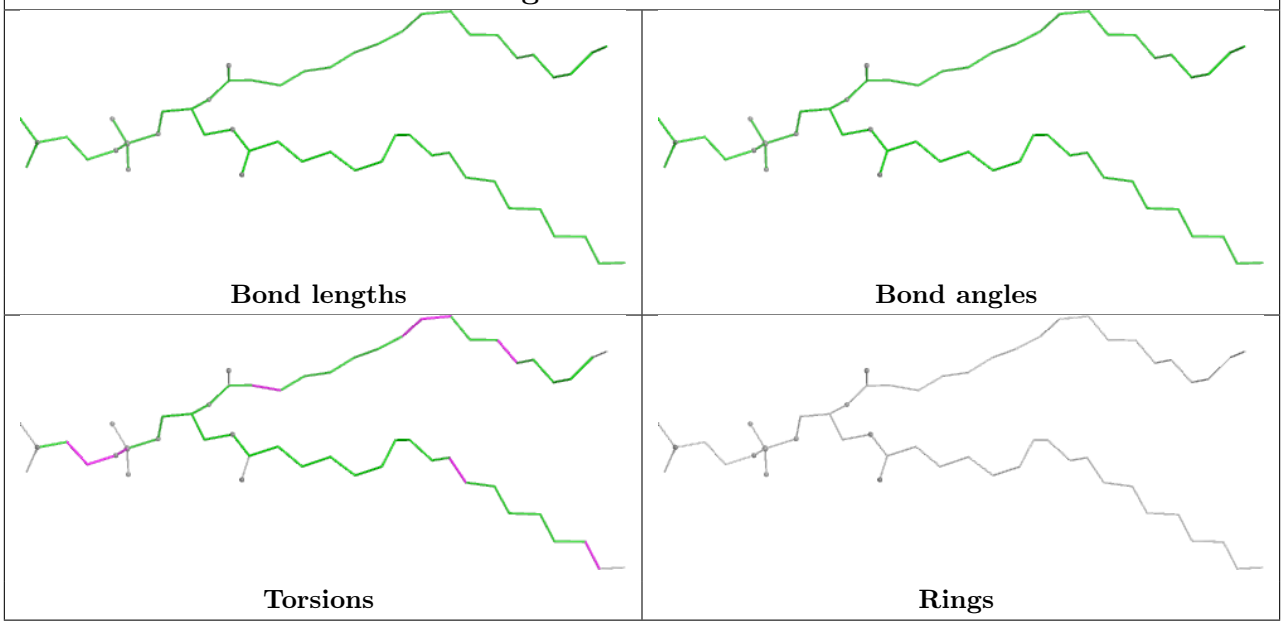
Ligand 3PE 4W 603



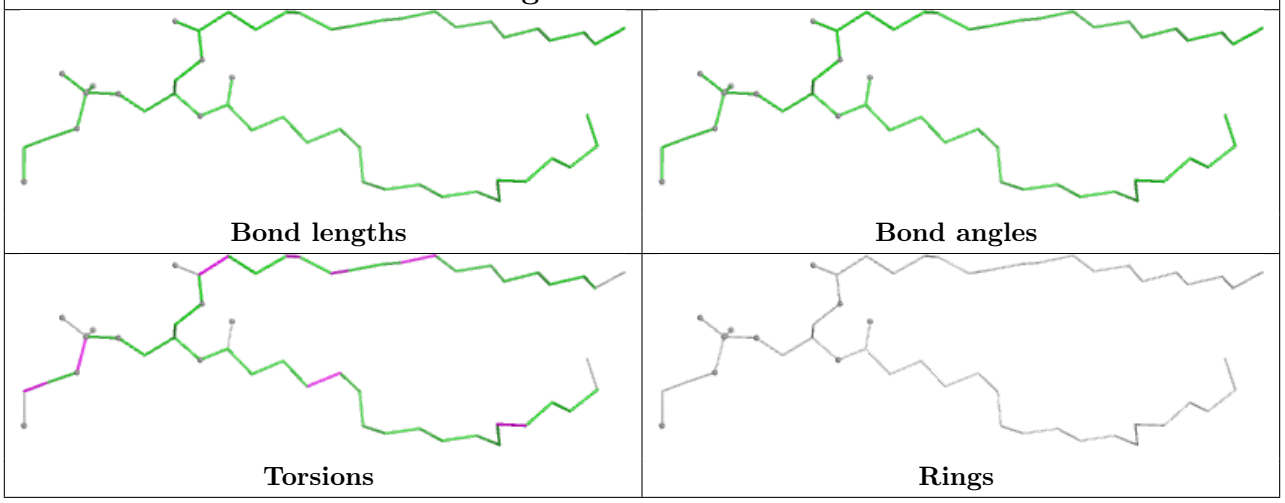
Ligand 3PE 4E 303



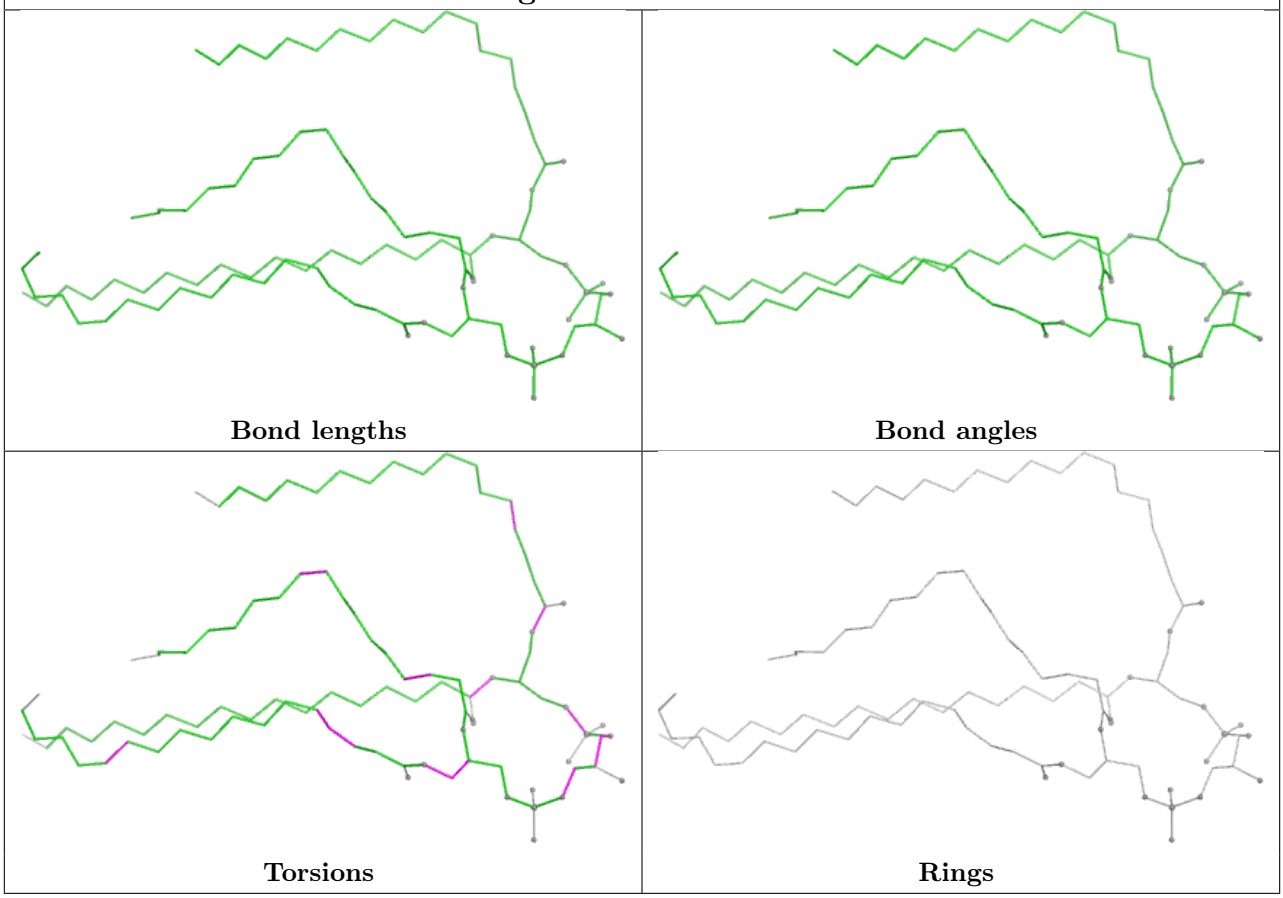
Ligand PC1 4L 202



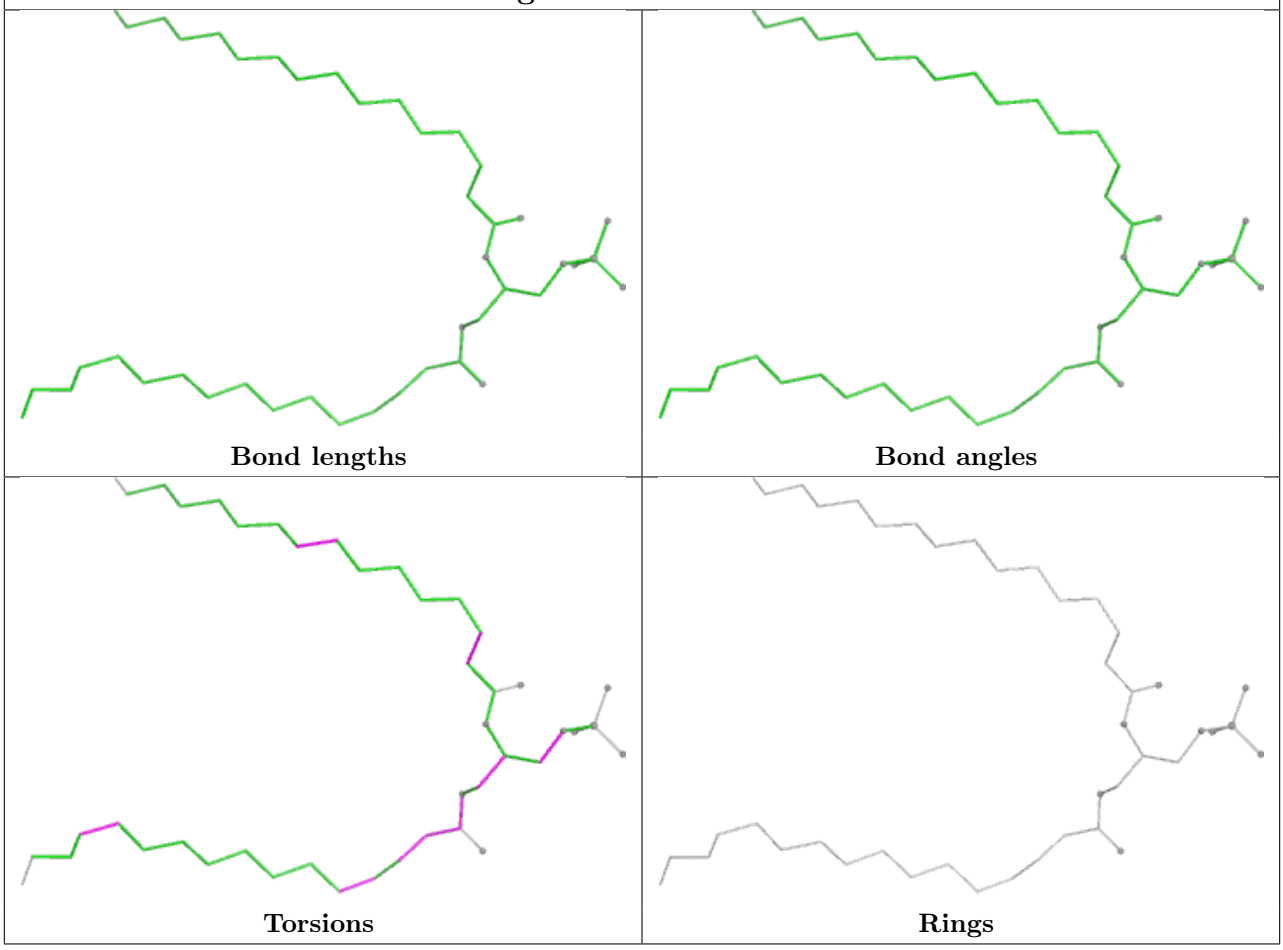
Ligand 3PE 4E 305



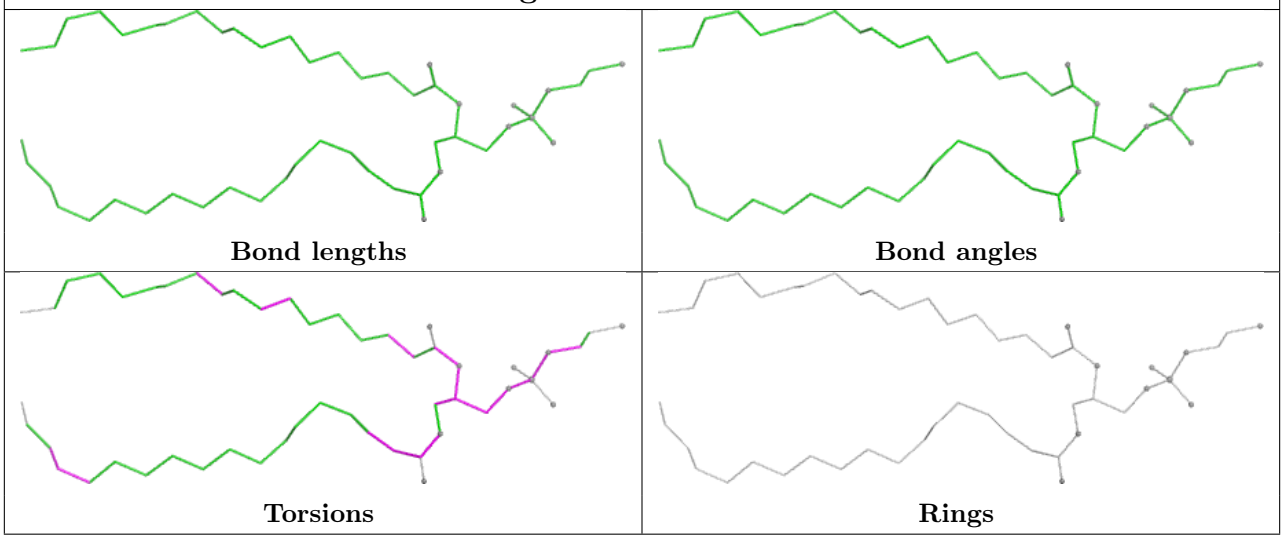
Ligand CDL 4L 201



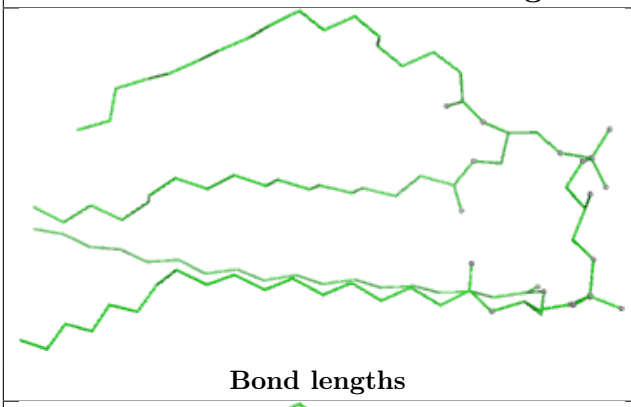
Ligand LPP 4D 201



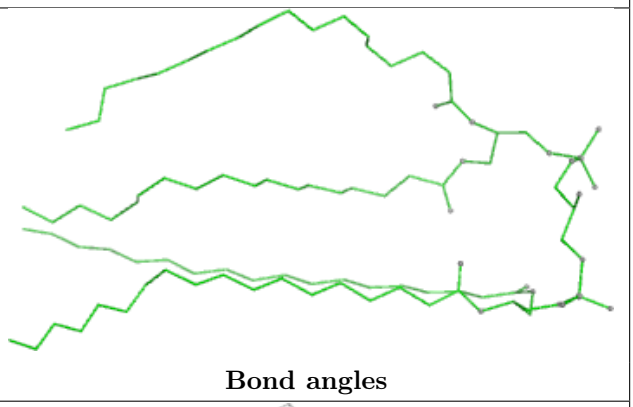
Ligand 3PE 4D 202



