



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 08:16 AM EDT

PDB ID : 8UGL / pdb_00008ugl
EMDB ID : EMD-42229
Title : High resolution in-situ structure of complex IV in respiratory supercomplex
Authors : Zheng, W.; Zhu, J.; Zhang, K.
Deposited on : 2023-10-05
Resolution : 3.00 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:

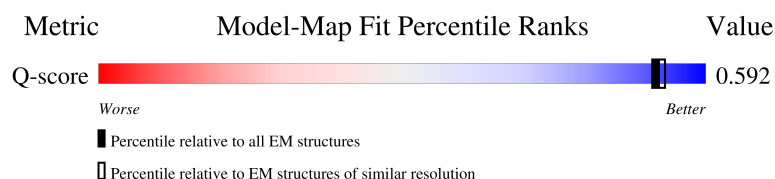
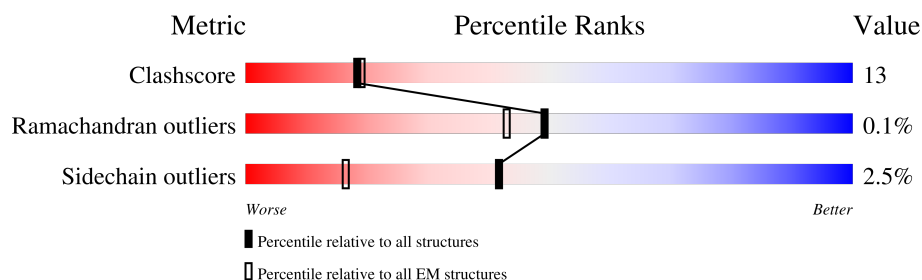
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	4A	514	69% 30%
2	4B	229	68% 31% ..
3	4C	261	71% 27% ..
4	4D	169	62% 20% 18%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	4E	152	
6	4F	129	
7	4G	97	
8	4H	86	
9	4I	75	
10	4J	80	
11	4K	80	
12	4L	63	
13	4M	70	
14	4N	82	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CUA	4B	303	-	-	X	-

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 16927 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	4A	513	Total	C	N	O	S	1	0
			4025	2692	625	677	31		

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	4B	227	Total	C	N	O	S	0	0
			1828	1190	281	339	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4C	259	Total	C	N	O	S	0	0
			2096	1399	336	351	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4D	139	Total	C	N	O	S	0	0
			1163	757	190	212	4		

- Molecule 5 is a protein called Cytochrome c oxidase subunit 5A, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4E	105	Total	C	N	O	S	0	0
			852	544	144	162	2		

- Molecule 6 is a protein called Cytochrome c oxidase subunit 5B, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	4F	97	Total	C	N	O	S	0	0
			734	455	130	143	6		

- Molecule 7 is a protein called Cytochrome c oxidase subunit 6A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	4G	75	Total	C	N	O	S	0	0
			617	398	118	100	1		

- Molecule 8 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	4H	82	Total	C	N	O	S	0	0
			687	434	125	123	5		

- Molecule 9 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	4I	67	Total	C	N	O	S	0	0
			550	359	97	91	3		

- Molecule 10 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	4J	58	Total	C	N	O	S	0	0
			456	293	78	82	3		

- Molecule 11 is a protein called Cytochrome c oxidase subunit 7B.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	4K	49	Total	C	N	O	S	0	0
			383	249	65	68	1		

- Molecule 12 is a protein called Cytochrome c oxidase subunit 7C, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	4L	46	Total	C	N	O	S	0	0
			381	254	64	61	2		

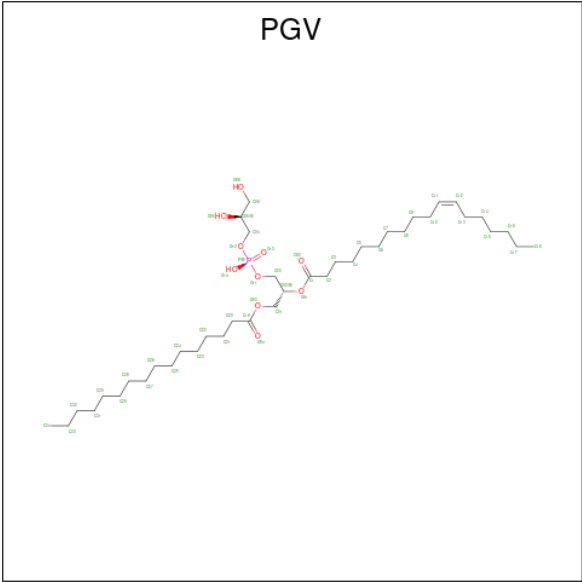
- Molecule 13 is a protein called Cytochrome c oxidase subunit 8.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	4M	43	Total	C	N	O	0	0
			338	222	57	59		

- Molecule 14 is a protein called Cytochrome c oxidase subunit NDUFA4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	4N	82	Total	C	N	O	S	0	0
			660	432	112	114	2		

- Molecule 15 is (1R)-2-{{[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



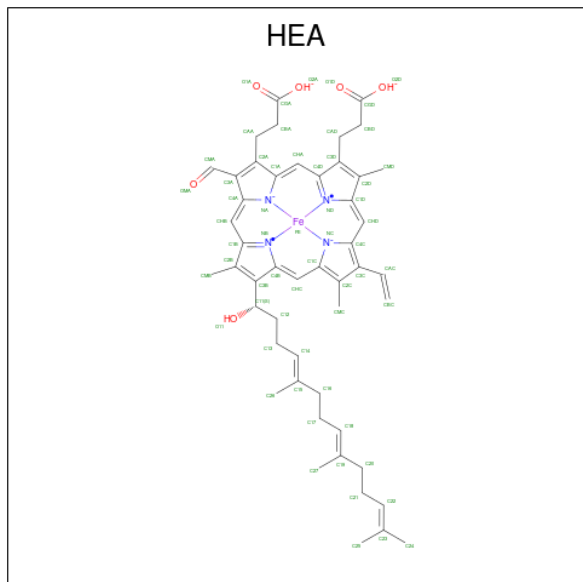
Mol	Chain	Residues	Atoms				AltConf
15	4A	1	Total	C	O	P	0
			51	40	10	1	
15	4A	1	Total	C	O	P	0
			51	40	10	1	
15	4A	1	Total	C	O	P	0
			51	40	10	1	
15	4B	1	Total	C	O	P	0
			51	40	10	1	
15	4C	1	Total	C	O	P	0
			51	40	10	1	
15	4C	1	Total	C	O	P	0
			51	40	10	1	
15	4C	1	Total	C	O	P	0
			51	40	10	1	
15	4C	1	Total	C	O	P	0
			51	40	10	1	
15	4C	1	Total	C	O	P	0
			51	40	10	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
15	4G	1	Total	C	O	P	0
			51	40	10	1	
15	4J	1	Total	C	O	P	0
			51	40	10	1	
15	4K	1	Total	C	O	P	0
			51	40	10	1	
15	4L	1	Total	C	O	P	0
			51	40	10	1	
15	4M	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 16 is HEME-A (CCD ID: HEA) (formula: $C_{49}H_{56}FeN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
16	4A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	
16	4A	1	Total	C	Fe	N	O	0
			60	49	1	4	6	

- Molecule 17 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		AltConf
17	4A	1	Total	Cu	0
			1	1	

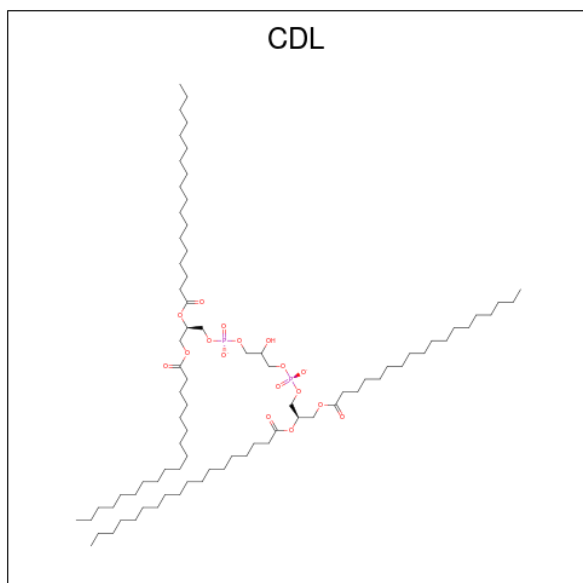
- Molecule 18 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
18	4A	1	Total	Mg	0
			1	1	

- Molecule 19 is SODIUM ION (CCD ID: NA) (formula: Na).

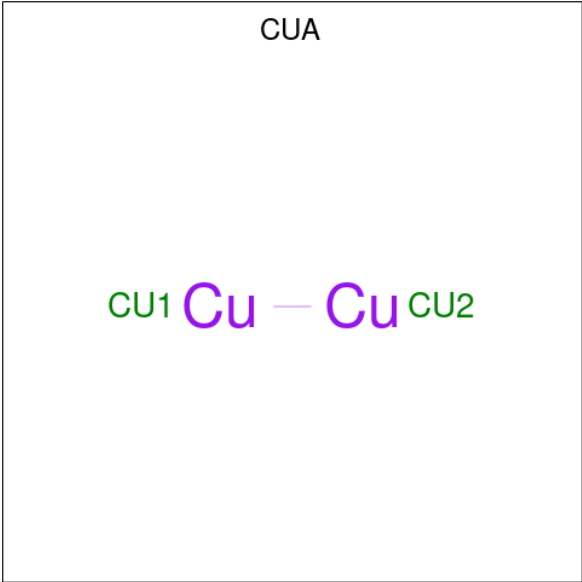
Mol	Chain	Residues	Atoms		AltConf
19	4A	1	Total	Na	0
			1	1	

- Molecule 20 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



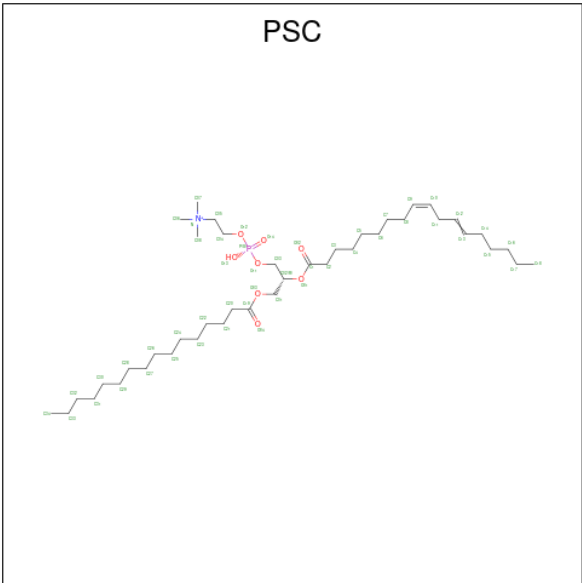
Mol	Chain	Residues	Atoms				AltConf
20	4B	1	Total	C	O	P	0
			100	81	17	2	
20	4C	1	Total	C	O	P	0
			100	81	17	2	
20	4D	1	Total	C	O	P	0
			100	81	17	2	

- Molecule 21 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu_2).



Mol	Chain	Residues	Atoms		AltConf
21	4B	1	Total	Cu	0
			2	2	

- Molecule 22 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: C₄₂H₈₁NO₈P).

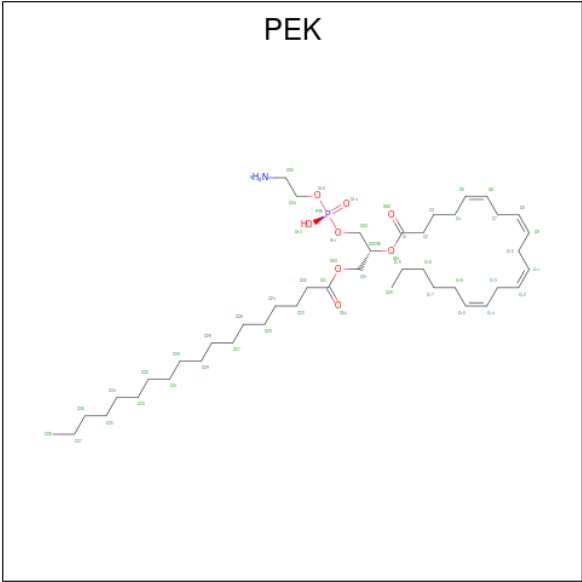


Mol	Chain	Residues	Atoms					AltConf
22	4B	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 23 is ZINC ION (CCD ID: ZN) (formula: Zn).

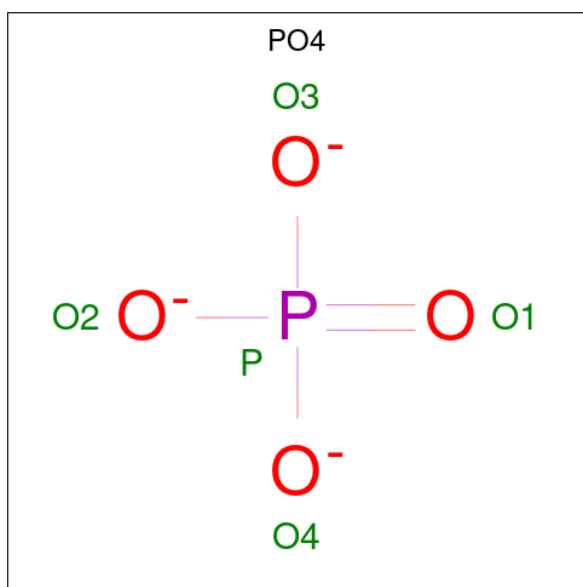
Mol	Chain	Residues	Atoms		AltConf
23	4F	1	Total	Zn	0
			1	1	

- Molecule 24 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: C₄₃H₇₈NO₈P).



Mol	Chain	Residues	Atoms					AltConf
24	4G	1	Total	C	N	O	P	0
			53	43	1	8	1	
24	4G	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 25 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			AltConf
25	4H	1	Total	O	P	0
			5	4	1	

- Molecule 26 is water.

Mol	Chain	Residues	Atoms		AltConf
26	4A	108	Total	O	0
			108	108	
26	4B	115	Total	O	0
			115	115	
26	4C	103	Total	O	0
			103	103	
26	4D	81	Total	O	0
			81	81	
26	4E	55	Total	O	0
			55	55	
26	4F	65	Total	O	0
			65	65	
26	4G	40	Total	O	0
			40	40	
26	4H	43	Total	O	0
			43	43	
26	4I	25	Total	O	0
			25	25	
26	4J	38	Total	O	0
			38	38	
26	4K	27	Total	O	0
			27	27	

Continued on next page...

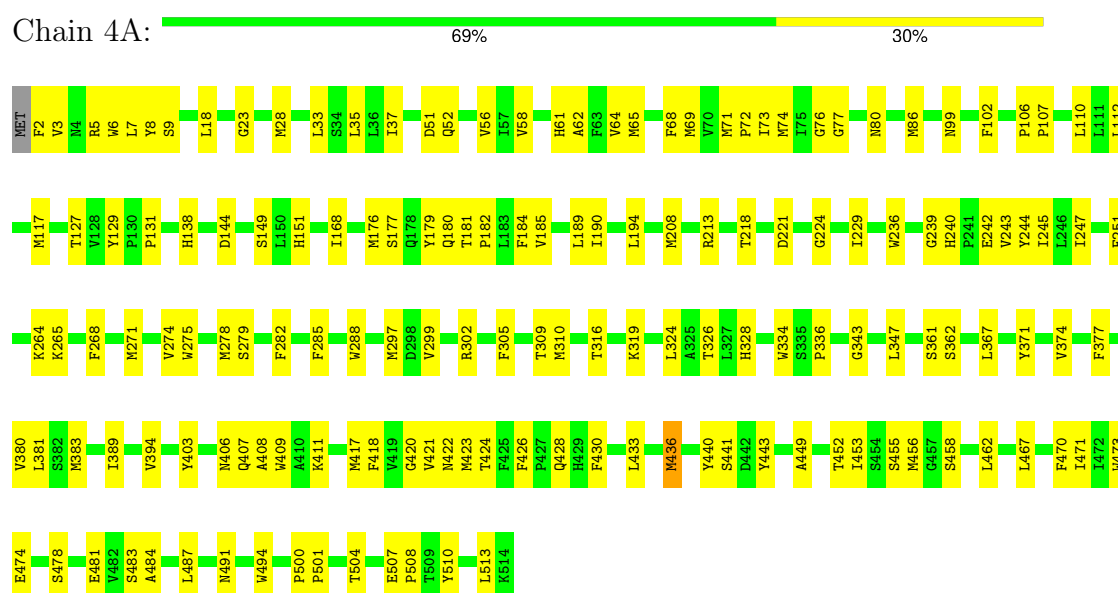
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
26	4L	23	Total 23	O 23	0
26	4M	28	Total 28	O 28	0
26	4N	53	Total 53	O 53	0

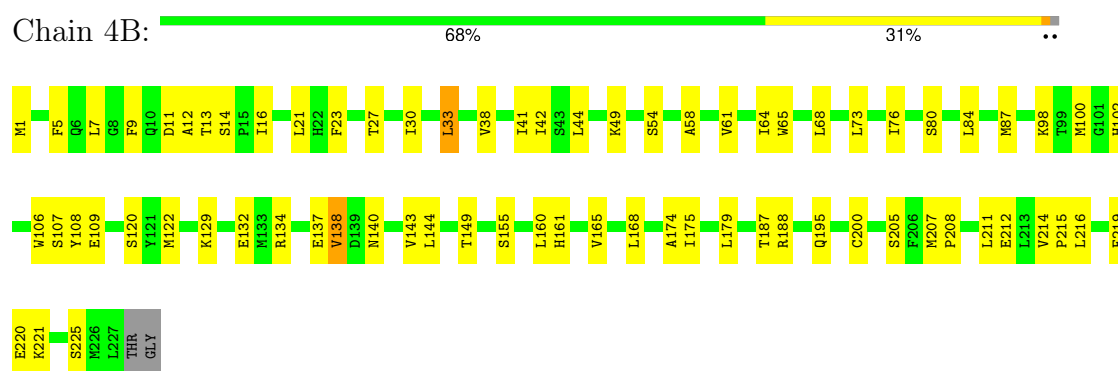
3 Residue-property plots

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

• Molecule 1: Cytochrome c oxidase subunit 1

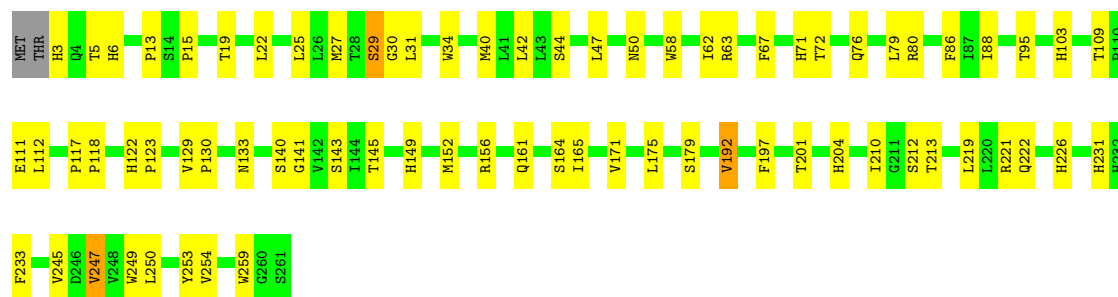


• Molecule 2: Cytochrome c oxidase subunit 2

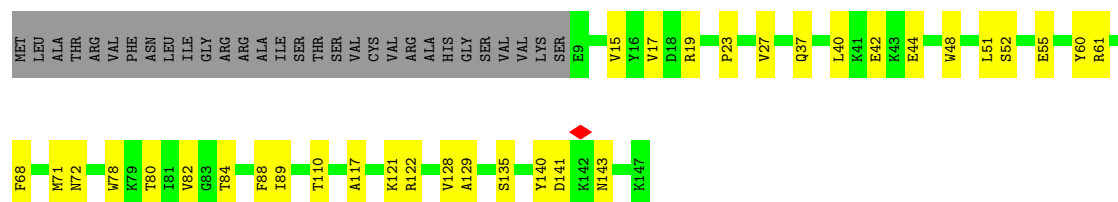


• Molecule 3: Cytochrome c oxidase subunit 3

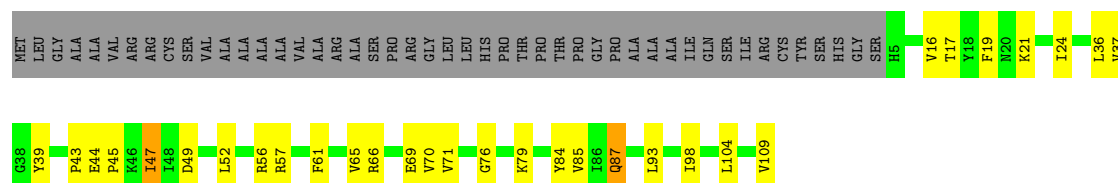




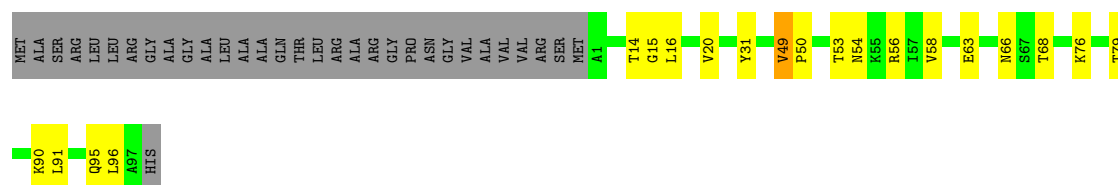
- Molecule 4: Cytochrome c oxidase subunit 4