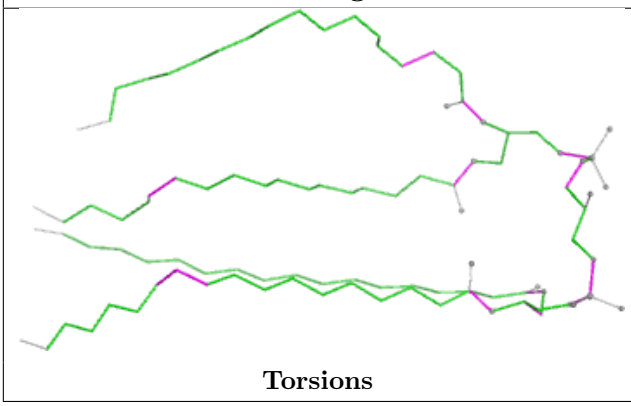
Ligand CDL B 502



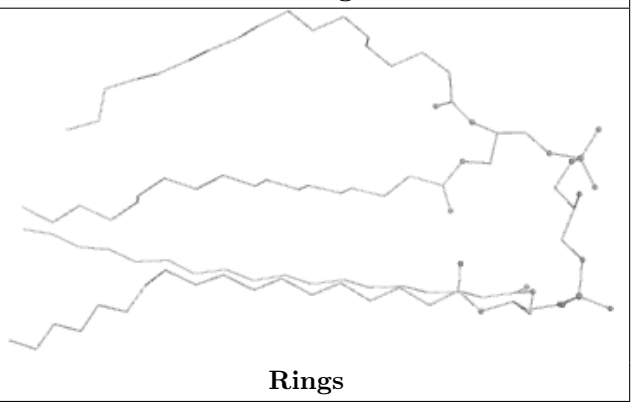
Bond lengths



Bond angles

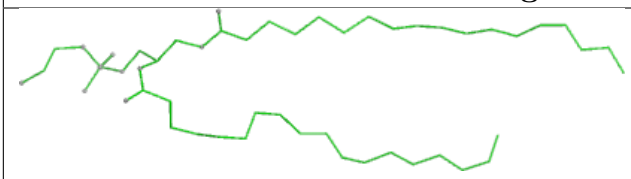


Torsions

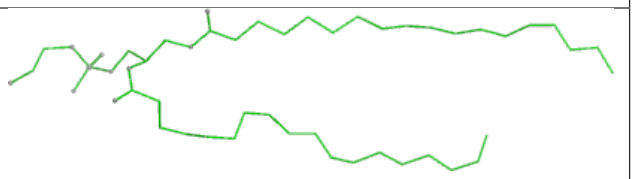


Rings

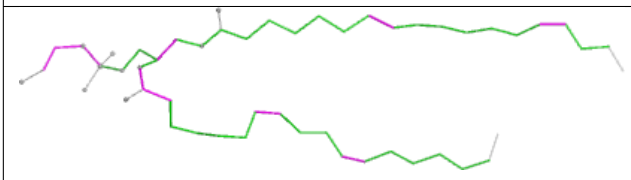
Ligand 3PE 4E 304



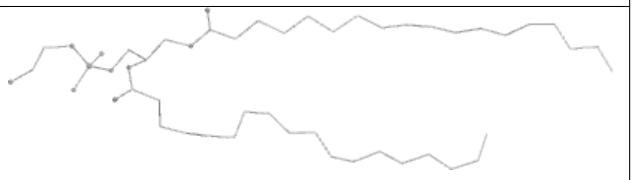
Bond lengths



Bond angles

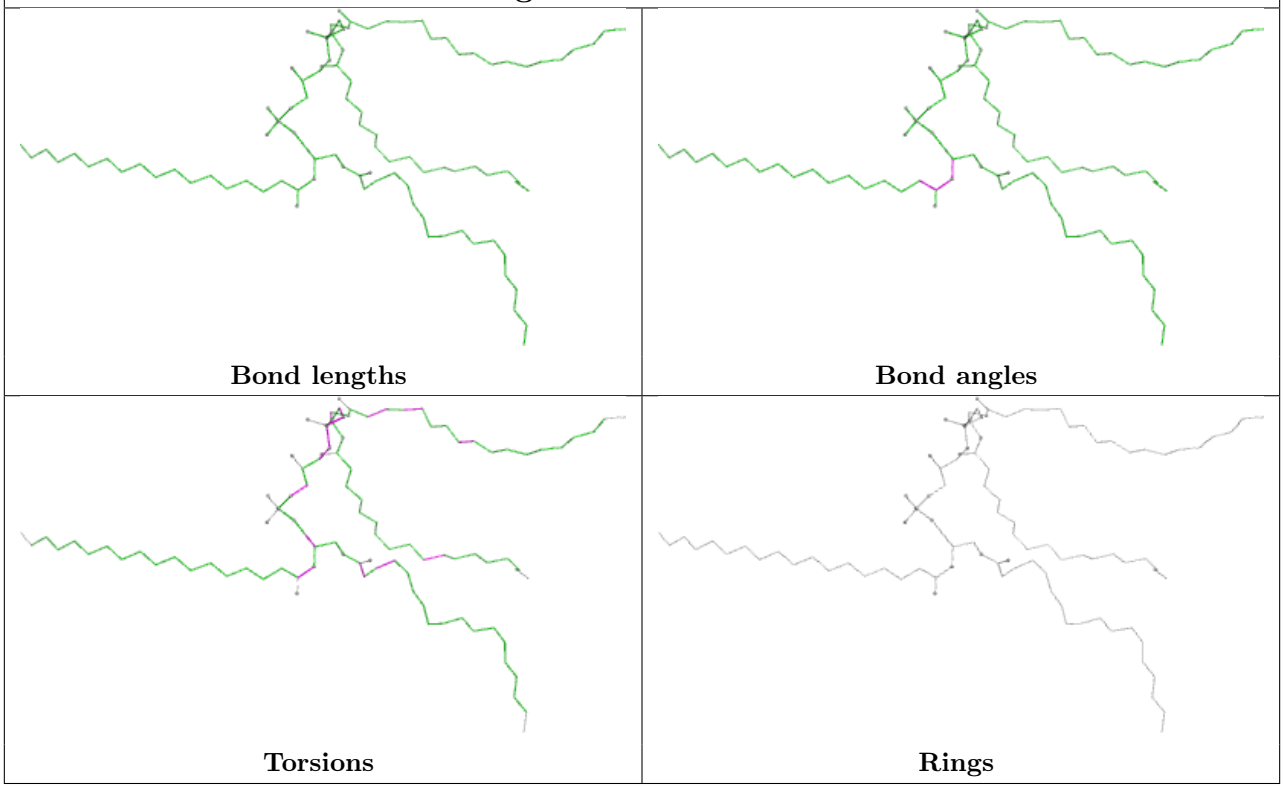


Torsions