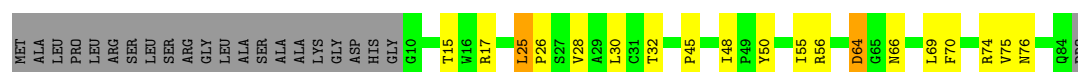
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial

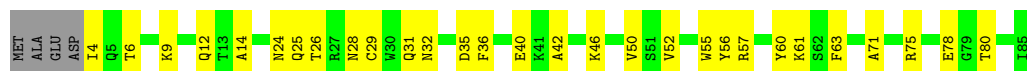


- Molecule 7: Cytochrome c oxidase subunit 6A2



- Molecule 8: Cytochrome c oxidase subunit 6B1

Chain 4H:  62% 34% 5%



- Molecule 9: Cytochrome c oxidase subunit 6C

Chain 4I:  72% 17% 11%



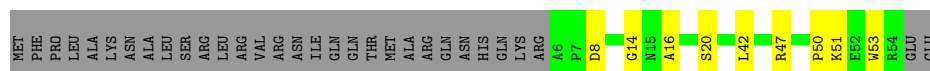
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial

Chain 4J:  56% 16% 28%



- Molecule 11: Cytochrome c oxidase subunit 7B

Chain 4K:  50% 11% 39%



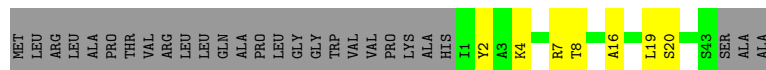
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial

Chain 4L:  54% 19% 27%



- Molecule 13: Cytochrome c oxidase subunit 8

Chain 4M:  51% 10% 39%



- Molecule 14: Cytochrome c oxidase subunit NDUF44

Chain 4N:  82% 17% 1%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	56000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.697	Depositor
Minimum map value	-1.154	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.025	Depositor
Map size (Å)	212.992, 212.992, 212.992	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.416, 0.416, 0.416	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CU, MG, FME, PEK, HEA, CUA, PSC, NA, PO4, ZN, CDL, PGV

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	4A	0.24	2/4165 (0.0%)	0.53	4/5691 (0.1%)
2	4B	0.13	0/1865	0.32	0/2544
3	4C	0.11	0/2179	0.26	0/2981
4	4D	0.10	0/1197	0.27	0/1617
5	4E	0.12	0/871	0.33	0/1182
6	4F	0.11	0/749	0.32	0/1016
7	4G	0.10	0/644	0.28	0/881
8	4H	0.12	0/708	0.34	0/956
9	4I	0.10	0/563	0.24	0/748
10	4J	0.09	0/466	0.23	0/631
11	4K	0.11	0/396	0.30	0/543
12	4L	0.10	0/394	0.28	0/528
13	4M	0.09	0/349	0.24	0/477
14	4N	0.12	0/680	0.39	0/921
All	All	0.16	2/15226 (0.0%)	0.37	4/20716 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4A	501	PRO	CG-CD	-9.47	1.18	1.50
1	4A	501	PRO	CB-CG	-9.12	1.04	1.49