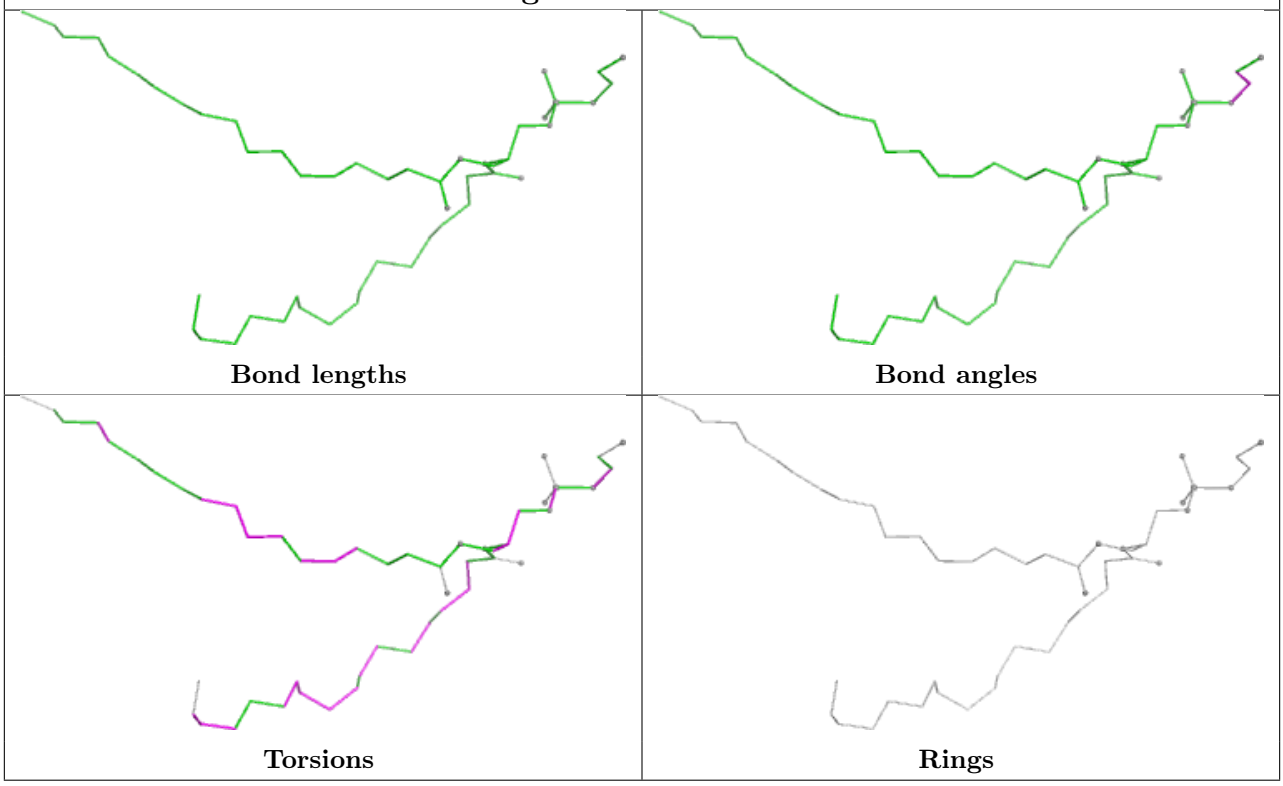


Rings

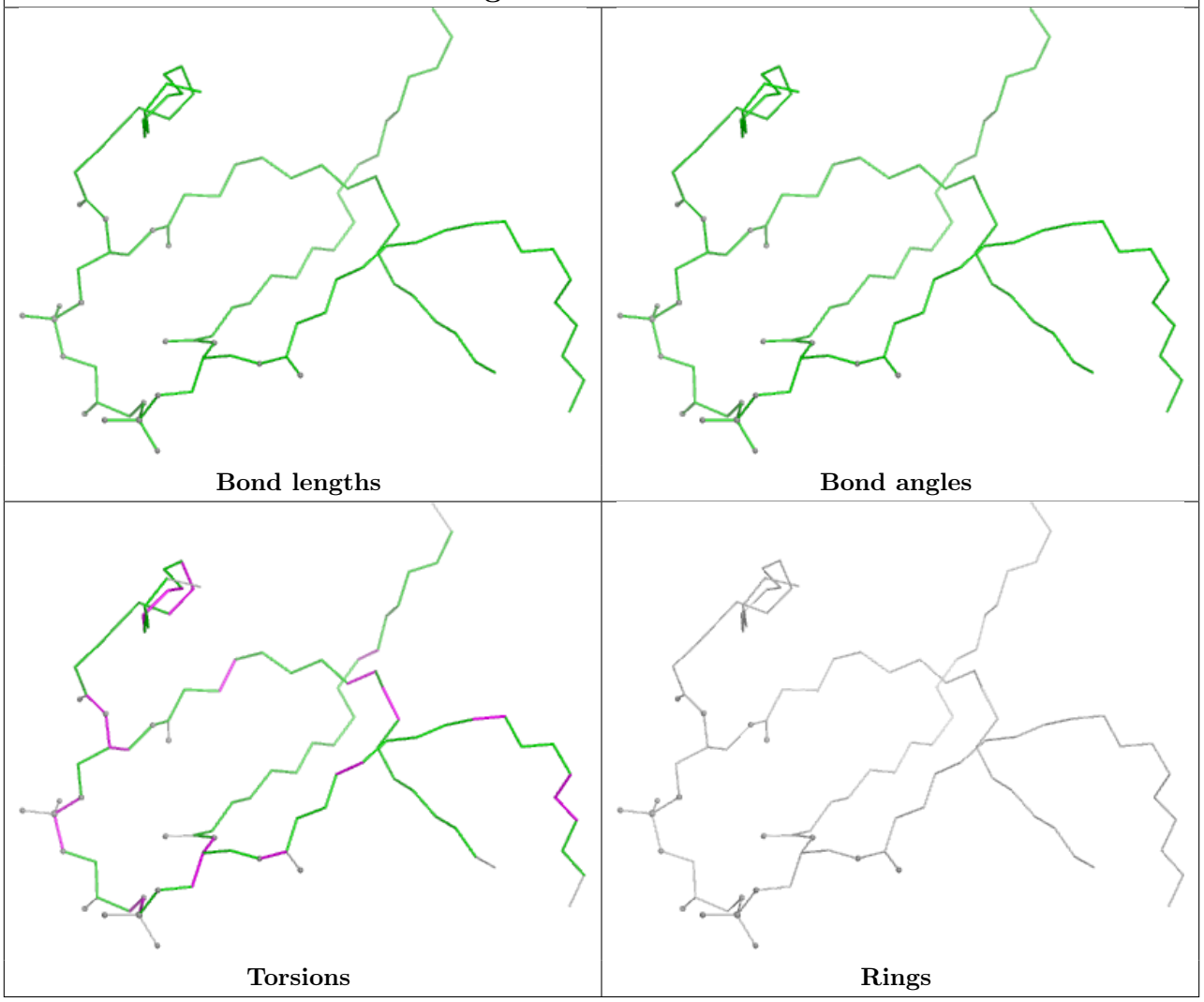
Ligand CDL 4U 201



Ligand 3PE 4E 302



Ligand CDL 4E 301



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

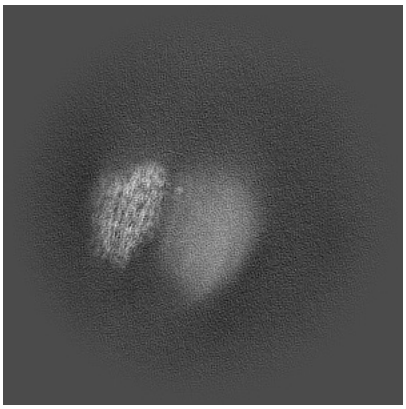
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-52622. These allow visual inspection of the internal detail of the map and identification of artifacts.

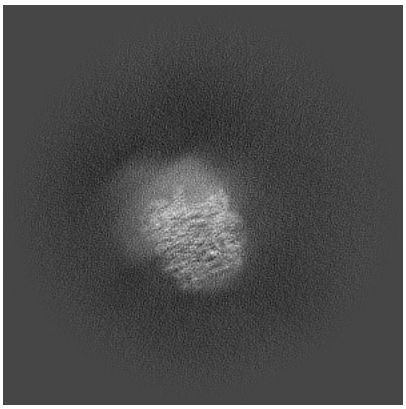