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4A	501	PRO	N-CD-CG	-19.90	73.35	103.20
1	4A	501	PRO	CA-CB-CG	-19.69	67.09	104.50
1	4A	501	PRO	CB-CG-CD	13.40	148.99	106.10
1	4A	501	PRO	CA-N-CD	-7.94	100.89	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	4A	4025	0	3999	128	0
2	4B	1828	0	1837	62	0
3	4C	2096	0	2027	60	0
4	4D	1163	0	1143	29	0
5	4E	852	0	845	20	0
6	4F	734	0	718	13	0
7	4G	617	0	585	16	0
8	4H	687	0	645	20	0
9	4I	550	0	560	9	0
10	4J	456	0	459	12	0
11	4K	383	0	366	9	0
12	4L	381	0	380	10	0
13	4M	338	0	345	9	0
14	4N	660	0	664	13	0
15	4A	153	0	228	22	0
15	4B	51	0	76	12	0
15	4C	306	0	456	40	0
15	4G	51	0	76	5	0
15	4J	51	0	76	3	0
15	4K	51	0	76	6	0
15	4L	51	0	76	10	0
15	4M	51	0	76	5	0
16	4A	120	0	108	7	0
17	4A	1	0	0	0	0
18	4A	1	0	0	0	0
19	4A	1	0	0	0	0
20	4B	100	0	156	9	0
20	4C	100	0	156	14	0
20	4D	100	0	156	20	0
21	4B	2	0	0	2	0
22	4B	52	0	80	9	0
23	4F	1	0	0	0	0
24	4G	105	0	149	9	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	4H	5	0	0	0	0
26	4A	108	0	0	6	0
26	4B	115	0	0	7	0
26	4C	103	0	0	3	0
26	4D	81	0	0	4	0
26	4E	55	0	0	1	0
26	4F	65	0	0	1	0
26	4G	40	0	0	1	0
26	4H	43	0	0	4	0
26	4I	25	0	0	0	0
26	4J	38	0	0	0	0
26	4K	27	0	0	0	0
26	4L	23	0	0	2	0
26	4M	28	0	0	0	0
26	4N	53	0	0	0	0
All	All	16927	0	16518	427	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (427) 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)
2:4B:200:CYS:SG	21:4B:303:CUA:CU1	1.48	1.03
12:4L:18:LYS:NZ	26:4L:201:HOH:O	2.09	0.84
20:4D:201:CDL:H351	20:4D:201:CDL:H551	1.60	0.82
15:4M:101:PGV:H221	15:4M:101:PGV:H61	1.60	0.82
15:4C:303:PGV:H21	15:4C:303:PGV:H92	1.62	0.81
8:4H:29:CYS:HB3	8:4H:63:PHE:HB3	1.66	0.78
1:4A:347:LEU:HD13	1:4A:383:MET:HG2	1.65	0.78
15:4A:601:PGV:H62	10:4J:40:LEU:HD11	1.65	0.77
2:4B:132:GLU:HB3	2:4B:137:GLU:HG3	1.67	0.76
1:4A:381:LEU:HD13	16:4A:604:HEA:HAC	1.68	0.75
3:4C:67:PHE:O	10:4J:13:GLN:NE2	2.20	0.74
3:4C:133:ASN:ND2	26:4C:401:HOH:O	2.21	0.73
1:4A:176:MET:HE3	1:4A:181:THR:HG22	1.71	0.72
5:4E:43:PRO:HB3	5:4E:47:ILE:HD11	1.70	0.72
4:4D:72:ASN:HB3	20:4D:201:CDL:H852	1.73	0.71
16:4A:604:HEA:H131	16:4A:604:HEA:HHC	1.71	0.70
2:4B:102:HIS:HE2	2:4B:107:SER:HG	1.35	0.70
2:4B:200:CYS:HG	21:4B:303:CUA:CU1	0.39	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4A:265:LYS:NZ	6:4F:68:THR:OG1	2.24	0.70
1:4A:138:HIS:O	1:4A:213:ARG:NH2	2.25	0.69
3:4C:109:THR:HG22	3:4C:111:GLU:H	1.57	0.69
1:4A:336:PRO:HB2	1:4A:394:VAL:HG11	1.75	0.68
1:4A:33:LEU:HB3	1:4A:61:HIS:HB2	1.74	0.68
15:4B:301:PGV:H212	20:4D:201:CDL:H331	1.74	0.68
11:4K:47:ARG:HH12	15:4K:101:PGV:H211	1.56	0.68
1:4A:129:TYR:OH	1:4A:236:TRP:NE1	2.27	0.67
20:4C:306:CDL:H322	20:4C:306:CDL:H191	1.75	0.67
6:4F:53:THR:O	26:4F:201:HOH:O	2.12	0.67
1:4A:179:TYR:OH	15:4A:602:PGV:O02	2.13	0.67
3:4C:259:TRP:O	14:4N:47:ARG:NH2	2.28	0.66
3:4C:62:ILE:HG13	15:4C:307:PGV:H21	1.76	0.66
1:4A:456:MET:O	26:4A:701:HOH:O	2.14	0.66
7:4G:76:ASN:OD1	24:4G:103:PEK:N	2.29	0.65
2:4B:30:ILE:HG21	2:4B:76:ILE:HD11	1.77	0.65
15:4C:304:PGV:H262	15:4C:304:PGV:H61	1.78	0.65
8:4H:28:ASN:O	8:4H:32:ASN:ND2	2.29	0.65
4:4D:52:SER:HB2	4:4D:55:GLU:HG3	1.77	0.65
7:4G:74:ARG:NH2	26:4G:201:HOH:O	2.29	0.64
12:4L:21:LEU:HA	12:4L:24:MET:HG2	1.80	0.64
15:4C:303:PGV:H11	15:4C:303:PGV:H272	1.80	0.64
2:4B:49:LYS:HE3	15:4B:301:PGV:H282	1.80	0.63
4:4D:84:THR:HG21	15:4M:101:PGV:H71	1.81	0.63
1:4A:310:MET:HB3	2:4B:73:LEU:HD22	1.81	0.63
3:4C:213:THR:HB	15:4C:307:PGV:H11	1.81	0.63
20:4C:306:CDL:H612	20:4C:306:CDL:H822	1.80	0.63
1:4A:343:GLY:HA2	15:4B:301:PGV:H062	1.79	0.62
1:4A:406:ASN:HB3	1:4A:409:TRP:HB2	1.82	0.62
5:4E:76:GLY:O	5:4E:79:LYS:NZ	2.32	0.62
26:4L:201:HOH:O	13:4M:8:THR:O	2.16	0.62
8:4H:52:VAL:O	26:4H:201:HOH:O	2.16	0.62
20:4C:306:CDL:H581	20:4C:306:CDL:H761	1.81	0.61
5:4E:21:LYS:HB2	5:4E:24:ILE:HB	1.81	0.61
2:4B:33:LEU:HB2	9:4I:32:ALA:HB2	1.81	0.61
15:4L:101:PGV:H81	15:4L:101:PGV:H301	1.82	0.61
1:4A:107:PRO:HB3	3:4C:25:LEU:HB2	1.83	0.61
1:4A:383:MET:HE2	1:4A:421:VAL:HB	1.80	0.61
3:4C:88:ILE:HG12	20:4C:306:CDL:H621	1.82	0.61
1:4A:117:MET:O	12:4L:46:LYS:NZ	2.33	0.61
4:4D:23:PRO:O	5:4E:66:ARG:NH1	2.34	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4D:19:ARG:O	26:4D:301:HOH:O	2.16	0.61
15:4L:101:PGV:H251	15:4L:101:PGV:H211	1.81	0.61
3:4C:95:THR:HG23	15:4C:304:PGV:H101	1.82	0.60
1:4A:297:MET:O	1:4A:302:ARG:NH1	2.34	0.60
2:4B:16:ILE:HG12	2:4B:87:MET:HG3	1.83	0.60
1:4A:279:SER:HB3	14:4N:22:ILE:HG12	1.83	0.60
11:4K:16:ALA:O	11:4K:20:SER:OG	2.16	0.60
1:4A:428:GLN:NE2	26:4A:703:HOH:O	2.26	0.60
1:4A:86:MET:HE1	1:4A:184:PHE:HB3	1.83	0.60
15:4A:601:PGV:H302	15:4L:101:PGV:H42	1.84	0.60
3:4C:210:ILE:HG12	15:4C:307:PGV:H141	1.84	0.60
3:4C:47:LEU:HD22	15:4C:303:PGV:H142	1.83	0.60
6:4F:49:VAL:HG22	6:4F:91:LEU:HD12	1.83	0.59
8:4H:25:GLN:O	26:4H:202:HOH:O	2.17	0.59
1:4A:426:PHE:HZ	20:4B:302:CDL:H142	1.67	0.59
15:4A:603:PGV:H211	15:4C:304:PGV:H62	1.84	0.59
3:4C:27:MET:SD	3:4C:50:ASN:ND2	2.74	0.59
3:4C:25:LEU:O	3:4C:29:SER:OG	2.20	0.59
20:4C:306:CDL:H473	14:4N:1:MET:HA	1.83	0.59
20:4C:306:CDL:H212	20:4C:306:CDL:H311	1.83	0.59
5:4E:19:PHE:O	5:4E:57:ARG:NH2	2.31	0.59
2:4B:102:HIS:CD2	2:4B:107:SER:HG	2.21	0.59
2:4B:161:HIS:HB2	2:4B:174:ALA:HB3	1.85	0.58
2:4B:212:GLU:O	26:4B:401:HOH:O	2.17	0.58
1:4A:483:SER:HB3	13:4M:4:LYS:HG3	1.86	0.58
15:4C:303:PGV:H183	15:4C:307:PGV:H172	1.86	0.58
1:4A:297:MET:HA	15:4A:603:PGV:H042	1.85	0.58
26:4D:301:HOH:O	5:4E:66:ARG:NH2	2.36	0.58
24:4G:103:PEK:H9	24:4G:103:PEK:H311	1.86	0.58
1:4A:371:TYR:CD1	1:4A:436:MET:HG2	2.38	0.58
15:4C:303:PGV:H241	15:4C:303:PGV:H91	1.85	0.58
4:4D:68:PHE:HA	4:4D:71:MET:HE2	1.86	0.57
1:4A:242[B]:GLU:HA	1:4A:245:ILE:HD12	1.87	0.57
1:4A:37:ILE:HD11	1:4A:58:VAL:HA	1.86	0.56
1:4A:240:HIS:O	1:4A:243:VAL:HG22	2.04	0.56
3:4C:164:SER:HB2	15:4C:302:PGV:H91	1.86	0.56
3:4C:212:SER:HB2	15:4C:305:PGV:H151	1.88	0.56
1:4A:244:TYR:HA	1:4A:247:ILE:HG22	1.86	0.56
2:4B:98:LYS:HE3	2:4B:109:GLU:HB2	1.88	0.56
4:4D:121:LYS:HE2	11:4K:50:PRO:HB2	1.87	0.56
7:4G:26:PRO:HG3	24:4G:102:PEK:H302	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:4B:301:PGV:H331	20:4D:201:CDL:H462	1.87	0.56
8:4H:31:GLN:NE2	8:4H:35:ASP:OD1	2.36	0.56
20:4C:306:CDL:H541	20:4C:306:CDL:H141	1.88	0.56
1:4A:218:THR:HG21	7:4G:55:ILE:HD12	1.88	0.55
1:4A:510:TYR:HB3	6:4F:58:VAL:HG22	1.87	0.55
6:4F:53:THR:HG22	6:4F:54:ASN:H	1.72	0.55
3:4C:165:ILE:HG12	15:4C:302:PGV:H11	1.88	0.55
2:4B:64:ILE:HG21	22:4B:304:PSC:H281	1.87	0.55
1:4A:240:HIS:NE2	1:4A:244:TYR:HE2	2.04	0.55
1:4A:52:GLN:O	1:4A:56:VAL:HG23	2.07	0.55
20:4B:302:CDL:H661	20:4B:302:CDL:H412	1.89	0.55
13:4M:19:LEU:HD23	15:4M:101:PGV:H271	1.89	0.55
1:4A:251:PHE:HB3	1:4A:319:LYS:HE2	1.89	0.55
8:4H:55:TRP:N	26:4H:201:HOH:O	2.38	0.55
3:4C:63:ARG:NH1	10:4J:20:VAL:O	2.39	0.54
1:4A:423:MET:HE2	1:4A:456:MET:HB2	1.89	0.54
3:4C:149:HIS:HA	3:4C:152:MET:HE2	1.90	0.54
15:4C:303:PGV:H51	7:4G:69:LEU:HD21	1.89	0.54
4:4D:19:ARG:NH2	26:4D:305:HOH:O	2.39	0.54
3:4C:15:PRO:HB2	10:4J:36:MET:HE1	1.89	0.54
5:4E:16:VAL:HG23	5:4E:47:ILE:HG22	1.87	0.54
15:4C:302:PGV:H012	15:4C:302:PGV:H42	1.89	0.54
2:4B:13:THR:O	2:4B:187:THR:OG1	2.24	0.54
2:4B:44:LEU:HD21	9:4I:20:HIS:HB3	1.89	0.54
2:4B:120:SER:OG	2:4B:140:ASN:O	2.24	0.54
7:4G:25:LEU:HD11	24:4G:102:PEK:H101	1.90	0.54
10:4J:38:LEU:HA	15:4J:101:PGV:H281	1.89	0.54
1:4A:129:TYR:HH	1:4A:236:TRP:NE1	2.06	0.54
15:4A:603:PGV:H211	15:4C:304:PGV:H32	1.90	0.54
1:4A:144:ASP:OD2	1:4A:213:ARG:NH1	2.41	0.53
6:4F:63:GLU:O	6:4F:66:ASN:HB2	2.08	0.53
3:4C:42:LEU:HD13	10:4J:45:TYR:HD2	1.73	0.53
7:4G:28:VAL:O	7:4G:32:THR:OG1	2.22	0.53
1:4A:268:PHE:HZ	2:4B:58:ALA:HB3	1.74	0.53
15:4K:101:PGV:H62	15:4K:101:PGV:H21	1.90	0.53
1:4A:3:VAL:HG11	15:4A:601:PGV:H32	1.91	0.53
2:4B:14:SER:HB3	2:4B:168:LEU:HD23	1.90	0.53
1:4A:218:THR:HG22	1:4A:221:ASP:HB3	1.90	0.52
1:4A:275:TRP:CE3	15:4A:602:PGV:H12	2.44	0.52
1:4A:420:GLY:O	1:4A:424:THR:OG1	2.23	0.52
1:4A:487:LEU:O	1:4A:491:ASN:ND2	2.36	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:4A:602:PGV:H131	14:4N:22:ILE:HG21	1.90	0.52
2:4B:9:PHE:HB2	2:4B:21:LEU:HD21	1.91	0.52
9:4I:61:GLU:OE1	9:4I:64:ARG:NH1	2.42	0.52
3:4C:31:LEU:HD12	15:4C:301:PGV:H181	1.91	0.52
1:4A:86:MET:HB3	1:4A:182:PRO:HG2	1.91	0.52
15:4J:101:PGV:H51	15:4J:101:PGV:H231	1.92	0.52
11:4K:8:ASP:OD1	11:4K:8:ASP:N	2.41	0.52
3:4C:72:THR:O	3:4C:76:GLN:HG3	2.10	0.52
3:4C:156:ARG:NH2	3:4C:222:GLN:O	2.43	0.52
9:4I:63:MET:HB3	9:4I:68:ILE:HD11	1.91	0.52
1:4A:430:PHE:HB3	2:4B:7:LEU:HA	1.93	0.51
20:4C:306:CDL:H541	20:4C:306:CDL:H162	1.91	0.51
1:4A:229:ILE:HG21	15:4A:603:PGV:H062	1.93	0.51
20:4D:201:CDL:H1O1	20:4D:201:CDL:HA62	1.75	0.51
20:4D:201:CDL:H742	20:4D:201:CDL:H181	1.91	0.51
1:4A:51:ASP:OD2	2:4B:205:SER:OG	2.23	0.51
1:4A:190:ILE:HG23	15:4A:602:PGV:H252	1.91	0.51
3:4C:175:LEU:HD12	15:4G:101:PGV:H182	1.92	0.51
1:4A:441:SER:OG	26:4A:702:HOH:O	2.14	0.51
3:4C:204:HIS:NE2	3:4C:249:TRP:HB2	2.26	0.51
15:4G:101:PGV:H012	15:4G:101:PGV:H241	1.91	0.51
4:4D:37:GLN:NE2	26:4D:307:HOH:O	2.42	0.51
4:4D:78:TRP:CZ2	20:4D:201:CDL:H592	2.45	0.51
12:4L:28:TYR:HD2	15:4L:101:PGV:H302	1.74	0.51
15:4B:301:PGV:O14	15:4B:301:PGV:O05	2.24	0.51
1:4A:443:TYR:O	2:4B:134:ARG:NH2	2.44	0.50
2:4B:134:ARG:HB2	4:4D:110:THR:HG21	1.92	0.50
3:4C:86:PHE:HZ	15:4C:307:PGV:H301	1.77	0.50
8:4H:71:ALA:O	8:4H:75:ARG:HG3	2.10	0.50
1:4A:51:ASP:CG	2:4B:205:SER:HG	2.20	0.50
1:4A:508:PRO:HG3	3:4C:6:HIS:HB3	1.93	0.50
2:4B:7:LEU:HD21	20:4B:302:CDL:H782	1.93	0.50
4:4D:89:ILE:HG21	15:4K:101:PGV:H151	1.92	0.50
8:4H:36:PHE:O	8:4H:40:GLU:HG3	2.12	0.50
1:4A:72:PRO:O	1:4A:77:GLY:N	2.45	0.50
15:4C:304:PGV:H183	20:4C:306:CDL:H861	1.94	0.49
15:4A:603:PGV:H012	15:4C:304:PGV:H202	1.93	0.49
3:4C:122:HIS:CE1	7:4G:45:PRO:HB3	2.47	0.49
15:4C:304:PGV:H201	14:4N:36:LEU:HB3	1.95	0.49
3:4C:71:HIS:NE2	15:4C:301:PGV:O06	2.39	0.49
4:4D:141:ASP:O	4:4D:143:ASN:N	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:4B:302:CDL:HB61	20:4B:302:CDL:HB21	1.94	0.49
5:4E:71:VAL:HG11	5:4E:85:VAL:HG11	1.94	0.49
15:4A:601:PGV:H282	15:4L:101:PGV:H42	1.94	0.49
1:4A:271:MET:HG3	14:4N:12:HIS:CE1	2.48	0.48
1:4A:474:GLU:OE1	1:4A:478:SER:OG	2.31	0.48
3:4C:58:TRP:HB3	15:4C:307:PGV:H32	1.95	0.48
15:4L:101:PGV:H92	15:4L:101:PGV:H52	1.94	0.48
14:4N:44:CYS:HB2	14:4N:53:PRO:HG3	1.95	0.48
22:4B:304:PSC:H261	22:4B:304:PSC:H10	1.94	0.48
5:4E:44:GLU:HG2	5:4E:45:PRO:HD2	1.94	0.48
1:4A:239:GLY:O	1:4A:242[B]:GLU:HG2	2.14	0.48
4:4D:60:TYR:OH	5:4E:69:GLU:OE2	2.20	0.48
1:4A:243:VAL:HB	16:4A:605:HEA:C3C	2.44	0.48
2:4B:129:LYS:HB2	2:4B:132:GLU:HG3	1.96	0.48
1:4A:64:VAL:HA	1:4A:68:PHE:HD2	1.79	0.48
1:4A:74:MET:HE3	1:4A:389:ILE:HG13	1.96	0.48
1:4A:264:LYS:NZ	1:4A:326:THR:O	2.34	0.48
1:4A:68:PHE:HE2	1:4A:112:LEU:HD22	1.78	0.48
1:4A:484:ALA:HB3	13:4M:2:TYR:HB2	1.96	0.48
4:4D:78:TRP:O	4:4D:82:VAL:HG23	2.14	0.48
1:4A:242[A]:GLU:HA	1:4A:245:ILE:HD12	1.96	0.47
3:4C:34:TRP:CD1	3:4C:40:MET:HG2	2.49	0.47
8:4H:57:ARG:HA	8:4H:60:TYR:CE2	2.49	0.47
15:4M:101:PGV:H242	15:4M:101:PGV:H81	1.96	0.47
1:4A:8:TYR:CZ	3:4C:15:PRO:HB3	2.49	0.47
1:4A:65:MET:HB3	16:4A:604:HEA:HBC1	1.95	0.47
1:4A:347:LEU:HD11	1:4A:418:PHE:CE1	2.49	0.47
4:4D:44:GLU:O	5:4E:56:ARG:NH2	2.47	0.47
2:4B:61:VAL:HG21	26:4B:406:HOH:O	2.14	0.47
15:4C:301:PGV:H281	15:4C:307:PGV:H312	1.95	0.47
15:4K:101:PGV:H292	15:4K:101:PGV:H61	1.96	0.47
1:4A:151:HIS:CD2	24:4G:103:PEK:H361	2.49	0.47
1:4A:168:ILE:HD13	1:4A:189:LEU:HB2	1.96	0.47
1:4A:275:TRP:HE3	15:4A:602:PGV:H12	1.79	0.47
1:4A:328:HIS:NE2	9:4I:17:LEU:HD22	2.30	0.47
1:4A:417:MET:O	1:4A:421:VAL:HG22	2.14	0.47
20:4D:201:CDL:H262	20:4D:201:CDL:H821	1.97	0.47
9:4I:55:ASP:HB3	9:4I:58:LYS:HB3	1.96	0.47
2:4B:138:VAL:HG23	26:4B:403:HOH:O	2.15	0.47
3:4C:58:TRP:CZ3	15:4C:307:PGV:H71	2.50	0.47
3:4C:141:GLY:O	3:4C:145:THR:OG1	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:4D:201:CDL:HB61	20:4D:201:CDL:H711	1.49	0.47
1:4A:35:LEU:HD11	1:4A:462:LEU:HB2	1.97	0.47
1:4A:374:VAL:HA	1:4A:377:PHE:CE2	2.51	0.47
10:4J:40:LEU:HD12	15:4J:101:PGV:H152	1.97	0.47
1:4A:500:PRO:HB2	1:4A:504:THR:HG21	1.96	0.46
15:4A:601:PGV:H201	15:4A:601:PGV:H011	1.46	0.46
15:4A:601:PGV:H142	3:4C:22:LEU:HD21	1.97	0.46
4:4D:40:LEU:HD11	4:4D:55:GLU:HB3	1.96	0.46
6:4F:20:VAL:HG12	6:4F:31:TYR:CD1	2.50	0.46
12:4L:17:ASN:HB3	12:4L:20:ARG:HB3	1.97	0.46
3:4C:76:GLN:O	3:4C:80:ARG:HG3	2.15	0.46
4:4D:40:LEU:HD21	4:4D:55:GLU:HB3	1.96	0.46
6:4F:79:THR:HG23	6:4F:90:LYS:HB2	1.97	0.46
2:4B:144:LEU:N	26:4B:401:HOH:O	2.45	0.46
4:4D:80:THR:HG22	11:4K:14:GLY:HA2	1.97	0.46
1:4A:131:PRO:HD3	2:4B:160:LEU:HD13	1.97	0.46
3:4C:250:LEU:O	3:4C:254:VAL:HG23	2.15	0.46
15:4C:304:PGV:H282	14:4N:45:TRP:HH2	1.80	0.46
6:4F:16:LEU:HD11	6:4F:31:TYR:CE2	2.50	0.46
2:4B:23:PHE:CZ	2:4B:80:SER:HB2	2.50	0.46
3:4C:130:PRO:HB2	3:4C:253:TYR:HE1	1.81	0.46
15:4L:101:PGV:O02	15:4L:101:PGV:H62	2.16	0.46
1:4A:507:GLU:HA	3:4C:5:THR:HB	1.97	0.46
15:4A:601:PGV:H161	15:4A:601:PGV:H332	1.98	0.46
3:4C:171:VAL:HG22	15:4C:305:PGV:H162	1.97	0.46
3:4C:247:VAL:HG21	20:4C:306:CDL:H842	1.98	0.46
15:4C:305:PGV:H02	15:4C:305:PGV:H22	1.69	0.46
14:4N:81:ASP:OD1	14:4N:81:ASP:N	2.49	0.46
2:4B:165:VAL:HG21	2:4B:211:LEU:HD11	1.97	0.46
6:4F:14:THR:OG1	6:4F:15:GLY:N	2.48	0.46
1:4A:299:VAL:HG11	14:4N:64:LYS:HD3	1.98	0.46
1:4A:408:ALA:HB3	15:4M:101:PGV:H21	1.97	0.45
3:4C:79:LEU:HB3	3:4C:233:PHE:CE2	2.51	0.45
5:4E:65:VAL:HG11	5:4E:104:LEU:HD12	1.98	0.45
1:4A:18:LEU:HB3	1:4A:102:PHE:CZ	2.52	0.45
1:4A:305:PHE:CZ	15:4A:603:PGV:H21	2.51	0.45
2:4B:122:MET:HG3	2:4B:208:PRO:HG2	1.98	0.45
20:4C:306:CDL:H251	20:4C:306:CDL:H371	1.98	0.45
20:4D:201:CDL:H272	20:4D:201:CDL:H412	1.98	0.45
26:4A:805:HOH:O	20:4B:302:CDL:H851	2.17	0.45
1:4A:62:ALA:HB2	16:4A:604:HEA:HBD1	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:4C:140:SER:HA	3:4C:143:SER:HB2	1.98	0.45
2:4B:11:ASP:HB2	4:4D:129:ALA:HA	1.98	0.45
2:4B:221:LYS:O	2:4B:225:SER:OG	2.26	0.45
20:4C:306:CDL:HB61	20:4C:306:CDL:H542	1.99	0.45
1:4A:76:GLY:O	1:4A:80:ASN:ND2	2.40	0.45
2:4B:214:VAL:HG22	26:4B:401:HOH:O	2.16	0.45
22:4B:304:PSC:H212	9:4I:18:ARG:HG2	1.99	0.45
15:4C:301:PGV:H22	15:4C:301:PGV:H242	1.98	0.45
2:4B:102:HIS:O	2:4B:161:HIS:NE2	2.50	0.45
2:4B:106:TRP:CE2	2:4B:207:MET:HE2	2.52	0.45
15:4B:301:PGV:H12	20:4D:201:CDL:C39	2.47	0.45
7:4G:70:PHE:HB2	24:4G:103:PEK:H041	1.99	0.45
1:4A:33:LEU:CB	1:4A:61:HIS:HB2	2.44	0.45
12:4L:15:VAL:HG12	12:4L:21:LEU:HD13	1.98	0.45
1:4A:189:LEU:HD11	26:4C:490:HOH:O	2.17	0.45
8:4H:75:ARG:HA	8:4H:78:GLU:HG2	1.98	0.45
1:4A:367:LEU:HD21	1:4A:433:LEU:HD23	1.99	0.45
2:4B:1:FME:HE3	4:4D:128:VAL:HG22	1.99	0.45
4:4D:19:ARG:HE	4:4D:19:ARG:HB3	1.62	0.45
6:4F:95:GLN:HG3	6:4F:96:LEU:H	1.81	0.45
2:4B:65:TRP:CD1	2:4B:65:TRP:C	2.95	0.44
7:4G:69:LEU:HD22	24:4G:103:PEK:H231	1.98	0.44
1:4A:7:LEU:HD23	15:4A:601:PGV:H71	1.98	0.44
3:4C:156:ARG:NH1	15:4C:302:PGV:O13	2.51	0.44
10:4J:31:LEU:O	10:4J:35:THR:HG22	2.18	0.44
2:4B:216:LEU:O	2:4B:220:GLU:HG2	2.18	0.44
7:4G:56:ARG:NH2	7:4G:66:ASN:O	2.32	0.44
8:4H:56:TYR:CZ	14:4N:80:PRO:HD2	2.52	0.44
13:4M:16:ALA:O	13:4M:20:SER:OG	2.30	0.44
1:4A:2:PHE:HZ	15:4L:101:PGV:H21	1.81	0.44
2:4B:61:VAL:HG11	22:4B:304:PSC:H41	2.00	0.44
15:4B:301:PGV:H05	20:4D:201:CDL:HA32	2.00	0.44
5:4E:61:PHE:HE1	5:4E:98:ILE:HA	1.82	0.44
15:4B:301:PGV:H011	20:4D:201:CDL:H111	2.00	0.44
3:4C:231:HIS:CD2	15:4C:307:PGV:H042	2.52	0.44
15:4C:307:PGV:H152	15:4C:307:PGV:H291	1.99	0.44
15:4L:101:PGV:C12	15:4L:101:PGV:H292	2.47	0.44
1:4A:149:SER:HA	26:4A:762:HOH:O	2.16	0.44
1:4A:481:GLU:OE1	12:4L:7:PRO:HG2	2.18	0.44
1:4A:324:LEU:HD22	2:4B:42:ILE:HG12	2.00	0.44
15:4A:602:PGV:H41	14:4N:1:MET:HE3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4B:38:VAL:O	2:4B:42:ILE:HG13	2.18	0.44
20:4C:306:CDL:HB4	20:4C:306:CDL:H512	1.44	0.44
10:4J:4:ARG:O	10:4J:8:LYS:HE2	2.18	0.43
1:4A:5:ARG:NH1	26:4A:715:HOH:O	2.47	0.43
1:4A:362:SER:HA	2:4B:87:MET:HE1	2.00	0.43
26:4C:402:HOH:O	7:4G:74:ARG:NH1	2.51	0.43
1:4A:418:PHE:O	1:4A:422:ASN:ND2	2.38	0.43
1:4A:481:GLU:HB2	13:4M:4:LYS:HB2	2.00	0.43
2:4B:5:PHE:HE2	11:4K:42:LEU:HD23	1.84	0.43
2:4B:216:LEU:HD12	26:4B:493:HOH:O	2.18	0.43
4:4D:48:TRP:HA	4:4D:51:LEU:HD13	2.00	0.43
4:4D:88:PHE:HZ	13:4M:19:LEU:HD21	1.84	0.43
2:4B:44:LEU:HD12	2:4B:44:LEU:HA	1.85	0.43
8:4H:4:ILE:HD11	8:4H:55:TRP:HB2	2.00	0.43
1:4A:8:TYR:O	3:4C:13:PRO:HB3	2.19	0.43
1:4A:168:ILE:HG12	1:4A:185:VAL:HG13	1.99	0.43
16:4A:604:HEA:H202	16:4A:604:HEA:H171	1.76	0.43
3:4C:219:LEU:HD21	15:4C:302:PGV:H231	2.00	0.43
1:4A:194:LEU:HD23	1:4A:285:PHE:CE2	2.53	0.43
1:4A:334:TRP:HB2	20:4D:201:CDL:H752	2.00	0.43
7:4G:64:ASP:N	7:4G:64:ASP:OD1	2.51	0.43
20:4B:302:CDL:H442	20:4B:302:CDL:H182	2.01	0.43
4:4D:61:ARG:HA	4:4D:61:ARG:HD2	1.87	0.43
8:4H:42:ALA:O	8:4H:46:LYS:HG2	2.18	0.43
16:4A:604:HEA:HBD2	16:4A:604:HEA:HHA	1.99	0.43
2:4B:100:MET:HE1	2:4B:155:SER:HB3	2.00	0.43
20:4D:201:CDL:H512	20:4D:201:CDL:HB4	1.44	0.43
12:4L:28:TYR:CD2	15:4L:101:PGV:H302	2.54	0.43
3:4C:117:PRO:HG2	3:4C:123:PRO:HG3	2.00	0.43
3:4C:221:ARG:HB3	3:4C:226:HIS:HB2	2.01	0.43
5:4E:49:ASP:HA	26:4E:202:HOH:O	2.18	0.43
5:4E:93:LEU:HD23	5:4E:98:ILE:HB	2.01	0.43
9:4I:22:VAL:O	9:4I:26:ILE:HG12	2.19	0.43
1:4A:106:PRO:HB2	1:4A:107:PRO:HD3	2.00	0.42
2:4B:143:VAL:HG12	2:4B:219:PHE:HD1	1.83	0.42
3:4C:179:SER:OG	15:4G:101:PGV:H101	2.19	0.42
15:4G:101:PGV:H162	24:4G:102:PEK:H181	2.00	0.42
1:4A:6:TRP:CE3	12:4L:12:PRO:HG3	2.54	0.42
1:4A:28:MET:N	1:4A:28:MET:HE2	2.33	0.42
1:4A:282:PHE:HA	15:4A:602:PGV:H292	2.00	0.42
1:4A:127:THR:HB	1:4A:129:TYR:CE1	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4A:177:SER:H	1:4A:180:GLN:HE21	1.66	0.42
2:4B:122:MET:HE2	2:4B:122:MET:HB3	1.90	0.42
1:4A:473:TRP:CE2	12:4L:22:LEU:HD13	2.54	0.42
3:4C:179:SER:HB3	15:4G:101:PGV:H82	2.02	0.42
15:4C:304:PGV:H231	15:4C:304:PGV:H52	2.01	0.42
8:4H:57:ARG:O	8:4H:61:LYS:HB2	2.18	0.42
15:4B:301:PGV:H252	20:4D:201:CDL:H261	2.01	0.42
15:4C:302:PGV:H02	15:4C:302:PGV:H21	1.73	0.42
1:4A:229:ILE:HD11	2:4B:175:ILE:HD13	2.02	0.42
1:4A:274:VAL:O	1:4A:278:MET:HG3	2.19	0.42
15:4B:301:PGV:H22	20:4D:201:CDL:H312	2.02	0.42
4:4D:44:GLU:OE2	5:4E:61:PHE:N	2.42	0.42
1:4A:236:TRP:O	1:4A:288:TRP:HB2	2.20	0.42
1:4A:361:SER:HG	2:4B:84:LEU:HD13	1.85	0.42
4:4D:117:ALA:HB1	11:4K:51:LYS:HG2	2.01	0.42
3:4C:63:ARG:HA	3:4C:67:PHE:CD2	2.55	0.42
1:4A:71:MET:HB2	1:4A:72:PRO:HD3	2.02	0.42
1:4A:467:LEU:O	1:4A:471:ILE:HG13	2.20	0.42
20:4B:302:CDL:H442	20:4B:302:CDL:H162	2.02	0.42
4:4D:135:SER:OG	4:4D:140:TYR:OH	2.29	0.42
1:4A:452:THR:HG22	1:4A:456:MET:HE3	2.01	0.42
2:4B:68:LEU:HB3	22:4B:304:PSC:H183	2.02	0.42
8:4H:56:TYR:CE2	14:4N:80:PRO:HD2	2.55	0.42
1:4A:305:PHE:O	1:4A:309:THR:HG22	2.20	0.41
4:4D:122:ARG:HG3	11:4K:53:TRP:CE2	2.55	0.41
5:4E:52:LEU:HD22	5:4E:98:ILE:HD13	2.02	0.41
10:4J:36:MET:HE2	10:4J:36:MET:HB2	1.84	0.41
1:4A:403:TYR:HE1	13:4M:7:ARG:NH2	2.18	0.41
8:4H:24:ASN:OD1	8:4H:26:THR:HG22	2.20	0.41
5:4E:37:VAL:HG11	5:4E:70:VAL:HG21	2.02	0.41
7:4G:48:ILE:O	7:4G:50:TYR:N	2.49	0.41
1:4A:455:SER:O	1:4A:458:SER:OG	2.38	0.41
3:4C:19:THR:HG23	10:4J:39:CYS:SG	2.61	0.41
15:4C:305:PGV:O13	15:4C:305:PGV:O05	2.32	0.41
7:4G:50:TYR:HA	8:4H:80:THR:HG23	2.02	0.41
3:4C:3:HIS:NE2	6:4F:96:LEU:HD11	2.36	0.41
6:4F:50:PRO:O	6:4F:56:ARG:NH1	2.52	0.41
1:4A:86:MET:HE3	1:4A:185:VAL:HG23	2.01	0.41
1:4A:110:LEU:HD22	15:4A:601:PGV:H181	2.01	0.41
1:4A:491:ASN:HB3	1:4A:494:TRP:HD1	1.84	0.41
2:4B:41:ILE:HG21	22:4B:304:PSC:H9	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:4C:304:PGV:O11	15:4C:304:PGV:O05	2.37	0.41
5:4E:84:TYR:HA	5:4E:87:GLN:HG2	2.03	0.41
1:4A:407:GLN:O	1:4A:411:LYS:HG3	2.21	0.41
1:4A:440:TYR:CZ	2:4B:205:SER:HA	2.56	0.41
3:4C:197:PHE:O	3:4C:201:THR:OG1	2.24	0.41
7:4G:17:ARG:NH2	24:4G:102:PEK:O04	2.53	0.41
15:4K:101:PGV:O14	15:4K:101:PGV:O05	2.38	0.41
1:4A:440:TYR:OH	2:4B:195:GLN:HB3	2.21	0.41
1:4A:470:PHE:CG	13:4M:19:LEU:HD13	2.56	0.41
3:4C:103:HIS:HA	15:4C:304:PGV:O02	2.21	0.41
20:4D:201:CDL:H721	20:4D:201:CDL:H141	2.03	0.41
10:4J:8:LYS:HA	10:4J:11:ILE:HD12	2.02	0.41
1:4A:23:GLY:HA3	1:4A:73:ILE:HG13	2.02	0.41
2:4B:215:PRO:HG2	9:4I:57:MET:HE1	2.02	0.41
20:4B:302:CDL:H242	20:4B:302:CDL:H811	2.03	0.41
15:4C:303:PGV:H302	15:4C:303:PGV:H343	2.03	0.41
20:4B:302:CDL:H811	20:4B:302:CDL:H262	2.03	0.41
22:4B:304:PSC:H073	22:4B:304:PSC:H041	1.82	0.41
20:4C:306:CDL:H111	20:4C:306:CDL:H152	2.03	0.41
5:4E:36:LEU:HA	5:4E:39:TYR:CE1	2.56	0.41
1:4A:449:ALA:O	1:4A:453:ILE:HG12	2.20	0.40
2:4B:12:ALA:O	2:4B:188:ARG:NH1	2.54	0.40
22:4B:304:PSC:H82	22:4B:304:PSC:H52	1.85	0.40
3:4C:161:GLN:O	3:4C:165:ILE:HG13	2.21	0.40
8:4H:9:LYS:HE3	8:4H:9:LYS:HB3	1.85	0.40
8:4H:14:ALA:HB3	8:4H:63:PHE:HE2	1.86	0.40
11:4K:42:LEU:HD22	15:4K:101:PGV:H202	2.03	0.40
2:4B:108:TYR:HD2	26:4B:423:HOH:O	2.03	0.40
3:4C:30:GLY:HA2	3:4C:42:LEU:HB3	2.03	0.40
3:4C:112:LEU:HB3	3:4C:118:PRO:HB3	2.03	0.40
1:4A:9:SER:HB3	1:4A:99:ASN:ND2	2.36	0.40
1:4A:224:GLY:O	3:4C:192:VAL:HG22	2.21	0.40
1:4A:418:PHE:CE1	15:4B:301:PGV:H061	2.57	0.40
2:4B:179:LEU:HD23	26:4H:202:HOH:O	2.22	0.40
15:4B:301:PGV:H232	20:4D:201:CDL:H401	2.03	0.40
22:4B:304:PSC:H271	22:4B:304:PSC:H241	1.87	0.40
8:4H:14:ALA:HB3	8:4H:63:PHE:CE2	2.57	0.40
1:4A:69:MET:HE3	1:4A:69:MET:HB3	1.98	0.40
1:4A:377:PHE:HA	1:4A:380:VAL:HG22	2.03	0.40
20:4D:201:CDL:H751	20:4D:201:CDL:H162	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4A	512/514 (100%)	500 (98%)	12 (2%)	0	100	100
2	4B	225/229 (98%)	216 (96%)	9 (4%)	0	100	100
3	4C	257/261 (98%)	249 (97%)	8 (3%)	0	100	100
4	4D	137/169 (81%)	131 (96%)	6 (4%)	0	100	100
5	4E	103/152 (68%)	99 (96%)	4 (4%)	0	100	100
6	4F	95/129 (74%)	94 (99%)	1 (1%)	0	100	100
7	4G	73/97 (75%)	69 (94%)	4 (6%)	0	100	100
8	4H	80/86 (93%)	77 (96%)	3 (4%)	0	100	100
9	4I	65/75 (87%)	64 (98%)	1 (2%)	0	100	100
10	4J	56/80 (70%)	55 (98%)	1 (2%)	0	100	100
11	4K	47/80 (59%)	46 (98%)	1 (2%)	0	100	100
12	4L	44/63 (70%)	43 (98%)	1 (2%)	0	100	100
13	4M	41/70 (59%)	41 (100%)	0	0	100	100
14	4N	80/82 (98%)	72 (90%)	7 (9%)	1 (1%)	9	38
All	All	1815/2087 (87%)	1756 (97%)	58 (3%)	1 (0%)	49	80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	4N	33	VAL