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

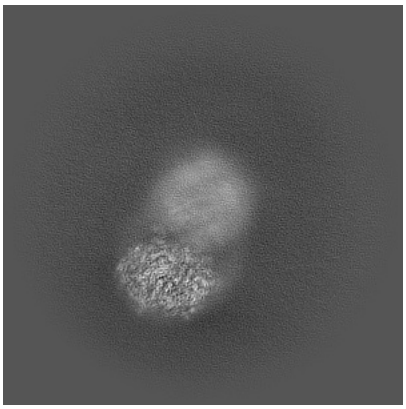
6.1.1 Primary map



X

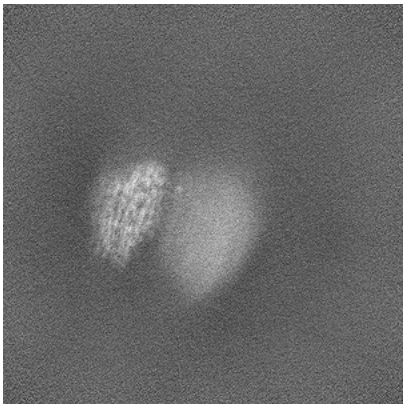


Y

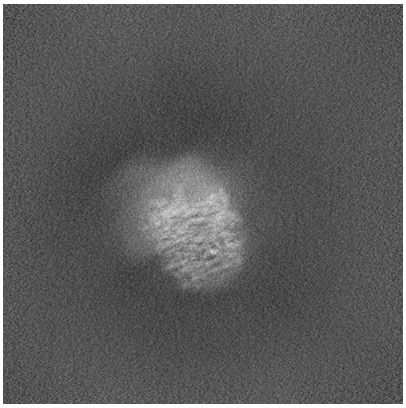


Z

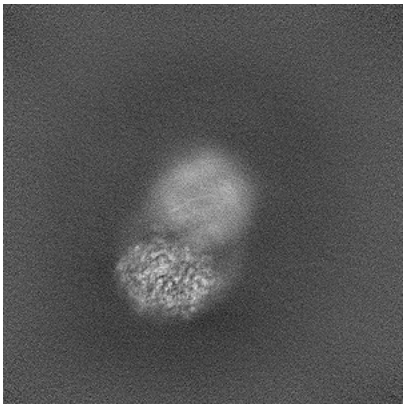
6.1.2 Raw map



X



Y

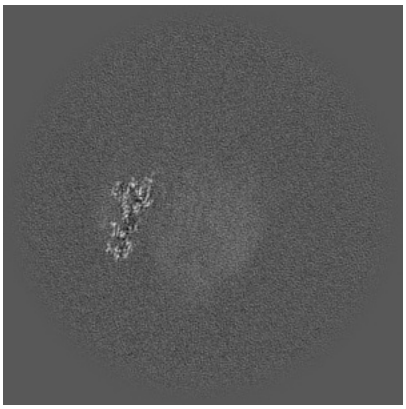


Z

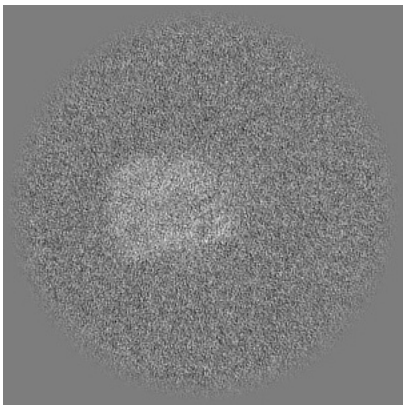
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