5.3.2 Protein sidechains

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	4A	425/425 (100%)	421 (99%)	4 (1%)	70	85
2	4B	210/211 (100%)	205 (98%)	5 (2%)	43	73
3	4C	223/225 (99%)	217 (97%)	6 (3%)	39	71
4	4D	124/149 (83%)	120 (97%)	4 (3%)	34	67
5	4E	92/124 (74%)	88 (96%)	4 (4%)	26	60
6	4F	80/101 (79%)	78 (98%)	2 (2%)	42	72
7	4G	65/80 (81%)	60 (92%)	5 (8%)	12	40
8	4H	73/76 (96%)	70 (96%)	3 (4%)	27	61
9	4I	54/61 (88%)	54 (100%)	0	100	100
10	4J	49/68 (72%)	48 (98%)	1 (2%)	48	76
11	4K	38/66 (58%)	38 (100%)	0	100	100
12	4L	39/55 (71%)	38 (97%)	1 (3%)	40	72
13	4M	37/57 (65%)	37 (100%)	0	100	100
14	4N	70/70 (100%)	66 (94%)	4 (6%)	18	52
All	All	1579/1768 (89%)	1540 (98%)	39 (2%)	42	72

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	4A	208	MET
1	4A	316	THR
1	4A	436	MET
1	4A	513	LEU
2	4B	27	THR
2	4B	33	LEU
2	4B	54	SER
2	4B	138	VAL
2	4B	149	THR
3	4C	29	SER
3	4C	44	SER
3	4C	129	VAL
3	4C	192	VAL
3	4C	245	VAL
3	4C	247	VAL
4	4D	15	VAL
4	4D	17	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	4D	27	VAL
4	4D	42	GLU
5	4E	17	THR
5	4E	47	ILE
5	4E	87	GLN
5	4E	109	VAL
6	4F	49	VAL
6	4F	76	LYS
7	4G	15	THR
7	4G	25	LEU
7	4G	30	LEU
7	4G	64	ASP
7	4G	75	VAL
8	4H	6	THR
8	4H	12	GLN
8	4H	50	VAL
10	4J	10	LYS
12	4L	14	SER
14	4N	6	ILE
14	4N	14	SER
14	4N	33	VAL
14	4N	69	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	4A	43	GLN
3	4C	76	GLN
4	4D	37	GLN
7	4G	72	ASN
7	4G	84	GLN
14	4N	8	GLN
14	4N	62	GLN
14	4N	69	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FME	4B	1	2	8,9,10	0.96	0	8,9,11	0.92	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	4B	1	2	-	4/7/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	4B	1	FME	O1-CN-N-CA
2	4B	1	FME	C-CA-CB-CG
2	4B	1	FME	N-CA-CB-CG
2	4B	1	FME	CB-CG-SD-CE

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	4B	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 4 are monoatomic - leaving 25 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$
15	PGV	4A	601	-	50,50,50	0.27	0	53,56,56	0.33	0
24	PEK	4G	102	-	52,52,52	0.46	0	55,57,57	0.46	0
22	PSC	4B	304	-	51,51,51	0.48	0	57,59,59	0.44	0
16	HEA	4A	604	1	67,67,67	2.45	25 (37%)	81,103,103	2.52	33 (40%)
15	PGV	4C	302	-	50,50,50	0.30	0	53,56,56	0.68	1 (1%)
15	PGV	4G	101	-	50,50,50	0.29	0	53,56,56	0.46	1 (1%)
20	CDL	4C	306	-	99,99,99	0.27	0	105,111,111	0.41	1 (0%)
15	PGV	4C	305	-	50,50,50	0.30	0	53,56,56	0.57	1 (1%)
15	PGV	4K	101	-	50,50,50	0.29	0	53,56,56	0.33	0
15	PGV	4C	304	-	50,50,50	0.30	0	53,56,56	0.39	0
15	PGV	4C	303	-	50,50,50	0.29	0	53,56,56	0.33	0
24	PEK	4G	103	-	51,51,52	0.48	0	54,56,57	0.46	0
15	PGV	4M	101	-	50,50,50	0.29	0	53,56,56	0.31	0
15	PGV	4L	101	-	50,50,50	0.30	0	53,56,56	0.39	0
15	PGV	4A	602	-	50,50,50	0.28	0	53,56,56	0.36	0
16	HEA	4A	605	1	67,67,67	2.46	25 (37%)	81,103,103	2.49	34 (41%)
21	CUA	4B	303	2	0,1,1	-	-	-	-	-
15	PGV	4A	603	-	50,50,50	0.30	0	53,56,56	0.35	0
15	PGV	4J	101	-	50,50,50	0.29	0	53,56,56	0.36	0
25	PO4	4H	101	-	4,4,4	0.98	0	6,6,6	0.44	0
15	PGV	4B	301	-	50,50,50	0.28	0	53,56,56	0.34	0
15	PGV	4C	307	-	50,50,50	0.29	0	53,56,56	0.36	0
20	CDL	4B	302	-	99,99,99	0.27	0	105,111,111	0.31	0
20	CDL	4D	201	-	99,99,99	0.27	0	105,111,111	0.38	0
15	PGV	4C	301	-	50,50,50	0.28	0	53,56,56	0.32	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
15	PGV	4A	601	-	-	10/55/55/55	-
24	PEK	4G	102	-	-	10/56/56/56	-
22	PSC	4B	304	-	-	17/55/55/55	-
16	HEA	4A	604	1	-	8/36/76/76	-
15	PGV	4C	302	-	-	6/55/55/55	-
15	PGV	4G	101	-	-	7/55/55/55	-
20	CDL	4C	306	-	-	24/110/110/110	-
15	PGV	4C	305	-	-	16/55/55/55	-
15	PGV	4K	101	-	-	14/55/55/55	-
15	PGV	4C	304	-	-	15/55/55/55	-
15	PGV	4C	303	-	-	10/55/55/55	-
24	PEK	4G	103	-	-	9/55/55/56	-
15	PGV	4M	101	-	-	8/55/55/55	-
15	PGV	4L	101	-	-	7/55/55/55	-
15	PGV	4A	602	-	-	6/55/55/55	-
16	HEA	4A	605	1	-	7/36/76/76	-
15	PGV	4A	603	-	-	11/55/55/55	-
15	PGV	4J	101	-	-	10/55/55/55	-
15	PGV	4B	301	-	-	11/55/55/55	-
15	PGV	4C	307	-	-	4/55/55/55	-
20	CDL	4B	302	-	-	15/110/110/110	-
20	CDL	4D	201	-	-	16/110/110/110	-
15	PGV	4C	301	-	-	1/55/55/55	-

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	4A	604	HEA	FE-ND	5.67	2.12	1.94
16	4A	605	HEA	FE-NB	5.63	2.12	1.94
16	4A	605	HEA	FE-ND	5.60	2.12	1.94
16	4A	604	HEA	FE-NB	5.57	2.12	1.94
16	4A	604	HEA	C3B-C2B	5.48	1.47	1.34
16	4A	605	HEA	C3B-C2B	5.48	1.47	1.34
16	4A	605	HEA	FE-NC	4.97	2.11	1.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	4A	605	HEA	C3D-C2D	4.94	1.47	1.36
16	4A	604	HEA	FE-NC	4.85	2.11	1.95
16	4A	604	HEA	C3D-C2D	4.80	1.47	1.36
16	4A	604	HEA	C3A-C2A	4.62	1.47	1.37
16	4A	605	HEA	C3A-C2A	4.60	1.47	1.37
16	4A	605	HEA	CHD-C1D	4.49	1.47	1.38
16	4A	604	HEA	CHD-C1D	4.47	1.47	1.38
16	4A	605	HEA	CHC-C4B	4.45	1.47	1.38
16	4A	605	HEA	C1A-NA	4.38	1.47	1.39
16	4A	604	HEA	CHC-C4B	4.35	1.47	1.38
16	4A	604	HEA	CHB-C4A	4.29	1.46	1.38
16	4A	604	HEA	CHA-C1A	4.20	1.46	1.38
16	4A	605	HEA	CHB-C4A	4.18	1.46	1.38
16	4A	604	HEA	C1A-NA	4.12	1.47	1.39
16	4A	605	HEA	C4A-NA	4.11	1.47	1.39
16	4A	605	HEA	CHA-C1A	4.08	1.46	1.38
16	4A	604	HEA	C4A-NA	3.96	1.47	1.39
16	4A	605	HEA	CHD-C4C	3.58	1.47	1.39
16	4A	604	HEA	CHD-C4C	3.53	1.47	1.39
16	4A	605	HEA	CHC-C1C	3.47	1.47	1.39
16	4A	604	HEA	CHC-C1C	3.45	1.47	1.39
16	4A	604	HEA	CHA-C4D	3.36	1.46	1.39
16	4A	604	HEA	CHB-C1B	3.32	1.46	1.39
16	4A	605	HEA	CHA-C4D	3.28	1.46	1.39
16	4A	605	HEA	CHB-C1B	3.28	1.46	1.39
16	4A	604	HEA	C4B-C3B	2.75	1.49	1.44
16	4A	605	HEA	C4B-C3B	2.69	1.49	1.44
16	4A	604	HEA	C1D-ND	-2.65	1.35	1.40
16	4A	605	HEA	C1D-ND	-2.59	1.35	1.40
16	4A	604	HEA	C4B-NB	-2.57	1.35	1.40
16	4A	605	HEA	C1C-C2C	2.56	1.49	1.43
16	4A	605	HEA	C4B-NB	-2.45	1.36	1.40
16	4A	604	HEA	C4D-C3D	2.45	1.49	1.45
16	4A	604	HEA	C1C-C2C	2.45	1.48	1.43
16	4A	605	HEA	C1D-C2D	2.32	1.49	1.44
16	4A	604	HEA	C1D-C2D	2.18	1.49	1.44
16	4A	605	HEA	C1A-C2A	2.13	1.48	1.45
16	4A	604	HEA	C4C-NC	-2.13	1.35	1.39
16	4A	604	HEA	C1A-C2A	2.11	1.48	1.45
16	4A	605	HEA	C4C-NC	-2.09	1.35	1.39
16	4A	605	HEA	C1B-C2B	2.05	1.48	1.44
16	4A	605	HEA	C4D-C3D	2.02	1.48	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	4A	604	HEA	C1B-C2B	2.02	1.48	1.44

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	4A	605	HEA	C3D-C4D-ND	6.70	116.83	110.35
16	4A	604	HEA	C3D-C4D-ND	6.50	116.64	110.35
16	4A	605	HEA	C2B-C1B-NB	5.82	116.63	109.90
16	4A	604	HEA	C2B-C1B-NB	5.71	116.51	109.90
16	4A	604	HEA	C3B-C4B-NB	5.64	116.33	109.84
16	4A	605	HEA	C3B-C4B-NB	5.57	116.24	109.84
16	4A	605	HEA	C3C-C2C-C1C	-5.55	100.62	107.17
16	4A	605	HEA	C2D-C1D-ND	5.53	116.20	109.84
16	4A	604	HEA	C2D-C1D-ND	5.43	116.09	109.84
16	4A	604	HEA	C3C-C2C-C1C	-5.41	100.79	107.17
16	4A	605	HEA	C3C-C4C-NC	5.24	114.21	109.80
16	4A	605	HEA	C2A-C1A-NA	5.19	115.33	110.32
16	4A	604	HEA	C3C-C4C-NC	5.18	114.16	109.80
16	4A	604	HEA	C2A-C1A-NA	4.98	115.12	110.32
16	4A	605	HEA	C1D-C2D-C3D	-4.29	102.47	106.98
16	4A	605	HEA	C2C-C1C-NC	4.14	116.77	110.14
16	4A	604	HEA	CHA-C4D-ND	-4.07	120.04	124.42
16	4A	604	HEA	C2C-C1C-NC	4.06	116.64	110.14
16	4A	604	HEA	C1D-C2D-C3D	-3.87	102.91	106.98
16	4A	605	HEA	C3A-C2A-C1A	-3.83	103.42	107.05
16	4A	604	HEA	C3A-C2A-C1A	-3.72	103.53	107.05
16	4A	605	HEA	C1B-C2B-C3B	-3.64	102.58	106.80
16	4A	604	HEA	C13-C14-C15	-3.60	119.38	127.62
16	4A	604	HEA	C1B-C2B-C3B	-3.48	102.76	106.80
16	4A	604	HEA	CAD-C3D-C4D	3.48	130.76	124.70
16	4A	604	HEA	C4D-C3D-C2D	-3.39	101.96	106.89
15	4C	302	PGV	O01-C1-C2	3.29	118.60	111.48
16	4A	605	HEA	C4A-NA-C1A	-3.26	100.51	105.82
16	4A	604	HEA	C4B-C3B-C2B	-3.23	102.00	107.44
16	4A	605	HEA	C4D-C3D-C2D	-3.19	102.25	106.89
16	4A	605	HEA	C4B-C3B-C2B	-3.08	102.27	107.44
16	4A	604	HEA	C13-C12-C11	-2.95	109.67	114.39
16	4A	604	HEA	C4A-NA-C1A	-2.95	101.01	105.82
16	4A	605	HEA	C13-C14-C15	-2.85	121.10	127.62
16	4A	604	HEA	CBA-CAA-C2A	-2.80	104.80	112.53
16	4A	605	HEA	C13-C12-C11	-2.74	110.02	114.39
16	4A	605	HEA	C26-C15-C16	2.73	119.96	115.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	4A	604	HEA	C17-C18-C19	-2.72	121.41	127.62
16	4A	605	HEA	C27-C19-C20	2.69	119.90	115.23
16	4A	605	HEA	C17-C18-C19	-2.68	121.49	127.62
16	4A	604	HEA	CHB-C1B-NB	-2.68	121.54	124.42
15	4C	305	PGV	O01-C1-C2	2.68	117.27	111.48
16	4A	604	HEA	CHA-C1A-NA	-2.66	121.56	124.45
16	4A	604	HEA	C26-C15-C16	2.64	119.81	115.23
16	4A	605	HEA	CHA-C4D-ND	-2.64	121.58	124.42
16	4A	605	HEA	CHB-C1B-NB	-2.60	121.62	124.42
16	4A	604	HEA	C27-C19-C20	2.55	119.66	115.23
16	4A	605	HEA	CHC-C1C-C2C	-2.52	120.11	127.43
16	4A	604	HEA	CHC-C1C-C2C	-2.50	120.17	127.43
16	4A	605	HEA	C1D-ND-C4D	-2.50	102.25	105.21
16	4A	605	HEA	C4B-NB-C1B	-2.47	102.28	105.21
16	4A	604	HEA	CMD-C2D-C1D	2.41	128.80	125.03
16	4A	605	HEA	CMB-C2B-C1B	2.38	128.75	125.03
16	4A	604	HEA	C4B-NB-C1B	-2.38	102.39	105.21
16	4A	604	HEA	C1D-ND-C4D	-2.37	102.40	105.21
16	4A	605	HEA	CMC-C2C-C1C	2.34	128.98	125.42
16	4A	605	HEA	C25-C23-C24	2.32	119.93	114.59
16	4A	605	HEA	CBA-CAA-C2A	-2.25	106.32	112.53
16	4A	605	HEA	CMD-C2D-C1D	2.25	128.54	125.03
16	4A	604	HEA	C25-C23-C24	2.24	119.73	114.59
16	4A	604	HEA	CMB-C2B-C1B	2.21	128.49	125.03
16	4A	604	HEA	CHD-C1D-C2D	-2.20	120.70	126.95
15	4G	101	PGV	O01-C1-C2	2.19	116.23	111.48
16	4A	604	HEA	CMC-C2C-C1C	2.19	128.75	125.42
16	4A	605	HEA	CHA-C4D-C3D	-2.19	121.58	124.77
16	4A	605	HEA	CHD-C1D-C2D	-2.14	120.87	126.95
16	4A	604	HEA	OMA-CMA-C3A	-2.11	120.85	125.62
16	4A	605	HEA	CHB-C1B-C2B	-2.08	121.74	125.03
20	4C	306	CDL	OB6-CB5-C51	2.05	115.92	111.48
16	4A	605	HEA	CHA-C1A-NA	-2.05	122.22	124.45
16	4A	605	HEA	C21-C22-C23	-2.02	120.91	127.64

There are no chirality outliers.