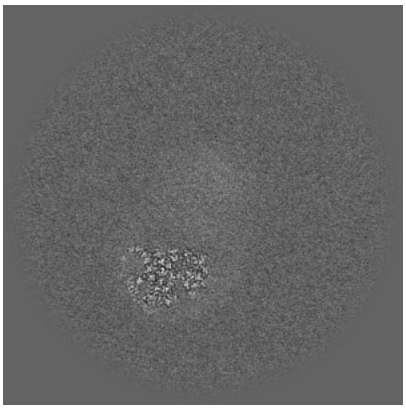
6.2.1 Primary map



X Index: 300

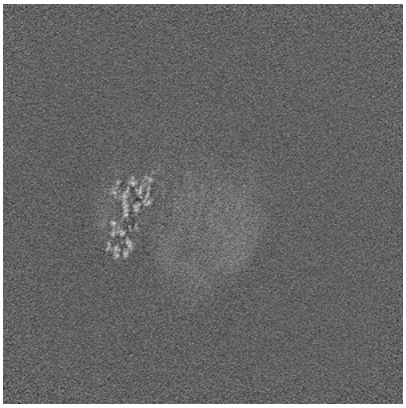


Y Index: 300

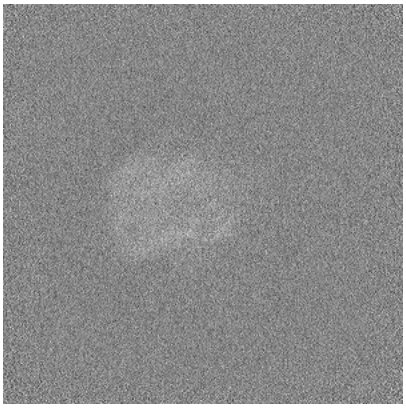


Z Index: 300

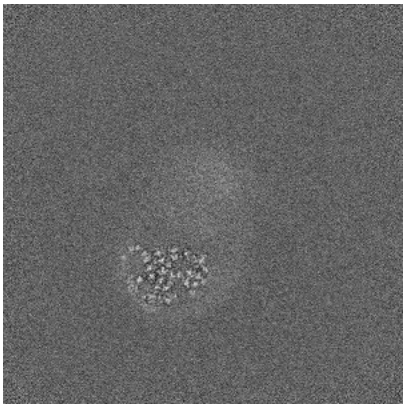
6.2.2 Raw map



X Index: 300



Y Index: 300

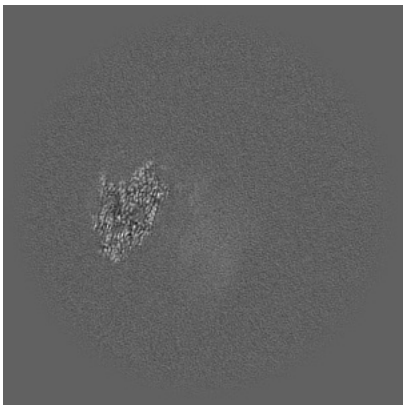


Z Index: 300

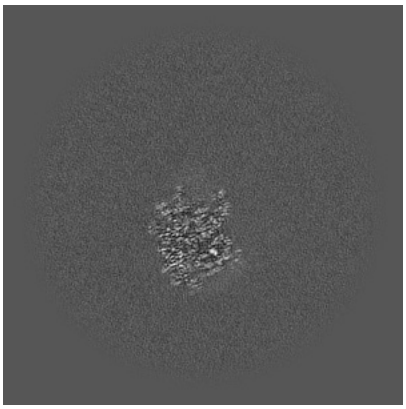
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

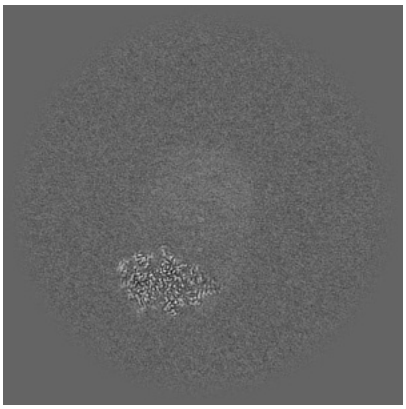
6.3.1 Primary map



X Index: 252

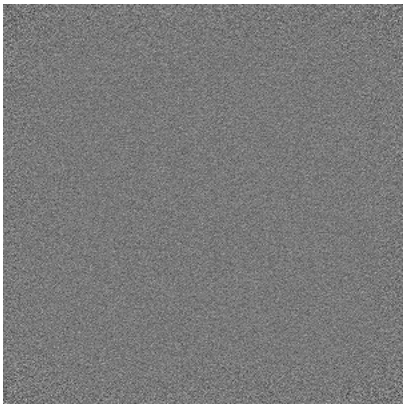


Y Index: 191

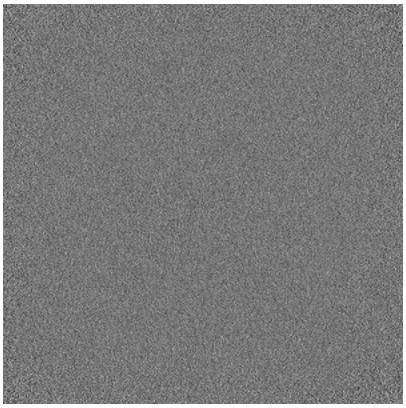


Z Index: 272

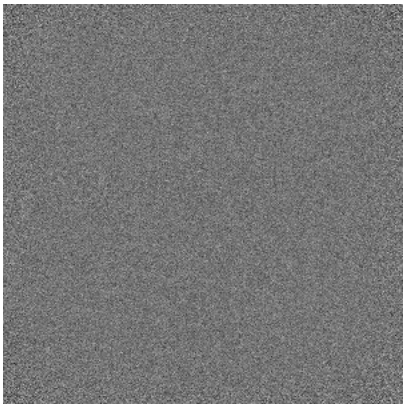
6.3.2 Raw map



X Index: 0



Y Index: 0

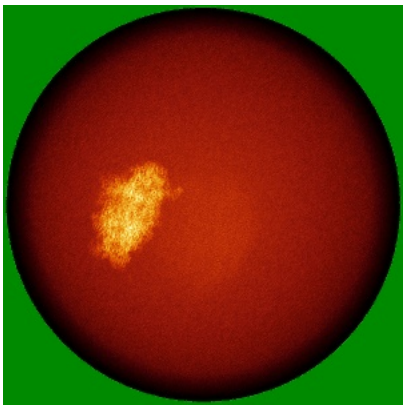


Z Index: 0

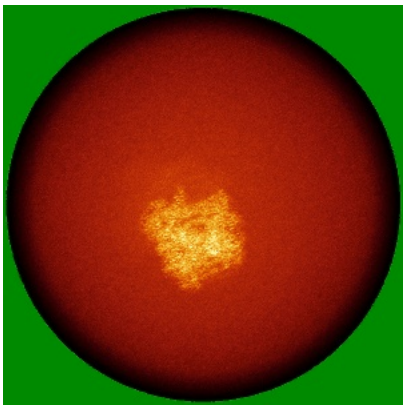
The images above show the largest variance slices of the map in three orthogonal directions.

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

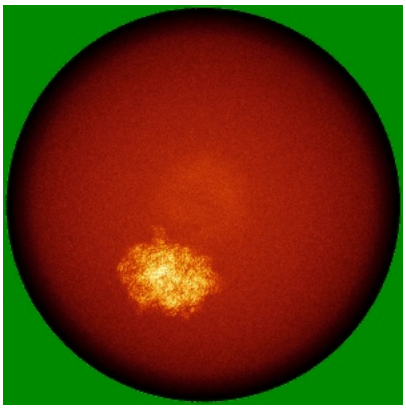
6.4.1 Primary map



X

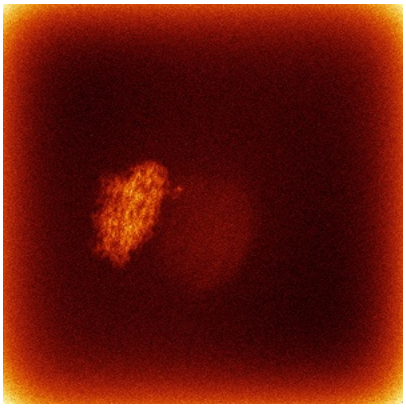


Y

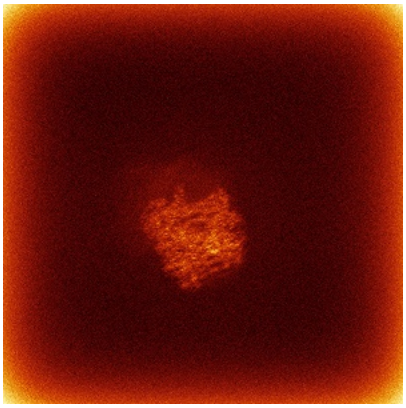


Z

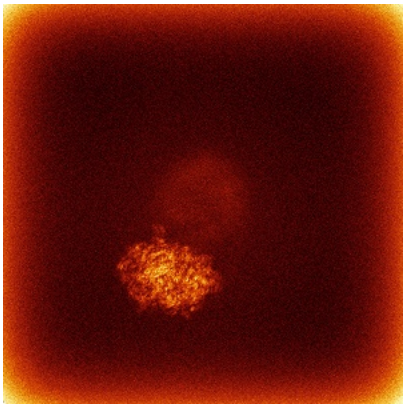
6.4.2 Raw map



X



Y

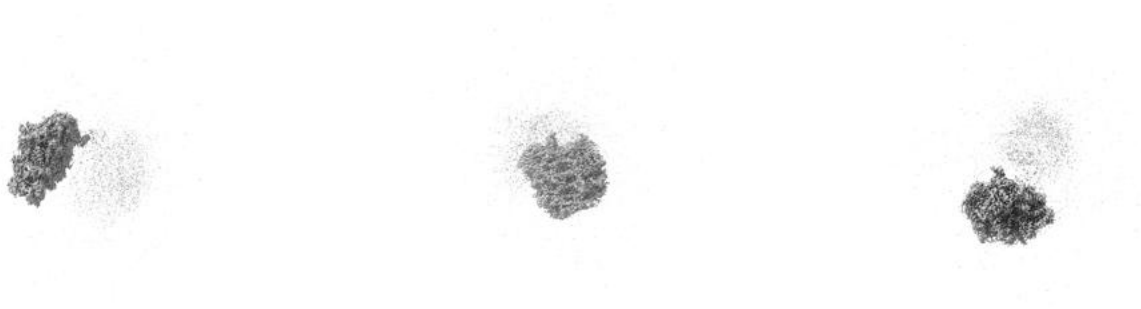


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

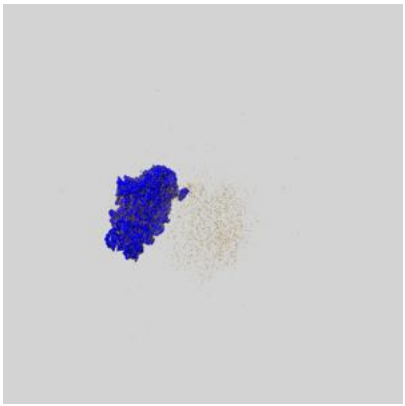
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

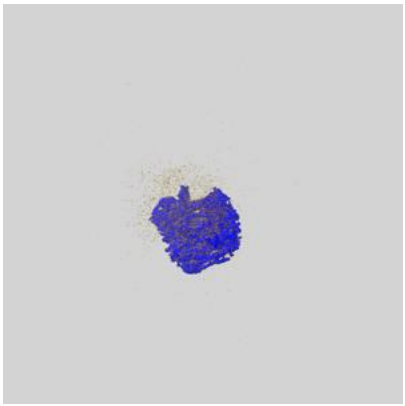
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

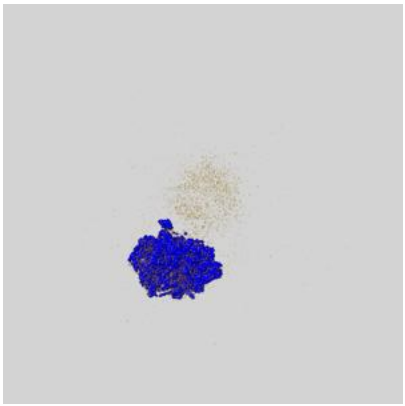
6.6.1 emd_52622_msk_1.map (i)



X



Y

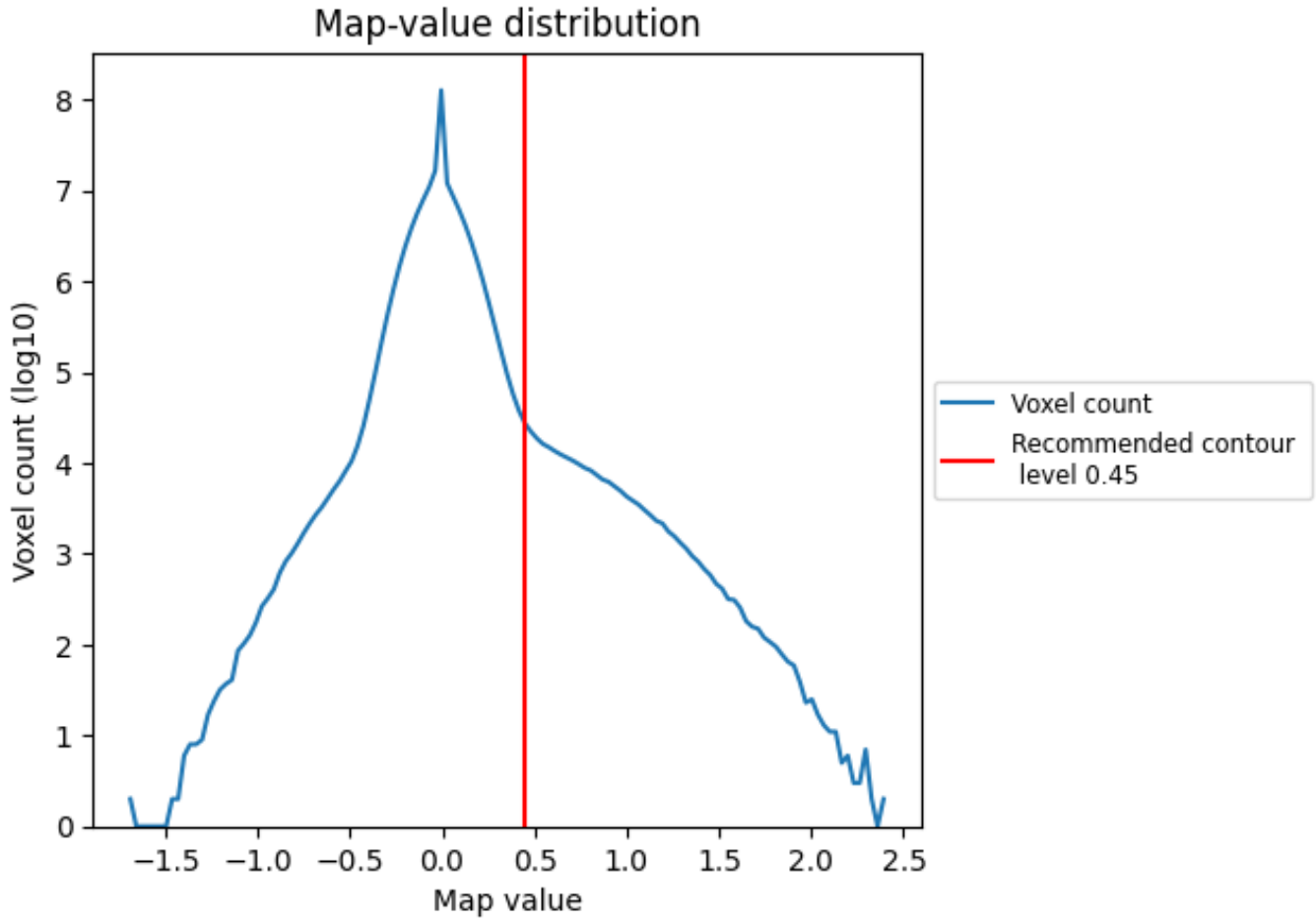


Z

7 Map analysis

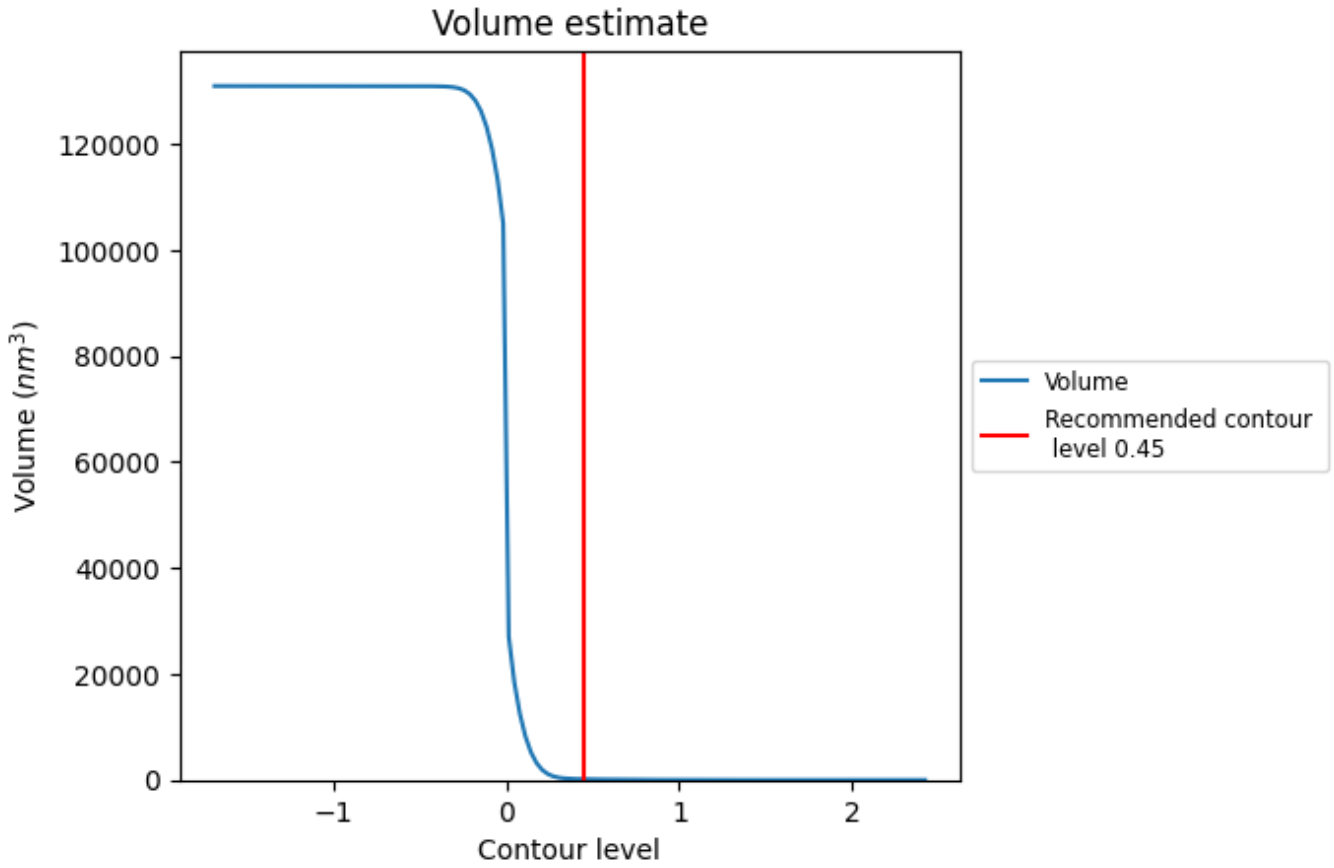
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