All (242) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	4A	601	PGV	C03-O11-P-O12
15	4A	601	PGV	C03-O11-P-O13
15	4A	601	PGV	O04-C19-O03-C01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	4A	601	PGV	C20-C19-O03-C01
15	4A	602	PGV	C02-C03-O11-P
15	4A	603	PGV	O03-C01-C02-O01
15	4B	301	PGV	C04-O12-P-O11
15	4C	302	PGV	C03-O11-P-O13
15	4C	302	PGV	O02-C1-O01-C02
15	4C	302	PGV	C2-C1-O01-C02
15	4C	303	PGV	C04-O12-P-O11
15	4C	303	PGV	C04-O12-P-O14
15	4C	303	PGV	O04-C19-O03-C01
15	4C	303	PGV	C20-C19-O03-C01
15	4C	304	PGV	C03-O11-P-O12
15	4C	304	PGV	C03-O11-P-O14
15	4C	304	PGV	C02-C03-O11-P
15	4C	305	PGV	C03-O11-P-O12
15	4C	305	PGV	C03-O11-P-O14
15	4C	305	PGV	C02-C03-O11-P
15	4C	305	PGV	O02-C1-O01-C02
15	4C	305	PGV	C2-C1-O01-C02
15	4G	101	PGV	O02-C1-O01-C02
15	4G	101	PGV	C2-C1-O01-C02
15	4G	101	PGV	O04-C19-O03-C01
15	4G	101	PGV	C20-C19-O03-C01
15	4K	101	PGV	C03-O11-P-O12
15	4K	101	PGV	C03-O11-P-O14
15	4K	101	PGV	O04-C19-O03-C01
15	4K	101	PGV	C20-C19-O03-C01
16	4A	604	HEA	C3B-C11-C12-C13
16	4A	604	HEA	O11-C11-C12-C13
20	4B	302	CDL	CA3-OA5-PA1-OA3
20	4B	302	CDL	OA9-CA7-OA8-CA6
20	4B	302	CDL	C31-CA7-OA8-CA6
20	4B	302	CDL	CB3-OB5-PB2-OB2
20	4B	302	CDL	CB3-OB5-PB2-OB3
20	4C	306	CDL	C1-CA2-OA2-PA1
20	4C	306	CDL	OB7-CB5-OB6-CB4
20	4C	306	CDL	C51-CB5-OB6-CB4
20	4C	306	CDL	OB9-CB7-OB8-CB6
20	4C	306	CDL	C71-CB7-OB8-CB6
20	4D	201	CDL	C1-CA2-OA2-PA1
20	4D	201	CDL	CB3-OB5-PB2-OB3
20	4D	201	CDL	OB7-CB5-OB6-CB4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	4D	201	CDL	C51-CB5-OB6-CB4
20	4D	201	CDL	OB9-CB7-OB8-CB6
20	4D	201	CDL	C71-CB7-OB8-CB6
22	4B	304	PSC	C03-O11-P-O12
22	4B	304	PSC	C03-O11-P-O13
22	4B	304	PSC	O02-C1-O01-C02
24	4G	102	PEK	C04-O12-P-O11
24	4G	102	PEK	C04-O12-P-O13
24	4G	103	PEK	O12-C04-C05-N
22	4B	304	PSC	C2-C1-O01-C02
15	4C	305	PGV	C05-C04-O12-P
22	4B	304	PSC	C19-C20-C21-C22
15	4J	101	PGV	C19-C20-C21-C22
15	4A	603	PGV	C05-C04-O12-P
15	4G	101	PGV	C1-C2-C3-C4
15	4L	101	PGV	C1-C2-C3-C4
15	4B	301	PGV	C4-C5-C6-C7
20	4C	306	CDL	O1-C1-CA2-OA2
15	4J	101	PGV	C22-C23-C24-C25
20	4D	201	CDL	C75-C76-C77-C78
15	4L	101	PGV	C2-C3-C4-C5
20	4D	201	CDL	O1-C1-CB2-OB2
20	4B	302	CDL	C59-C60-C61-C62
24	4G	102	PEK	C26-C27-C28-C29
22	4B	304	PSC	C27-C28-C29-C30
22	4B	304	PSC	C22-C23-C24-C25
15	4C	307	PGV	C02-C03-O11-P
15	4C	304	PGV	C24-C25-C26-C27
22	4B	304	PSC	C25-C26-C27-C28
22	4B	304	PSC	C20-C21-C22-C23
20	4D	201	CDL	C38-C39-C40-C41
24	4G	103	PEK	C21-C22-C23-C24
15	4C	305	PGV	O03-C01-C02-O01
15	4B	301	PGV	C27-C28-C29-C30
15	4C	303	PGV	C05-C04-O12-P
20	4C	306	CDL	CB2-C1-CA2-OA2
15	4B	301	PGV	C6-C7-C8-C9
24	4G	102	PEK	C22-C23-C24-C25
15	4C	305	PGV	O03-C01-C02-C03
15	4J	101	PGV	O03-C01-C02-C03
20	4C	306	CDL	C81-C82-C83-C84
15	4L	101	PGV	C5-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
20	4D	201	CDL	C62-C63-C64-C65
15	4C	303	PGV	C5-C6-C7-C8
24	4G	102	PEK	C21-C22-C23-C24
20	4C	306	CDL	C75-C76-C77-C78
20	4D	201	CDL	C14-C15-C16-C17
16	4A	605	HEA	C3B-C11-C12-C13
15	4K	101	PGV	C22-C23-C24-C25
15	4A	603	PGV	C02-C03-O11-P
15	4B	301	PGV	C05-C04-O12-P
15	4K	101	PGV	C02-C03-O11-P
22	4B	304	PSC	C1-C2-C3-C4
24	4G	103	PEK	C23-C24-C25-C26
15	4A	603	PGV	O03-C01-C02-C03
22	4B	304	PSC	O03-C01-C02-C03
20	4C	306	CDL	C59-C60-C61-C62
15	4K	101	PGV	C05-C04-O12-P
20	4B	302	CDL	C1-CA2-OA2-PA1
22	4B	304	PSC	O03-C01-C02-O01
20	4C	306	CDL	C36-C37-C38-C39
15	4B	301	PGV	C2-C3-C4-C5
15	4A	603	PGV	C1-C2-C3-C4
15	4C	305	PGV	C26-C27-C28-C29
20	4C	306	CDL	C51-C52-C53-C54
15	4B	301	PGV	C01-C02-C03-O11
15	4C	304	PGV	C05-C04-O12-P
15	4C	304	PGV	C23-C24-C25-C26
15	4C	302	PGV	C22-C23-C24-C25
20	4C	306	CDL	C16-C17-C18-C19
15	4B	301	PGV	O01-C02-C03-O11
20	4B	302	CDL	OA5-CA3-CA4-OA6
20	4B	302	CDL	CB3-CB4-CB6-OB8
20	4B	302	CDL	OB6-CB4-CB6-OB8
15	4C	303	PGV	C02-C03-O11-P
20	4C	306	CDL	C71-C72-C73-C74
16	4A	604	HEA	C4D-C3D-CAD-CBD
20	4B	302	CDL	OA5-CA3-CA4-CA6
20	4C	306	CDL	C79-C80-C81-C82
15	4K	101	PGV	C3-C4-C5-C6
20	4C	306	CDL	C52-C53-C54-C55
15	4C	301	PGV	C11-C12-C13-C14
15	4M	101	PGV	C9-C10-C11-C12
15	4J	101	PGV	O03-C01-C02-O01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	4A	601	PGV	C03-O11-P-O14
15	4A	603	PGV	C03-O11-P-O13
15	4B	301	PGV	C04-O12-P-O13
15	4C	305	PGV	C04-O12-P-O13
15	4G	101	PGV	C04-O12-P-O14
15	4K	101	PGV	C04-O12-P-O13
15	4L	101	PGV	C03-O11-P-O13
20	4B	302	CDL	CB3-OB5-PB2-OB4
20	4C	306	CDL	CB2-OB2-PB2-OB3
20	4C	306	CDL	CB3-OB5-PB2-OB3
20	4D	201	CDL	CA3-OA5-PA1-OA3
20	4D	201	CDL	CB2-OB2-PB2-OB3
15	4K	101	PGV	C9-C10-C11-C12
20	4C	306	CDL	C11-C12-C13-C14
15	4A	603	PGV	C2-C3-C4-C5
15	4C	305	PGV	C24-C25-C26-C27
15	4B	301	PGV	C1-C2-C3-C4
20	4B	302	CDL	C38-C39-C40-C41
15	4C	304	PGV	C11-C12-C13-C14
15	4G	101	PGV	C11-C12-C13-C14
15	4J	101	PGV	C11-C12-C13-C14
15	4C	304	PGV	O03-C01-C02-O01
16	4A	604	HEA	C2D-C3D-CAD-CBD
15	4C	304	PGV	O03-C19-C20-C21
15	4A	601	PGV	C11-C10-C9-C8
15	4M	101	PGV	C11-C12-C13-C14
15	4C	304	PGV	C3-C4-C5-C6
15	4C	303	PGV	C11-C12-C13-C14
15	4M	101	PGV	C22-C23-C24-C25
15	4M	101	PGV	C3-C4-C5-C6
20	4D	201	CDL	OB6-CB4-CB6-OB8
15	4C	302	PGV	C21-C22-C23-C24
24	4G	103	PEK	C02-C03-O11-P
15	4K	101	PGV	C1-C2-C3-C4
15	4A	601	PGV	O03-C01-C02-C03
16	4A	604	HEA	CAD-CBD-CGD-O2D
22	4B	304	PSC	C5-C6-C7-C8
15	4A	602	PGV	C11-C12-C13-C14
15	4J	101	PGV	C5-C6-C7-C8
20	4C	306	CDL	C38-C39-C40-C41
15	4L	101	PGV	C21-C22-C23-C24
16	4A	605	HEA	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	4M	101	PGV	C01-C02-C03-O11
15	4C	305	PGV	C9-C10-C11-C12
24	4G	102	PEK	O03-C01-C02-O01
24	4G	102	PEK	C6-C7-C8-C9
24	4G	102	PEK	C9-C10-C11-C12
24	4G	103	PEK	C11-C12-C13-C14
16	4A	604	HEA	CAD-CBD-CGD-O1D
16	4A	605	HEA	CAD-CBD-CGD-O2D
15	4J	101	PGV	C2-C3-C4-C5
16	4A	605	HEA	C26-C15-C16-C17
15	4K	101	PGV	C5-C6-C7-C8
16	4A	605	HEA	C2A-CAA-CBA-CGA
20	4D	201	CDL	C12-C13-C14-C15
16	4A	604	HEA	C19-C20-C21-C22
15	4A	603	PGV	C5-C6-C7-C8
20	4C	306	CDL	C72-C73-C74-C75
24	4G	103	PEK	O01-C02-C03-O11
15	4C	304	PGV	C9-C10-C11-C12
15	4K	101	PGV	C11-C12-C13-C14
20	4B	302	CDL	C12-C11-CA5-OA6
24	4G	103	PEK	C01-C02-C03-O11
20	4D	201	CDL	C73-C74-C75-C76
20	4C	306	CDL	C18-C19-C20-C21
22	4B	304	PSC	C2-C3-C4-C5
16	4A	604	HEA	C26-C15-C16-C17
24	4G	103	PEK	O03-C21-C22-C23
15	4C	303	PGV	C14-C15-C16-C17
15	4C	305	PGV	C6-C7-C8-C9
15	4A	603	PGV	C24-C25-C26-C27
15	4J	101	PGV	C9-C10-C11-C12
15	4C	304	PGV	C29-C30-C31-C32
15	4C	305	PGV	C4-C5-C6-C7
20	4B	302	CDL	C60-C61-C62-C63
15	4A	601	PGV	C9-C10-C11-C12
15	4C	307	PGV	C11-C12-C13-C14
15	4C	302	PGV	C24-C25-C26-C27
15	4A	602	PGV	C6-C7-C8-C9
15	4L	101	PGV	C24-C25-C26-C27
20	4C	306	CDL	C22-C23-C24-C25
22	4B	304	PSC	O03-C19-C20-C21
15	4L	101	PGV	C9-C10-C11-C12
15	4A	602	PGV	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
15	4M	101	PGV	C27-C28-C29-C30
24	4G	103	PEK	C22-C23-C24-C25
24	4G	102	PEK	C14-C15-C16-C17
15	4C	307	PGV	C5-C6-C7-C8
15	4C	304	PGV	C02-C01-O03-C19
22	4B	304	PSC	C24-C25-C26-C27
15	4A	603	PGV	C20-C21-C22-C23
15	4A	602	PGV	C28-C29-C30-C31
15	4A	601	PGV	O03-C19-C20-C21
15	4C	305	PGV	O03-C19-C20-C21
15	4M	101	PGV	C20-C21-C22-C23
15	4A	602	PGV	C2-C3-C4-C5
24	4G	102	PEK	C23-C24-C25-C26
20	4C	306	CDL	CA2-C1-CB2-OB2
15	4C	304	PGV	C01-C02-O01-C1
15	4J	101	PGV	C6-C7-C8-C9
15	4C	304	PGV	C21-C22-C23-C24
15	4A	603	PGV	C26-C27-C28-C29
15	4C	303	PGV	C2-C3-C4-C5
15	4C	307	PGV	C14-C15-C16-C17
15	4B	301	PGV	C23-C24-C25-C26
15	4J	101	PGV	C26-C27-C28-C29
22	4B	304	PSC	O04-C19-C20-C21
15	4C	305	PGV	O04-C19-C20-C21
16	4A	605	HEA	CAA-CBA-CGA-O2A
15	4K	101	PGV	C2-C3-C4-C5
15	4M	101	PGV	O01-C1-C2-C3
16	4A	605	HEA	CAA-CBA-CGA-O1A
15	4A	601	PGV	O04-C19-C20-C21

There are no ring outliers.

24 monomers are involved in 158 short contacts:

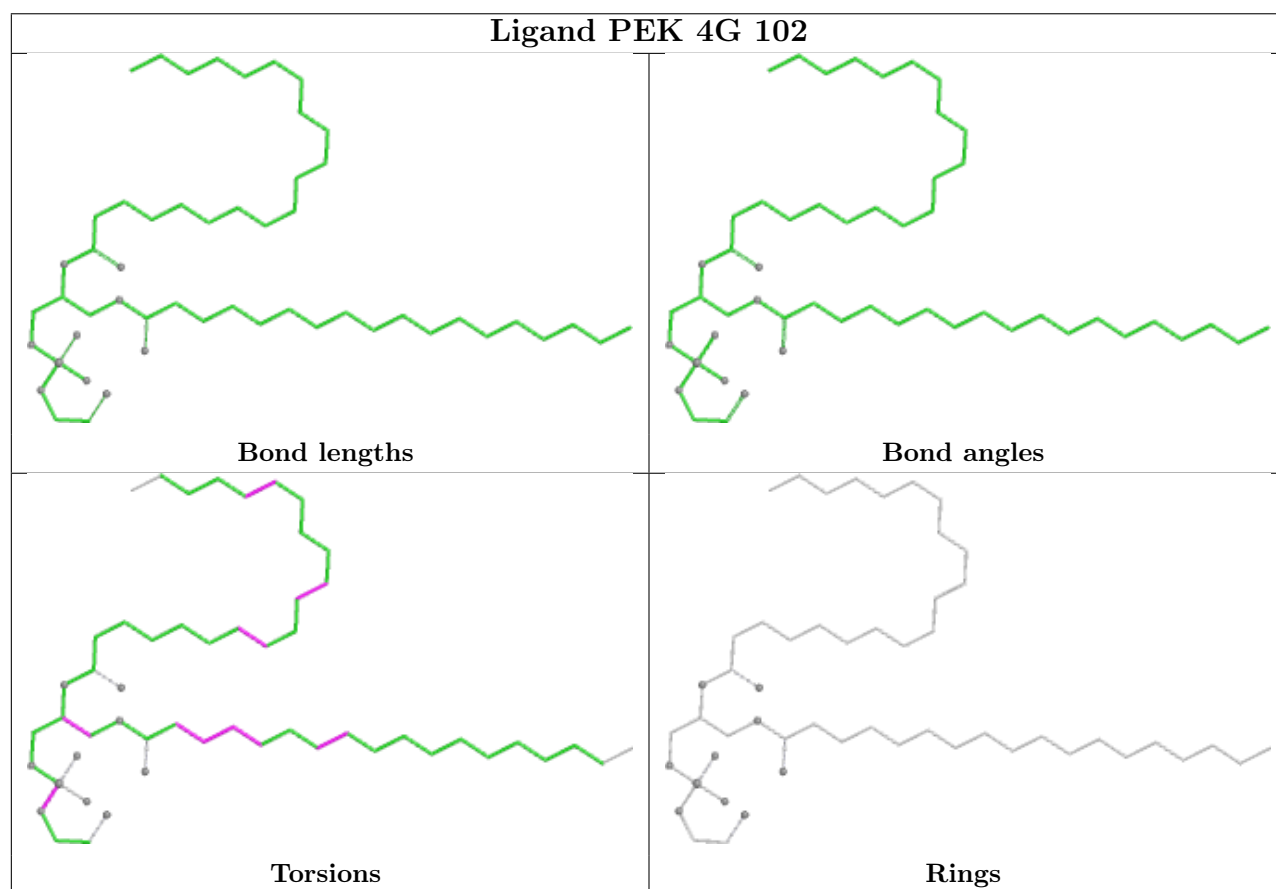
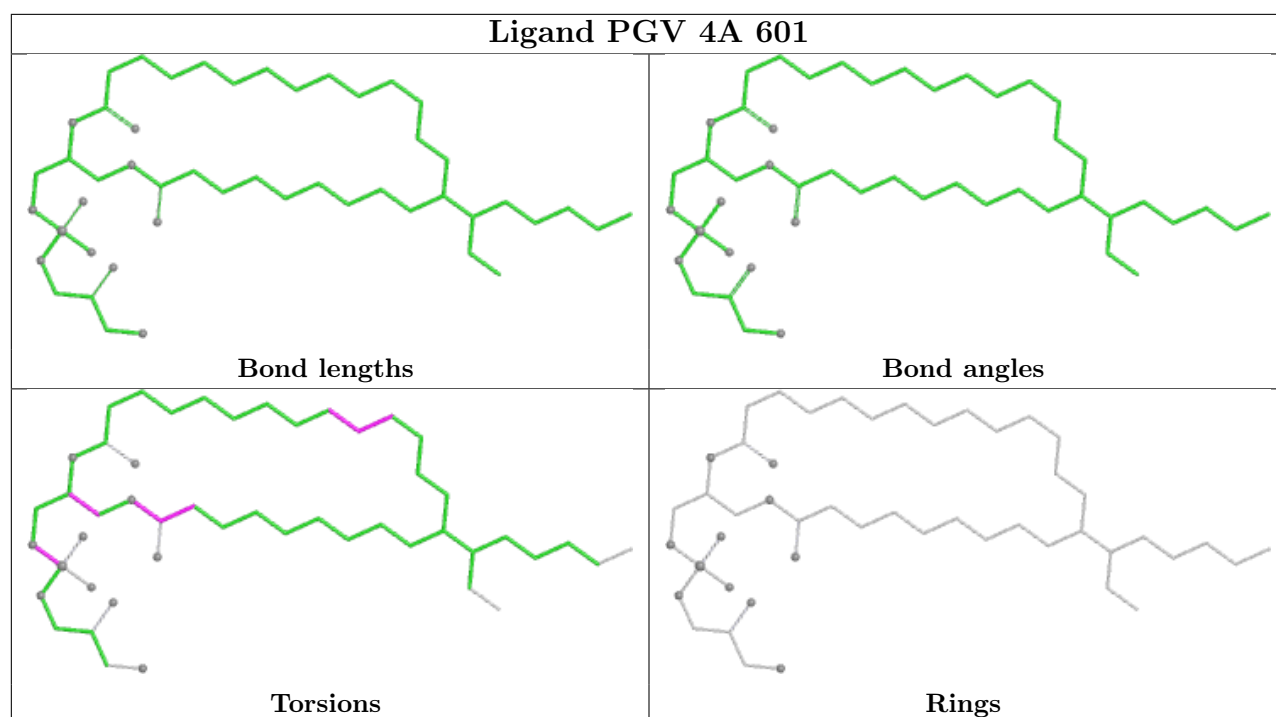
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	4A	601	PGV	9	0
24	4G	102	PEK	4	0
22	4B	304	PSC	9	0
16	4A	604	HEA	6	0
15	4C	302	PGV	6	0
15	4G	101	PGV	5	0
20	4C	306	CDL	14	0
15	4C	305	PGV	4	0

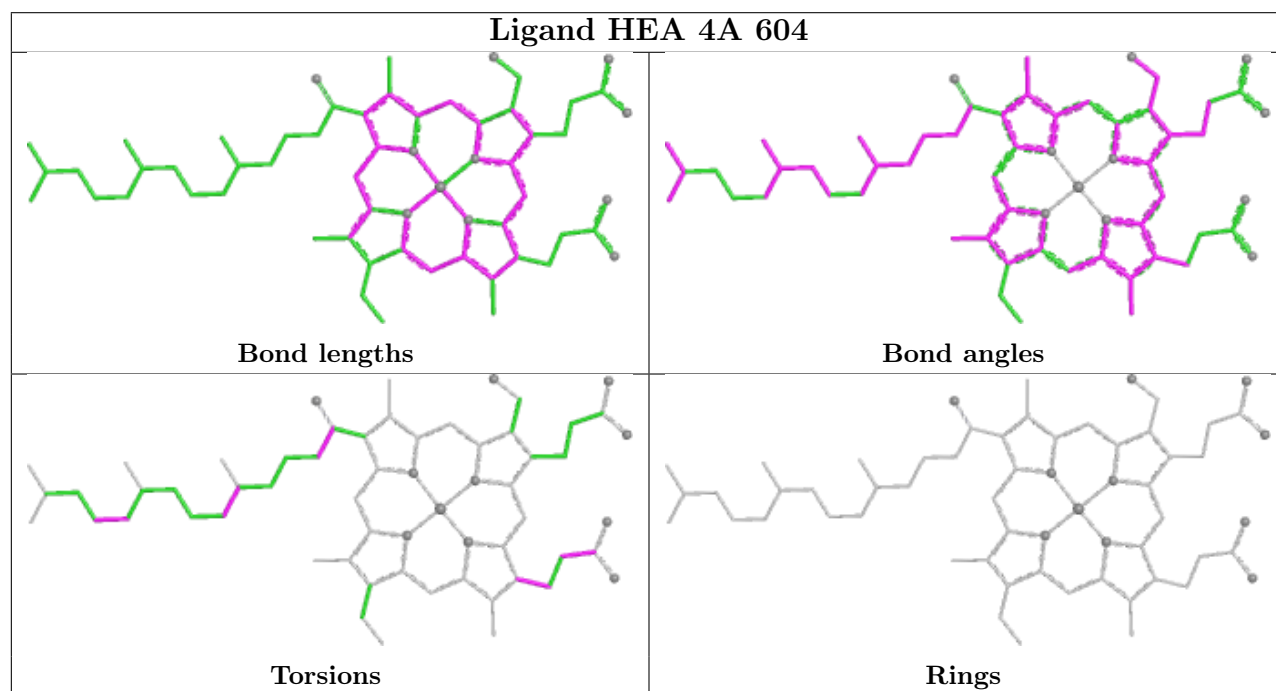
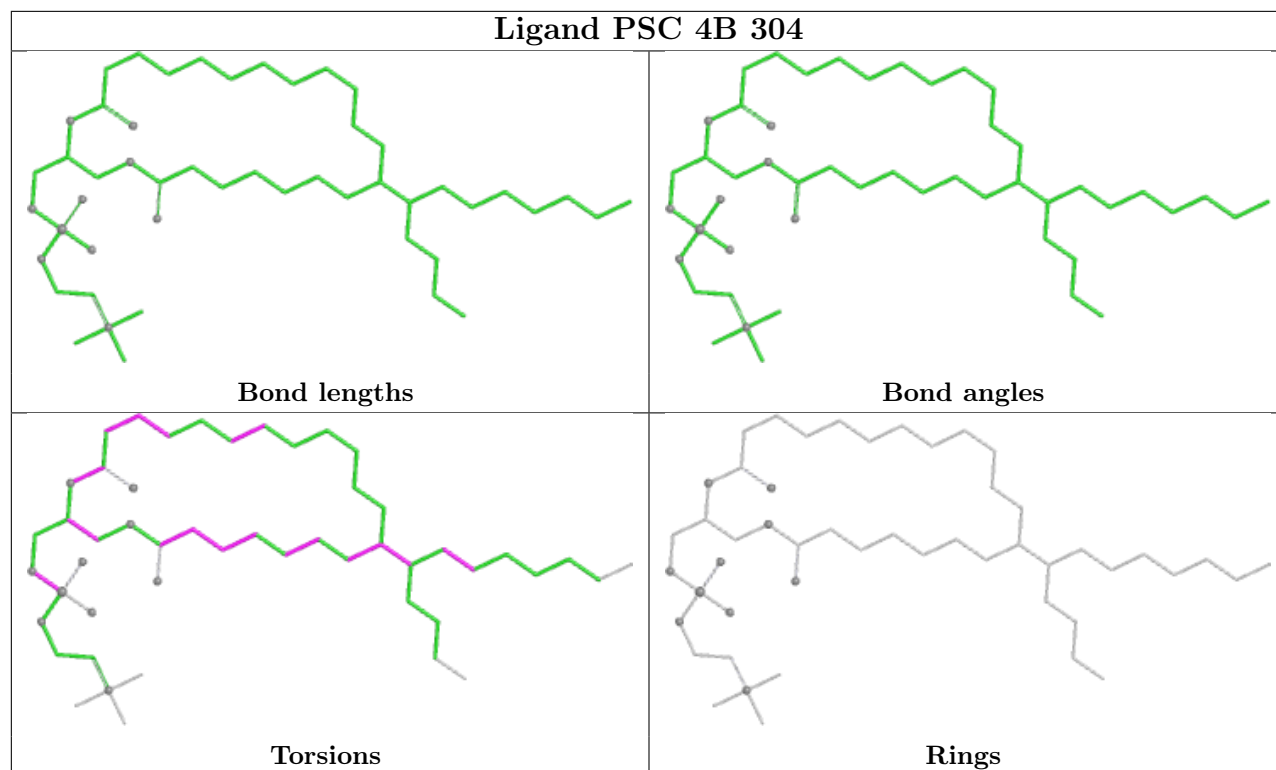
Continued on next page...