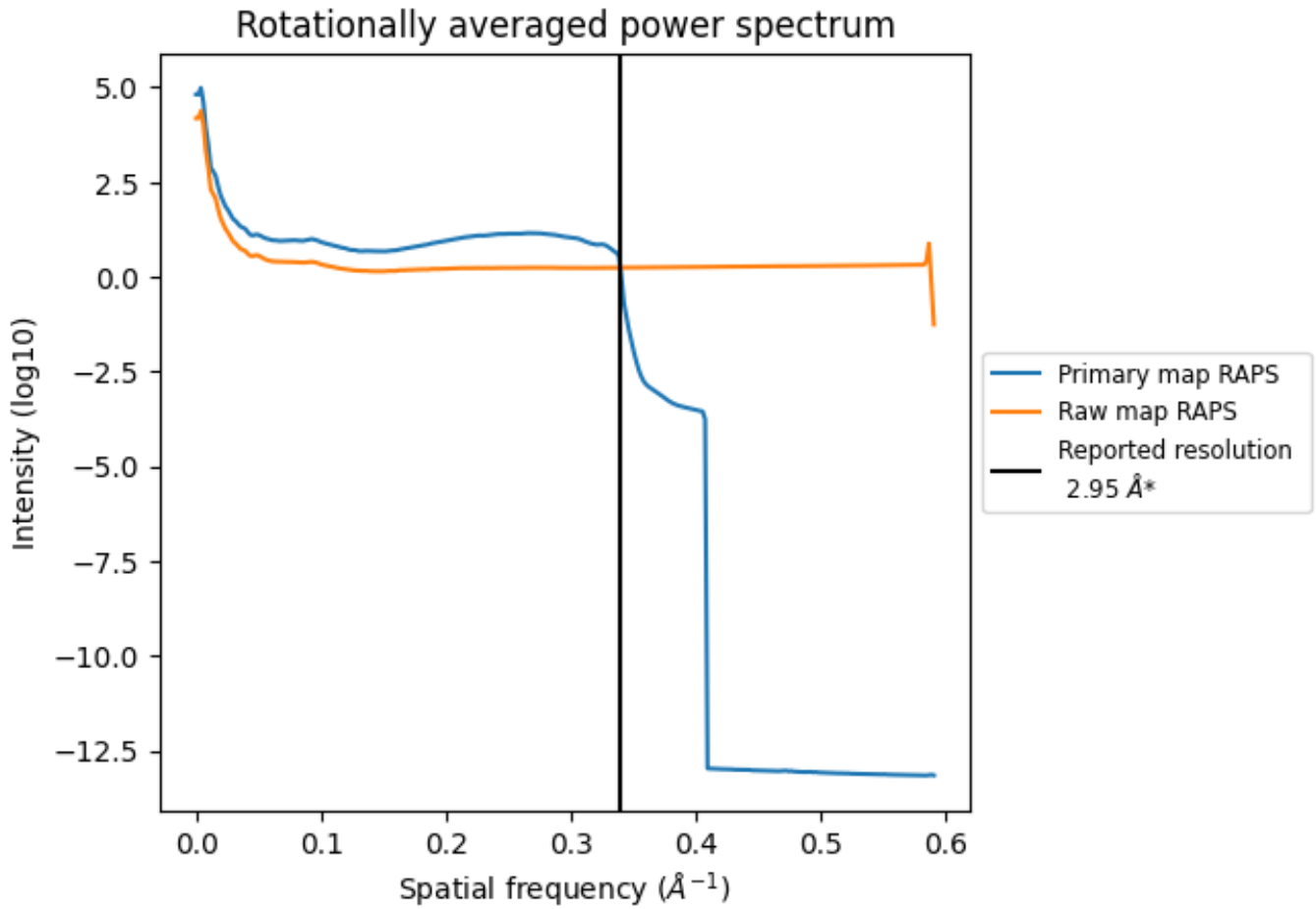
7.2 Volume estimate



The volume at the recommended contour level is 145 nm^3; this corresponds to an approximate mass of 131 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)

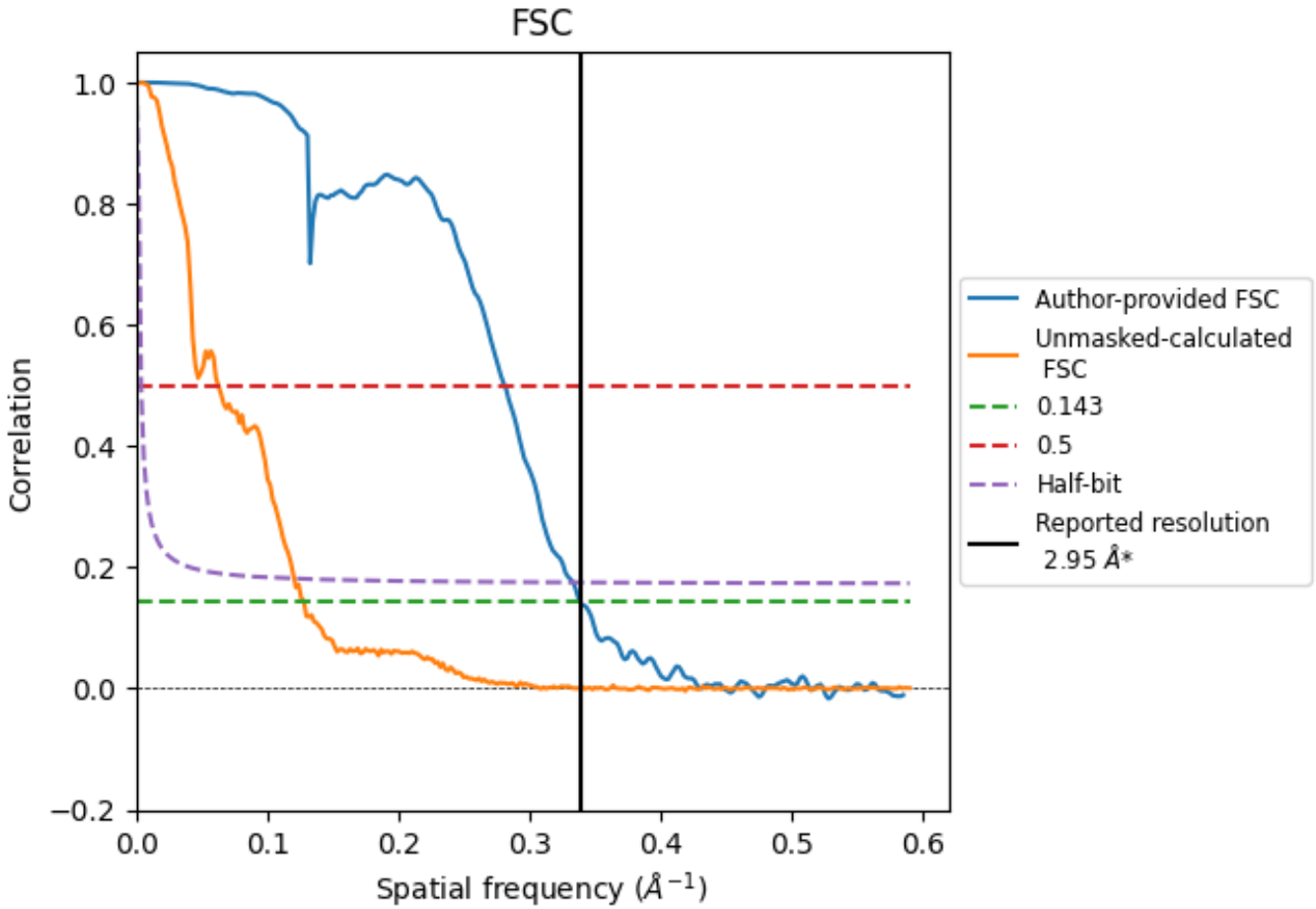


*Reported resolution corresponds to spatial frequency of 0.339 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.339 Å^{-1}

8.2 Resolution estimates (i)

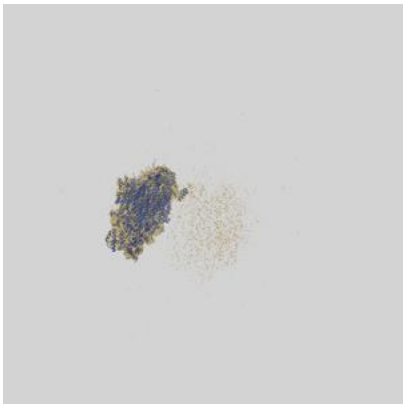
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.95	-	-
Author-provided FSC curve	2.95	3.55	3.00
Unmasked-calculated*	7.81	15.92	8.29

*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 7.81 differs from the reported value 2.95 by more than 10 %

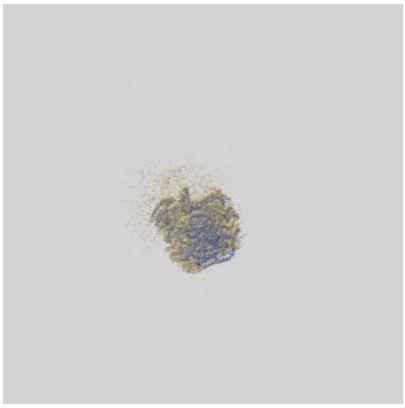
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-52622 and PDB model 9I4Y. Per-residue inclusion information can be found in section 3 on page 14.