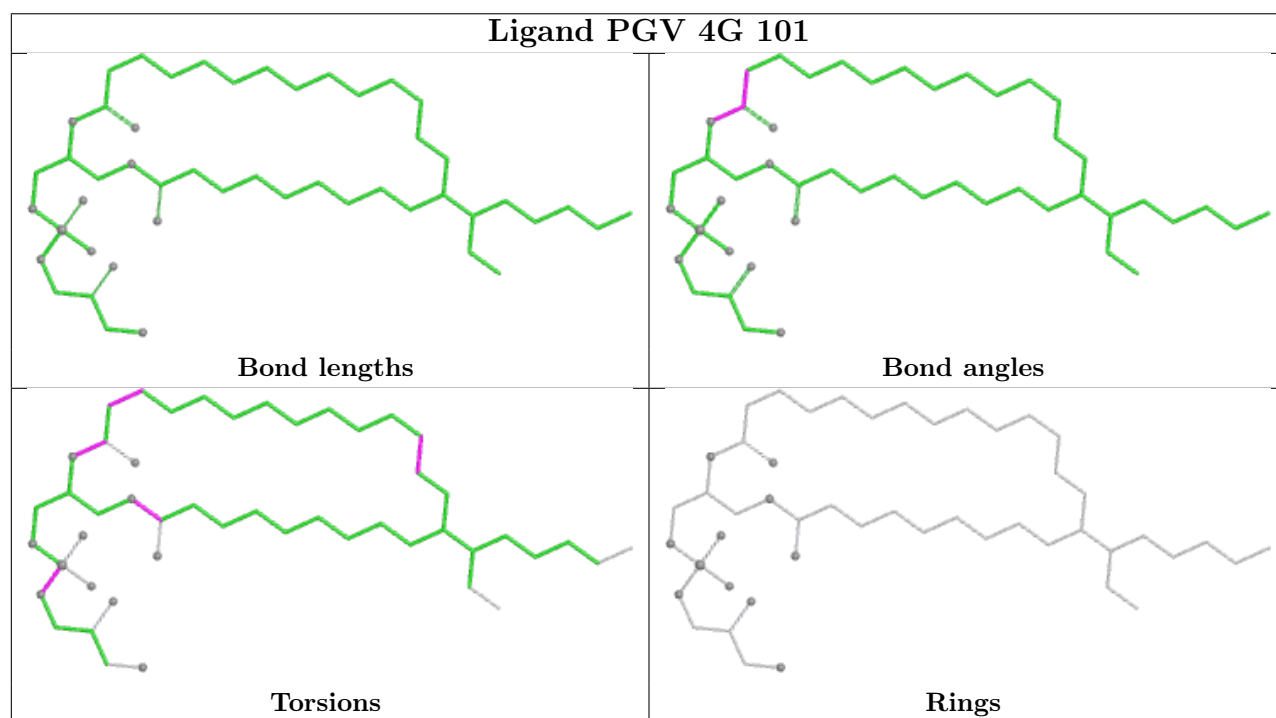
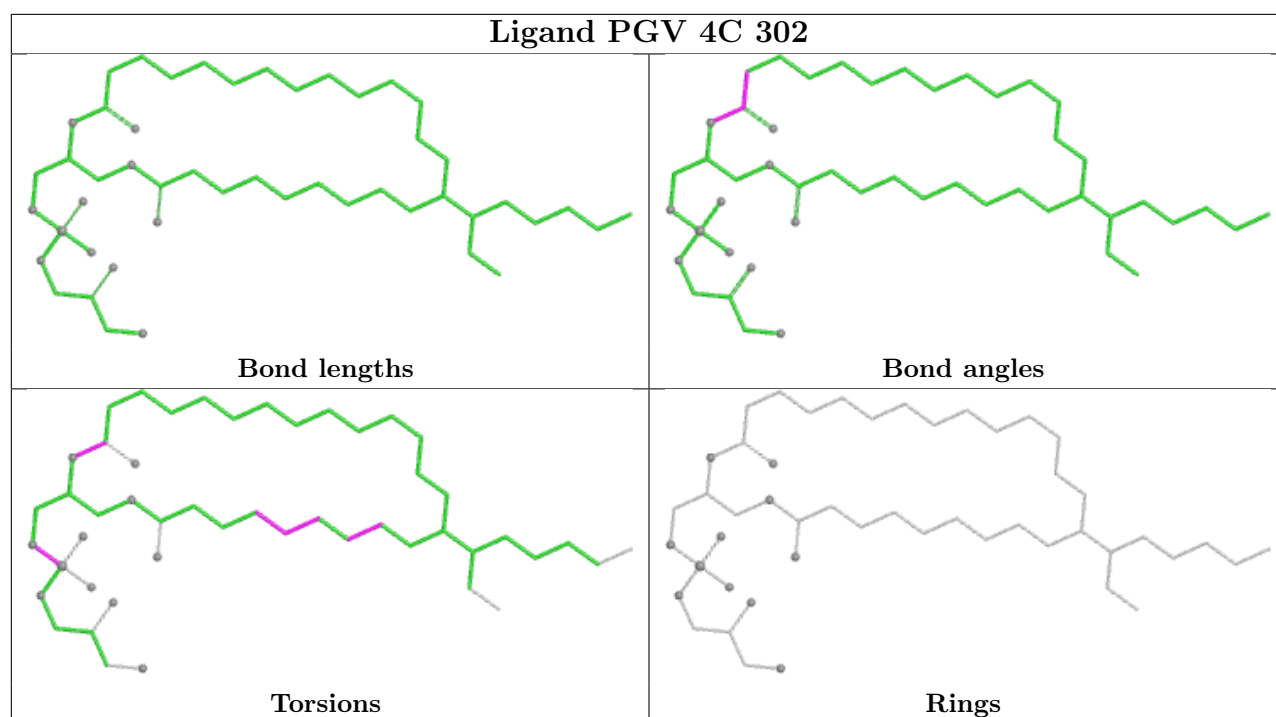
Continued from previous page...

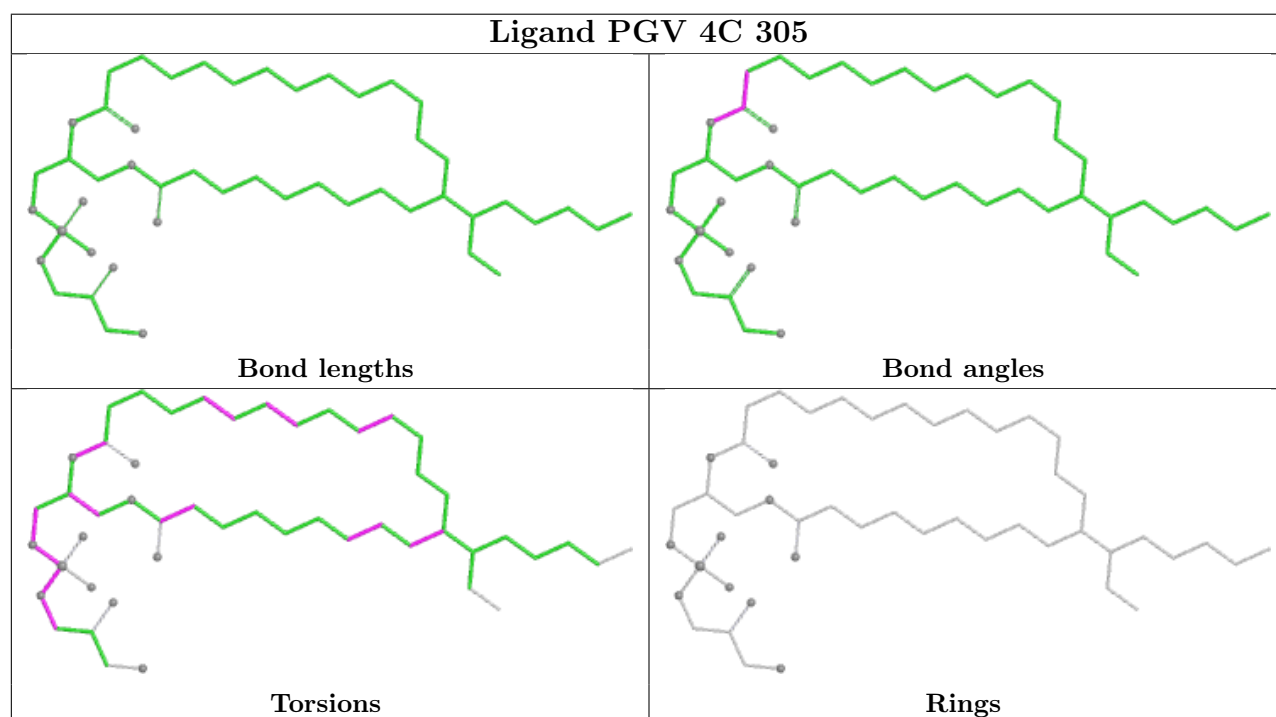
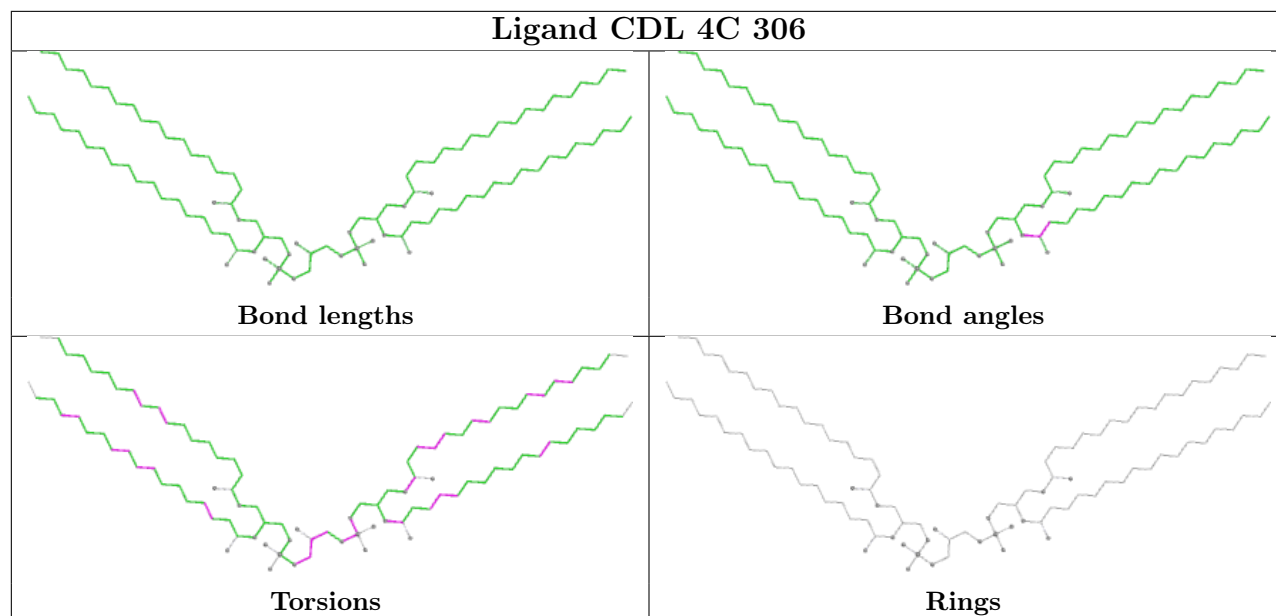
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	4K	101	PGV	6	0
15	4C	304	PGV	11	0
15	4C	303	PGV	7	0
24	4G	103	PEK	5	0
15	4M	101	PGV	5	0
15	4L	101	PGV	10	0
15	4A	602	PGV	7	0
16	4A	605	HEA	1	0
21	4B	303	CUA	2	0
15	4A	603	PGV	6	0
15	4J	101	PGV	3	0
15	4B	301	PGV	12	0
15	4C	307	PGV	10	0
20	4B	302	CDL	9	0
20	4D	201	CDL	20	0
15	4C	301	PGV	4	0

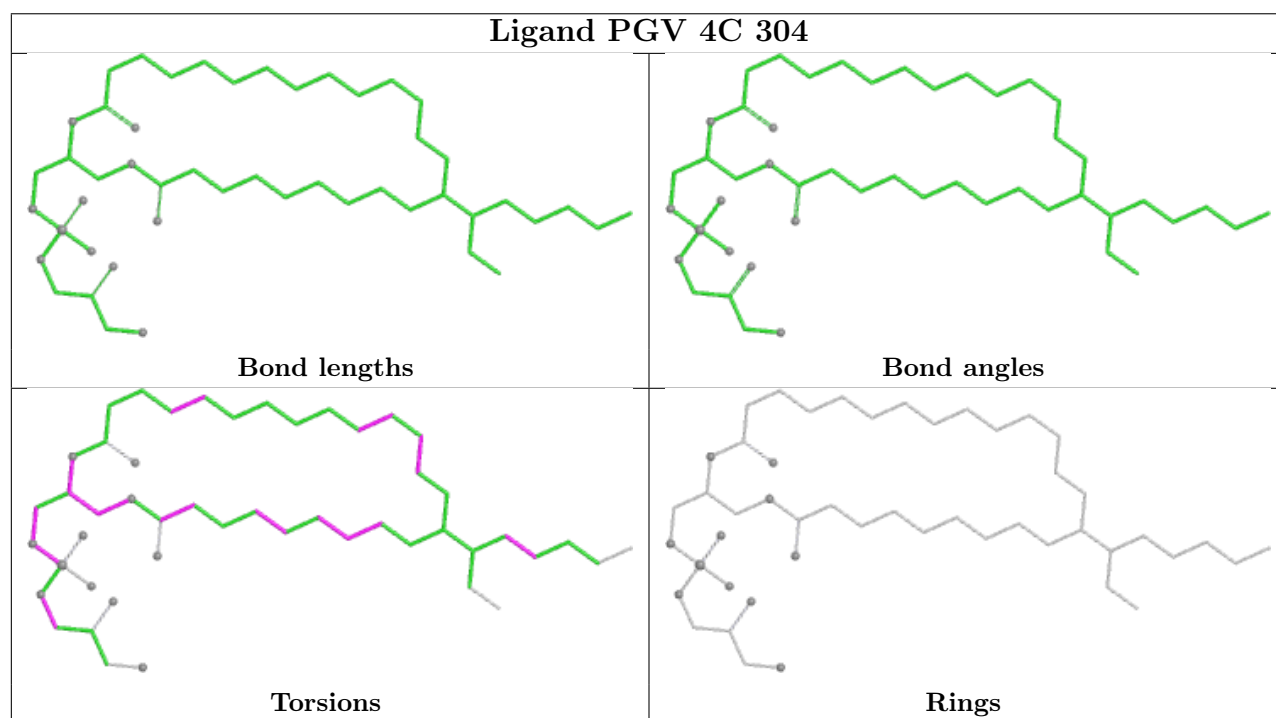
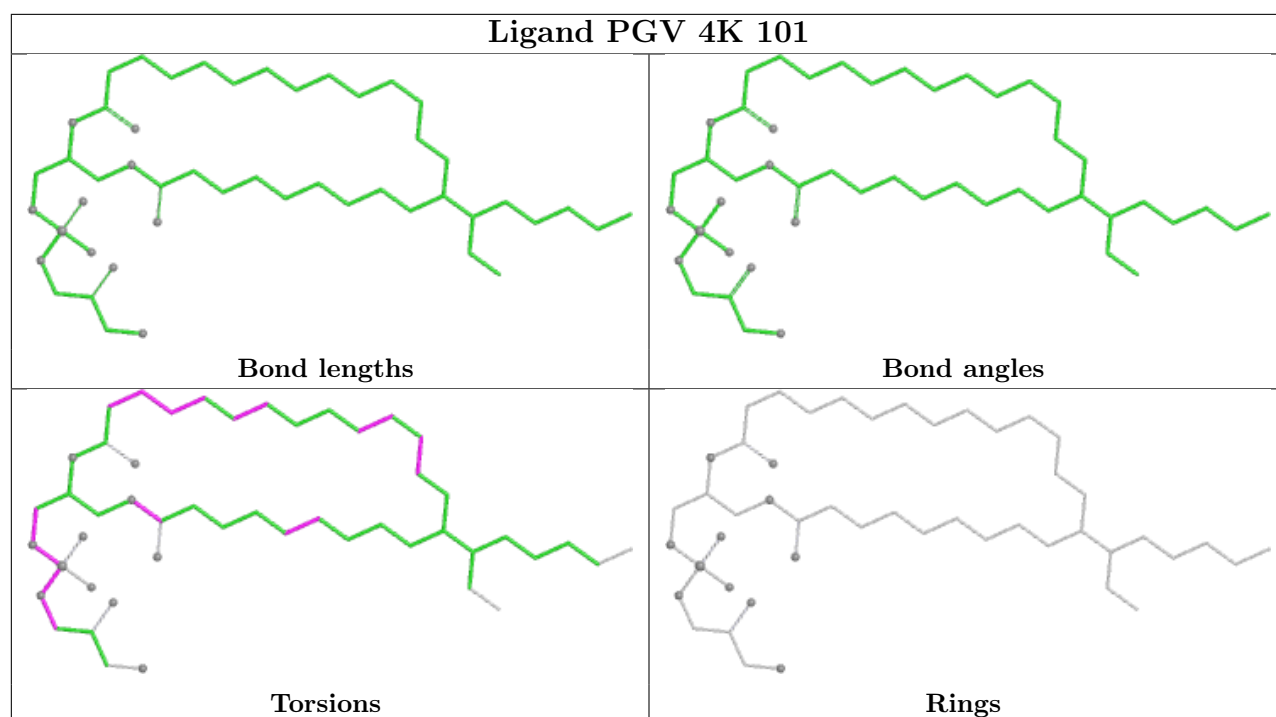
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

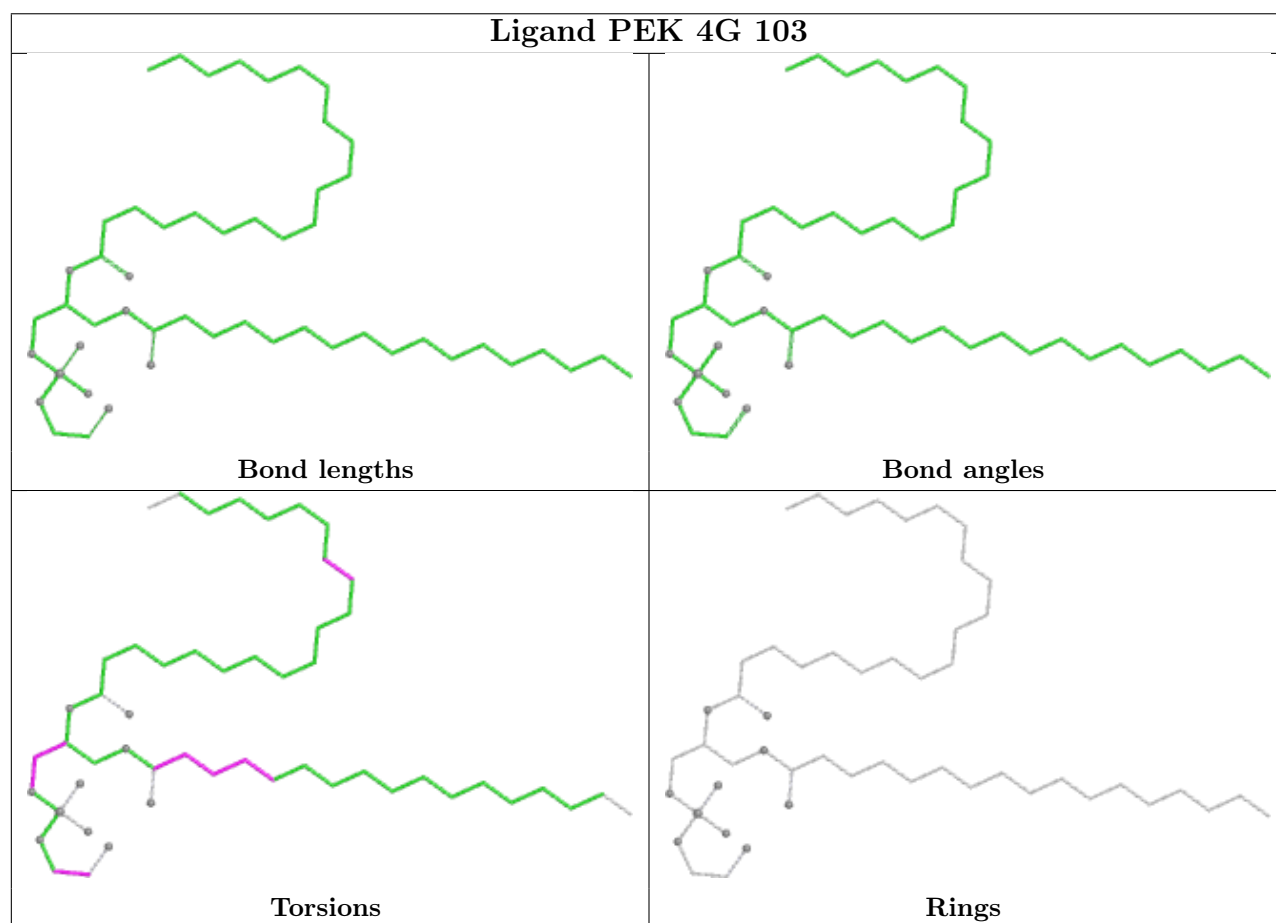
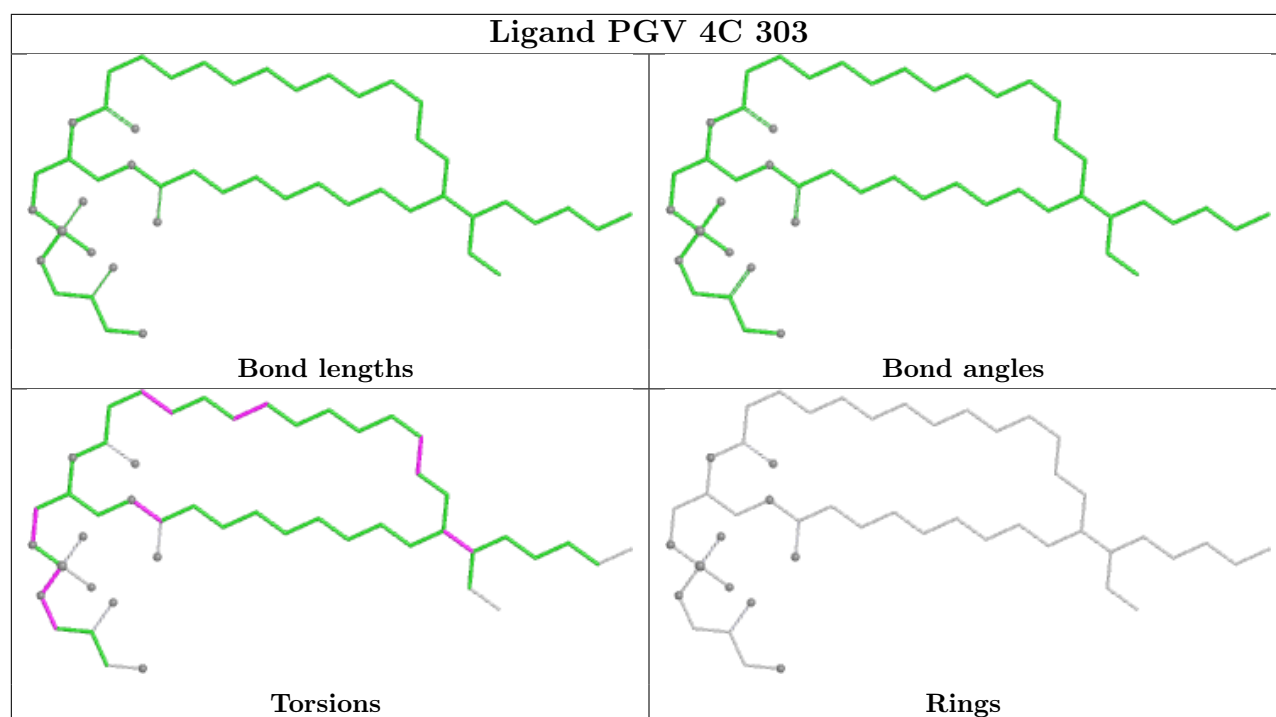


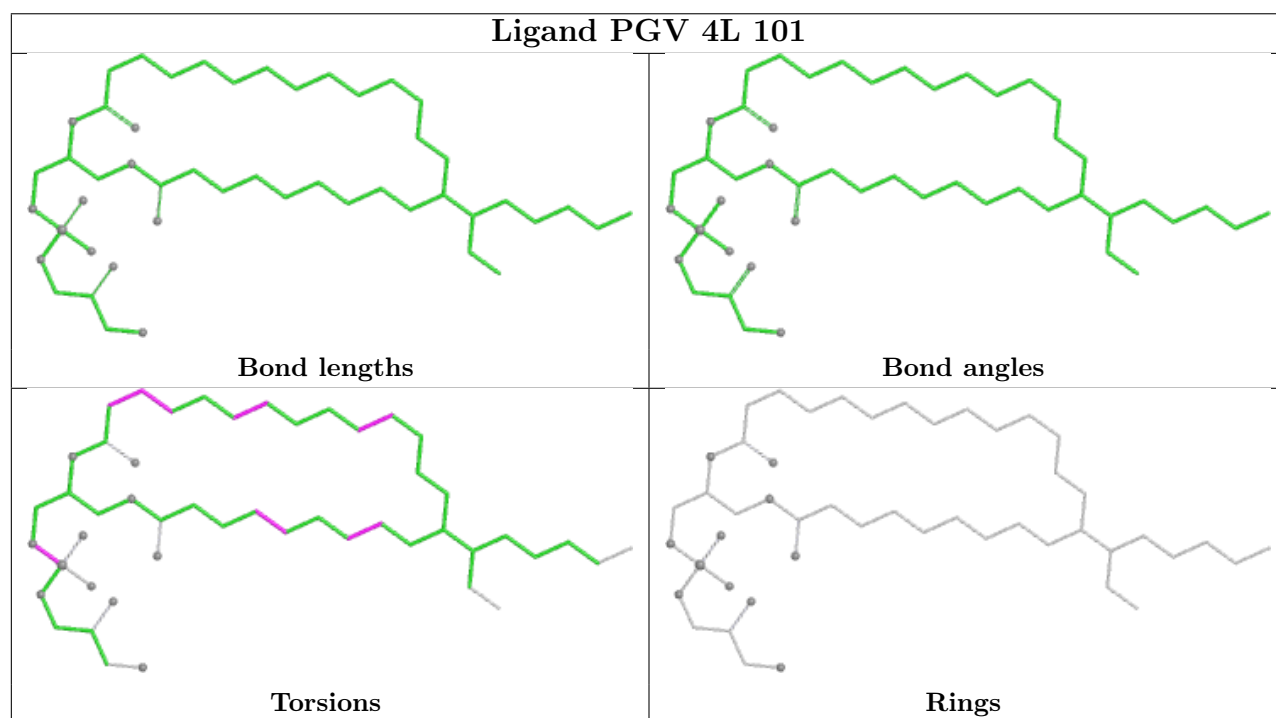
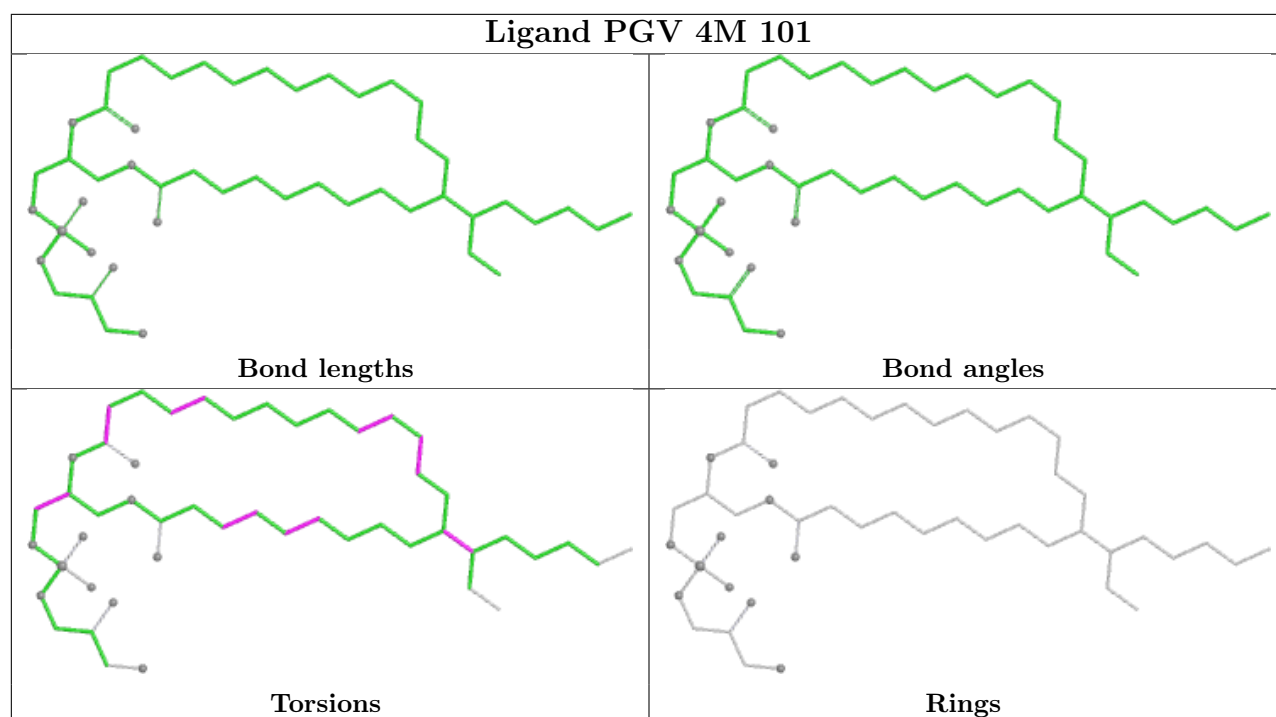


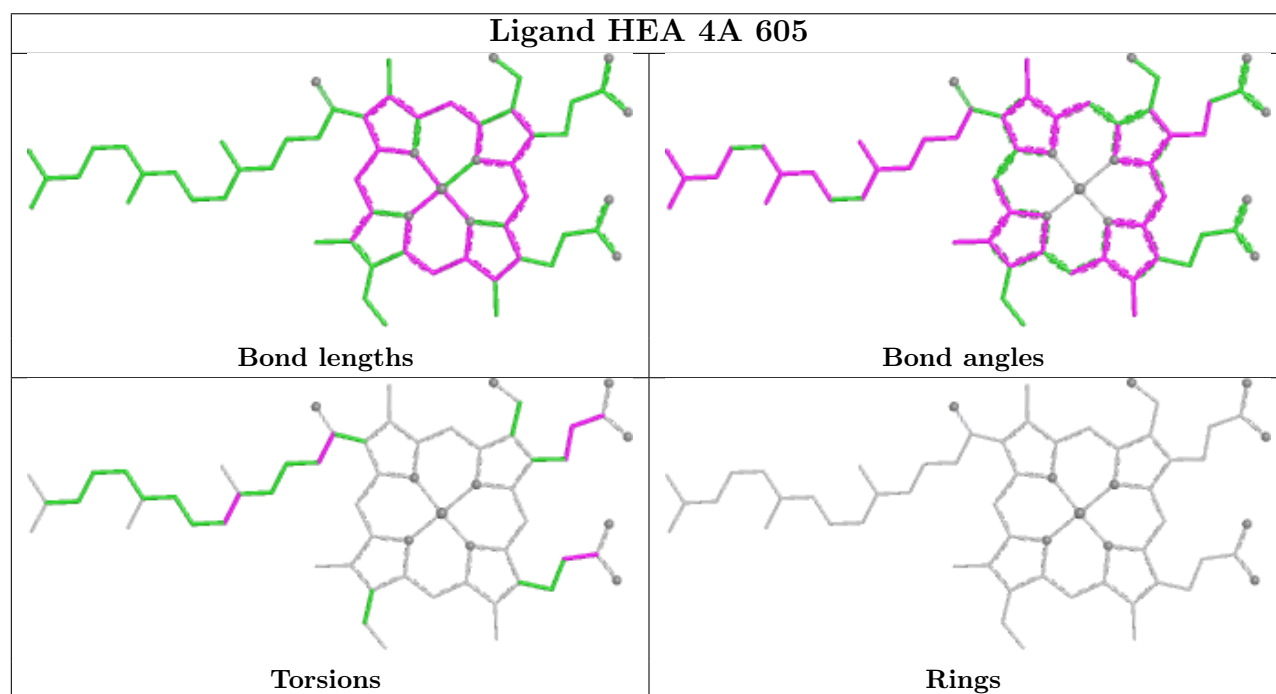
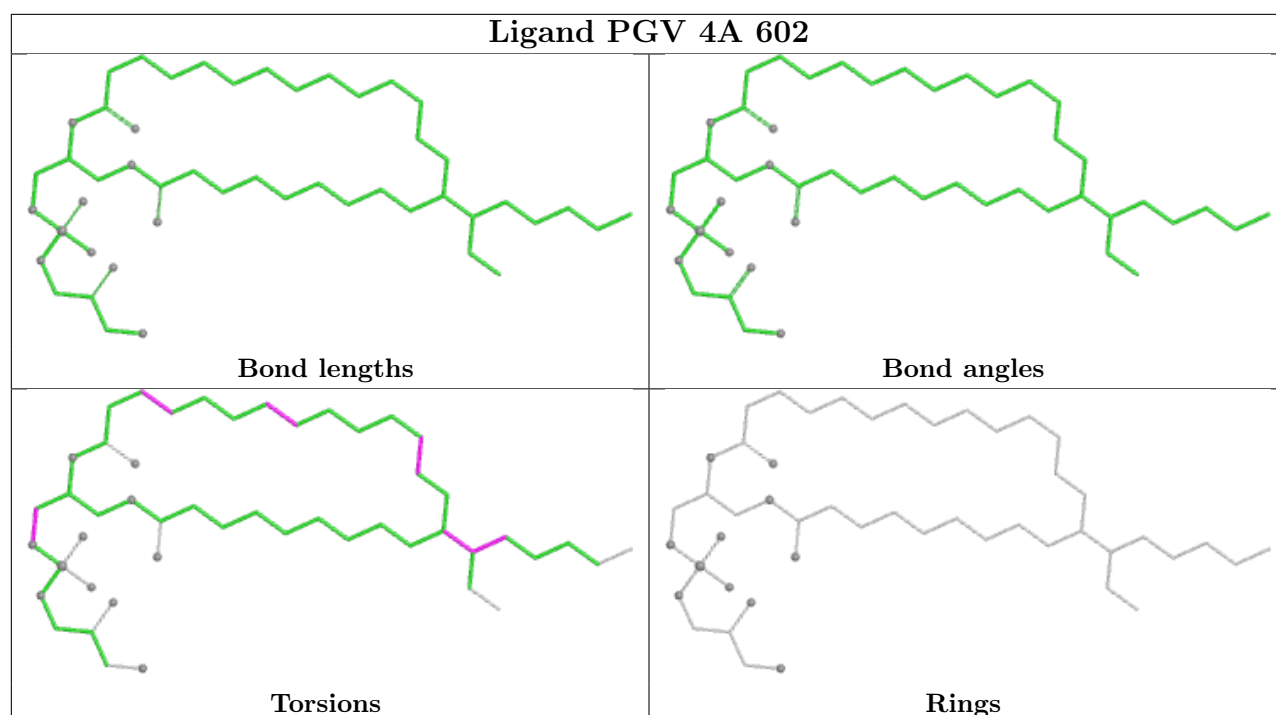


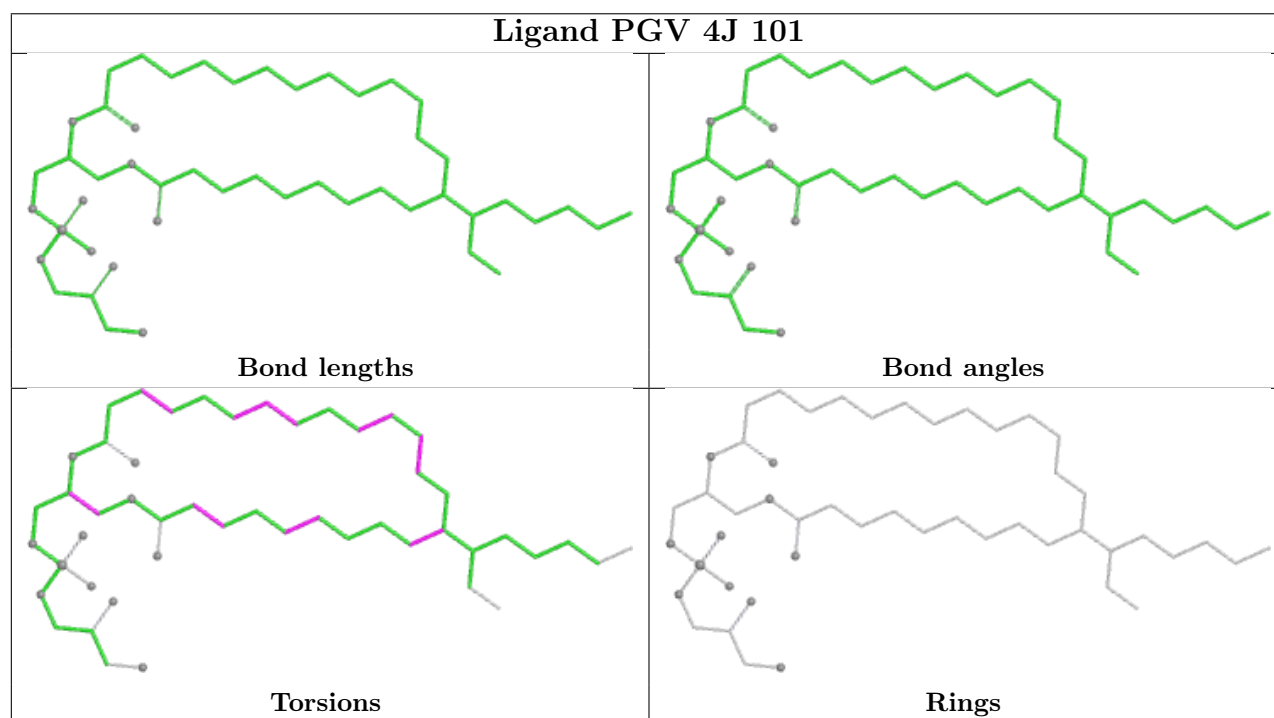
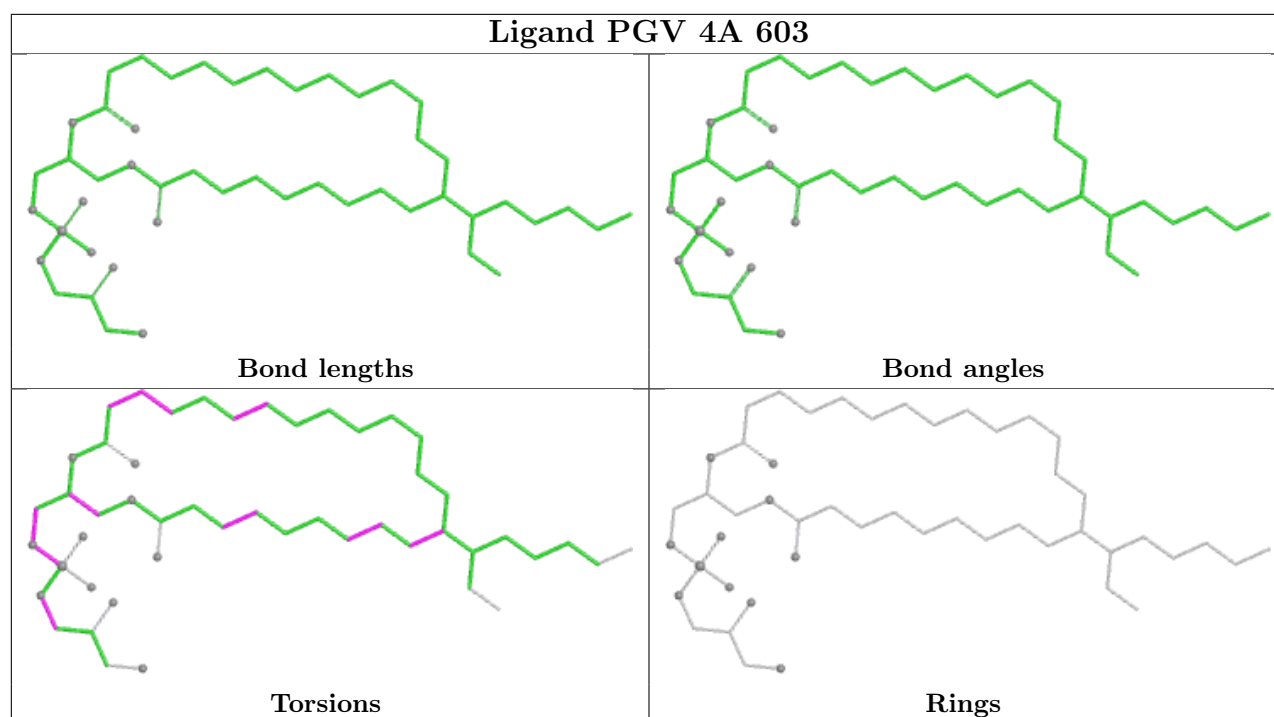