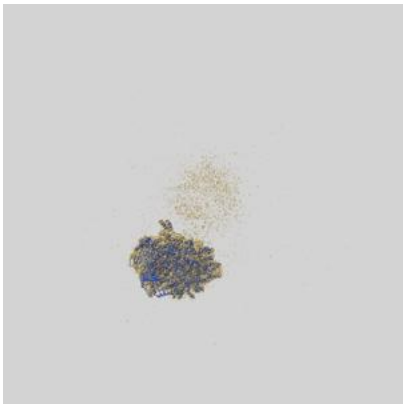
9.1 Map-model overlay



X



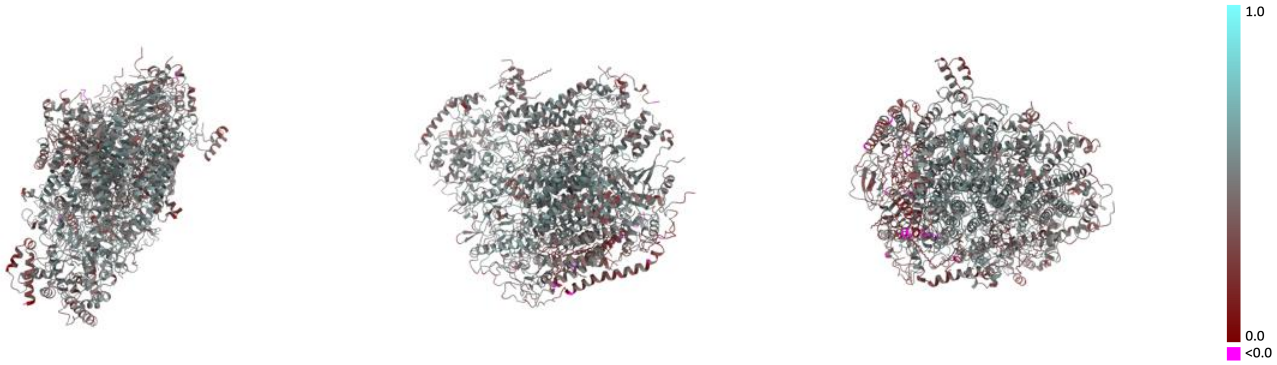
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.45 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.

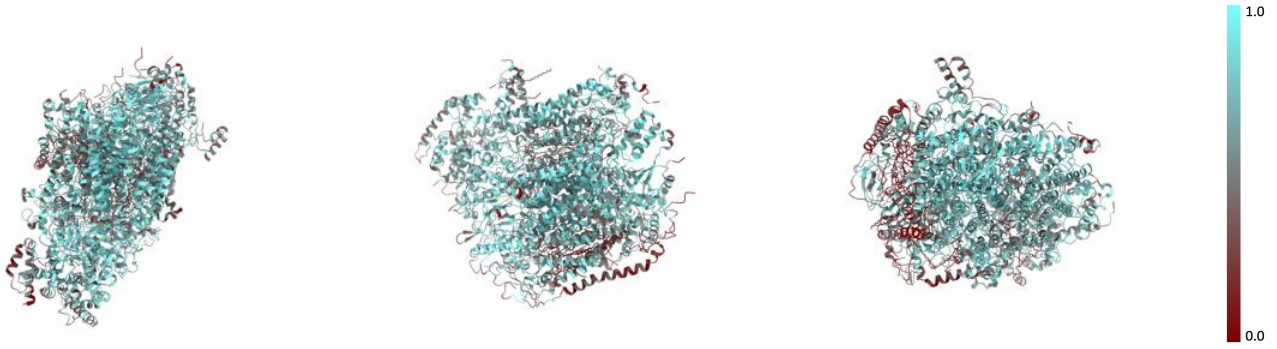
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

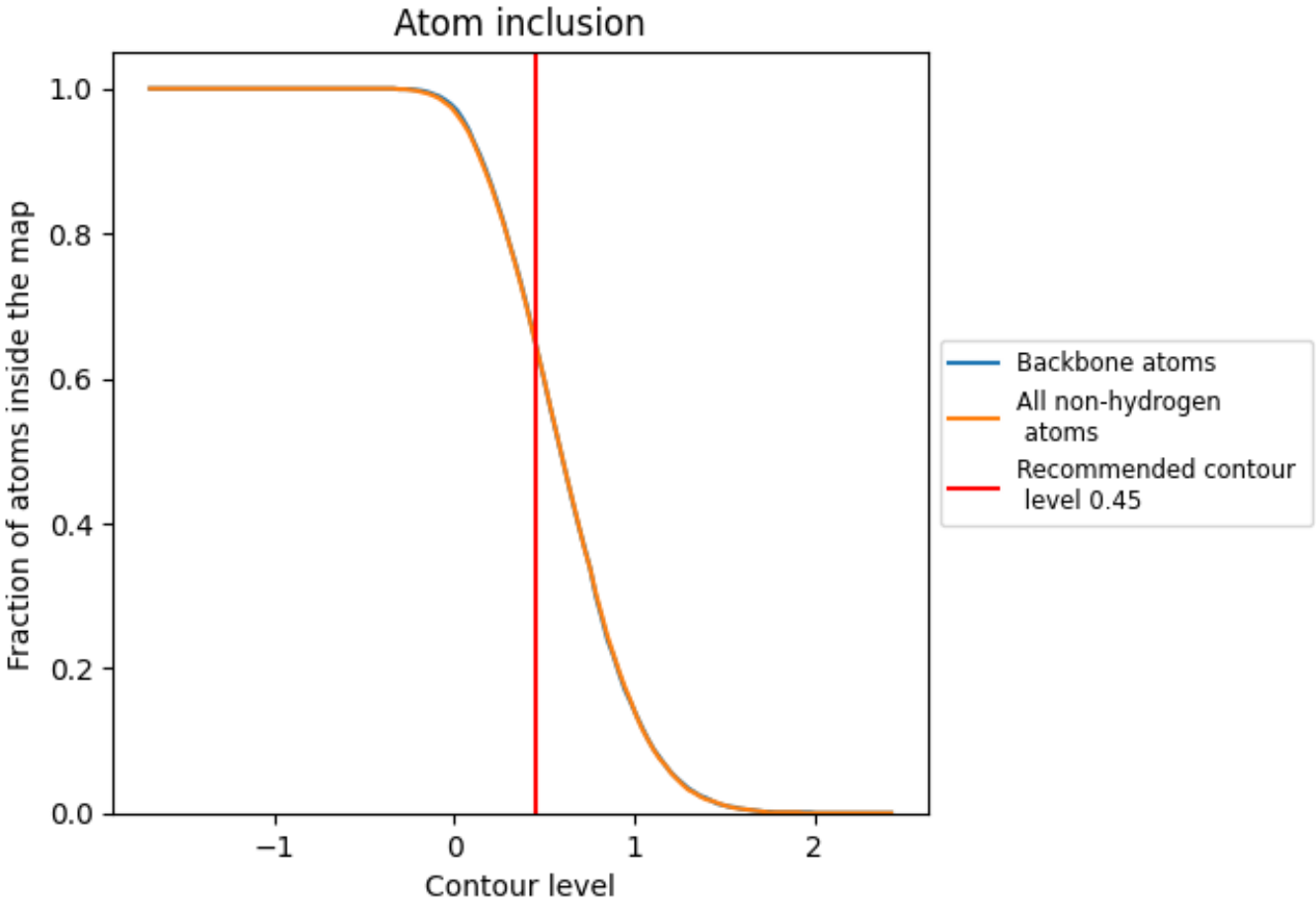
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.45).

9.4 Atom inclusion (i)



At the recommended contour level, 65% of all backbone atoms, 65% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6490	0.4590
4B	0.6720	0.4790
4C	0.7500	0.4870
4D	0.6310	0.4460
4E	0.6910	0.4860
4F	0.5050	0.3780
4G	0.6710	0.4690
4H	0.6410	0.4480
4I	0.7320	0.4650
4J	0.7410	0.4970
4K	0.7110	0.4680
4L	0.5940	0.4450
4M	0.1700	0.2760
4N	0.7370	0.5050
4O	0.5960	0.4260
4P	0.6940	0.4630
4Q	0.3070	0.3440
4R	0.5470	0.4060
4S	0.7650	0.5080
4T	0.7750	0.5130
4U	0.5190	0.4160
4V	0.5470	0.4140
4W	0.5990	0.4050
4X	0.5640	0.4050
4Y	0.5640	0.4340
B	0.7540	0.5030