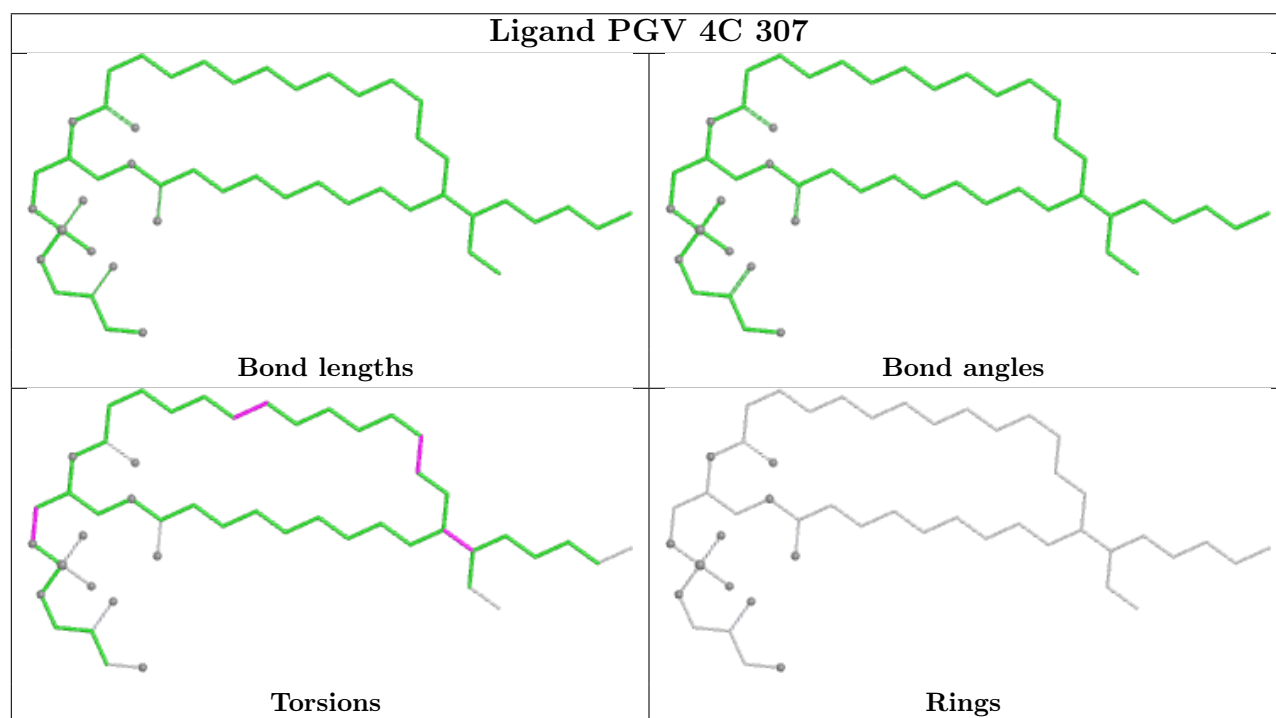
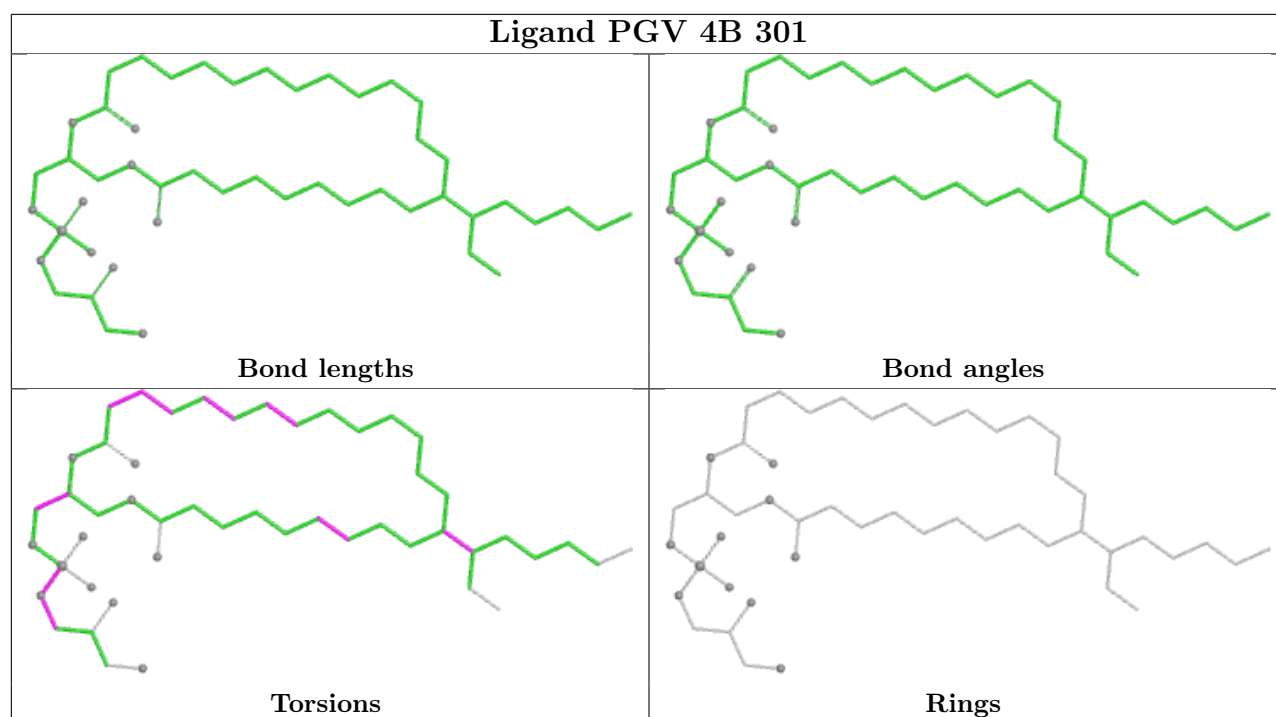


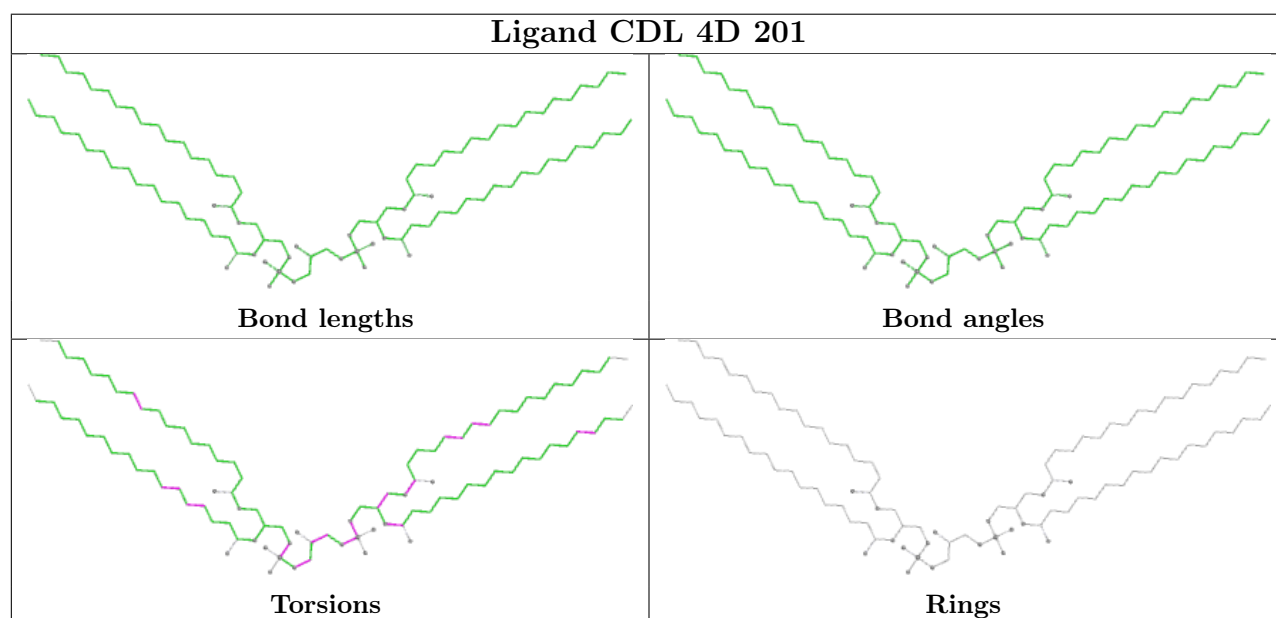
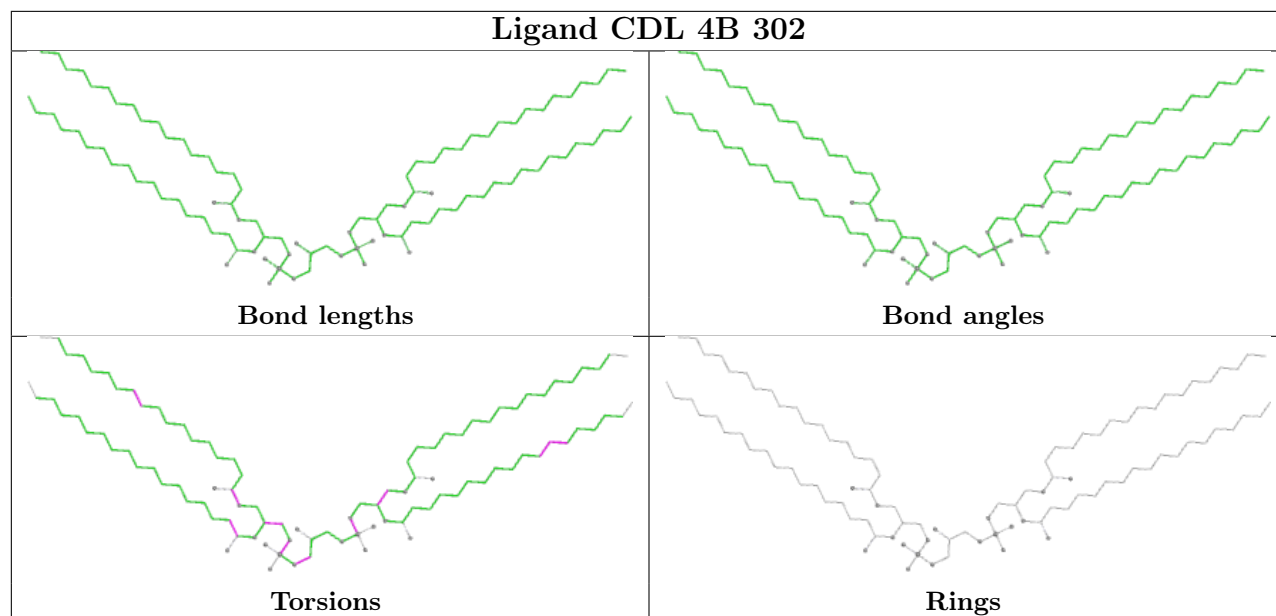


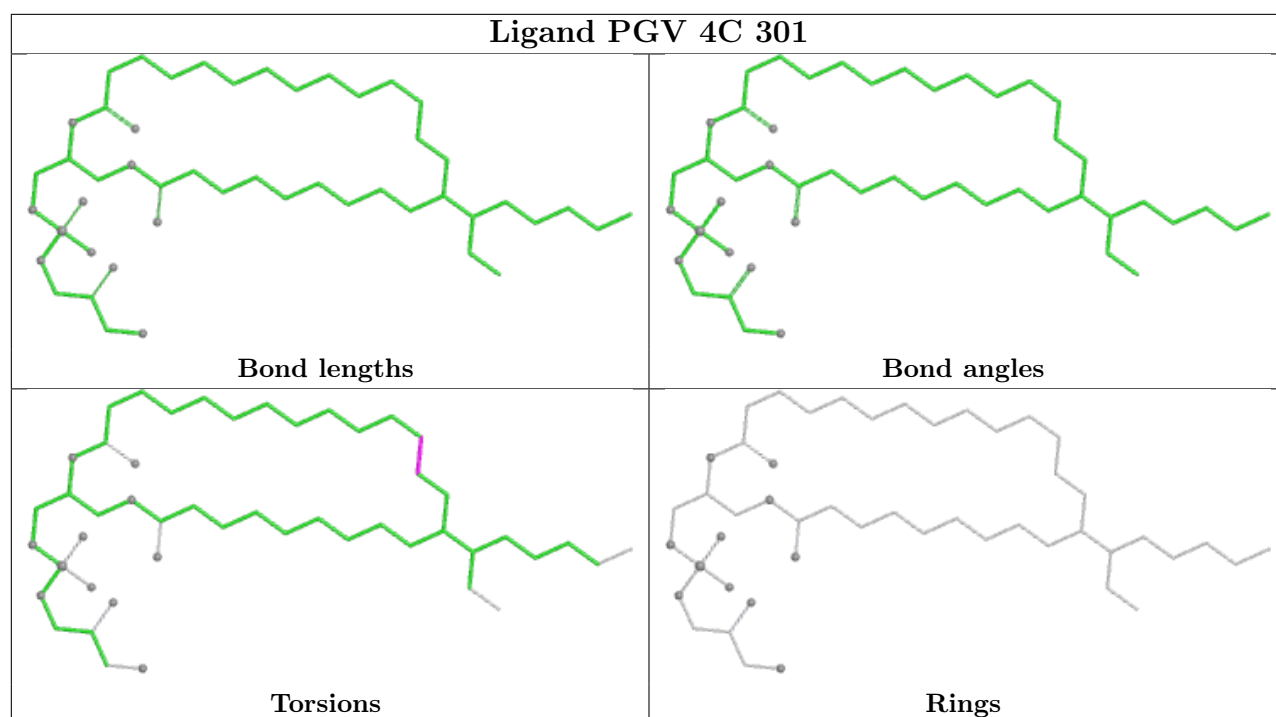












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

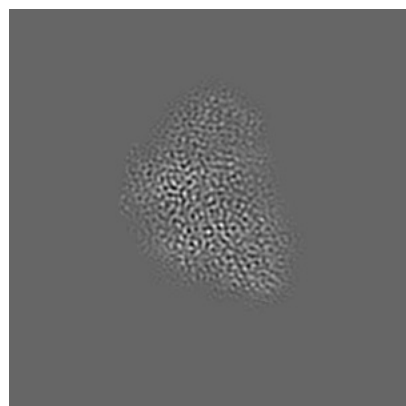
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42229. These allow visual inspection of the internal detail of the map and identification of artifacts.

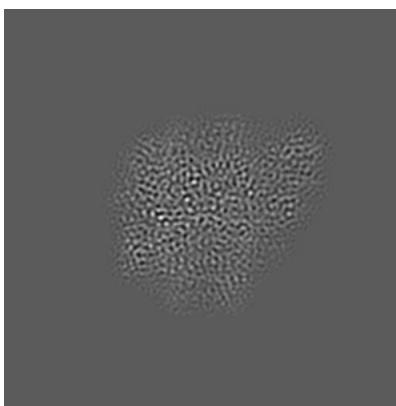
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

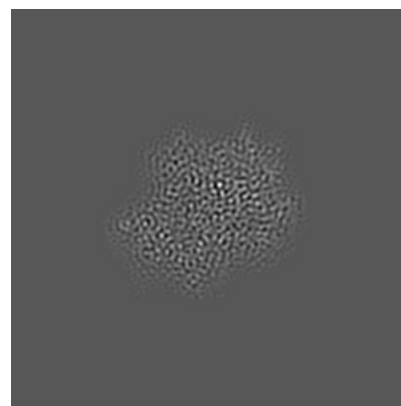
6.1.1 Primary map



X



Y



Z

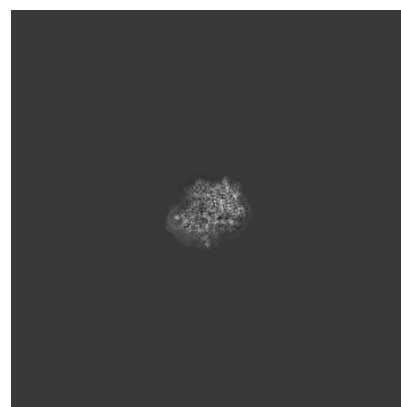
6.1.2 Raw map



X



Y

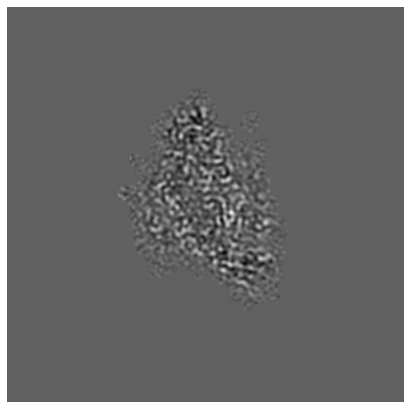


Z

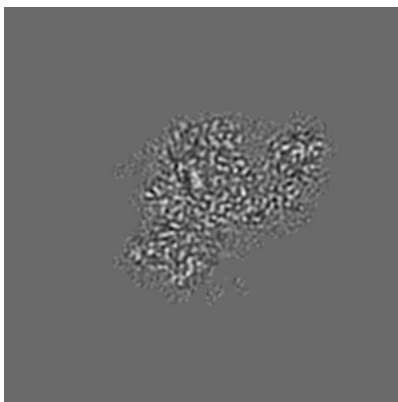
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

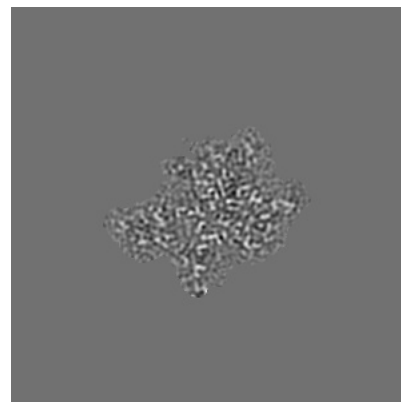
6.2.1 Primary map



X Index: 256

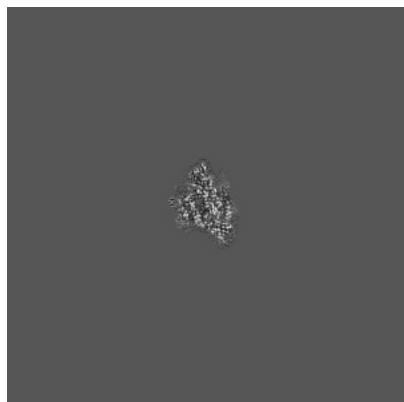


Y Index: 256

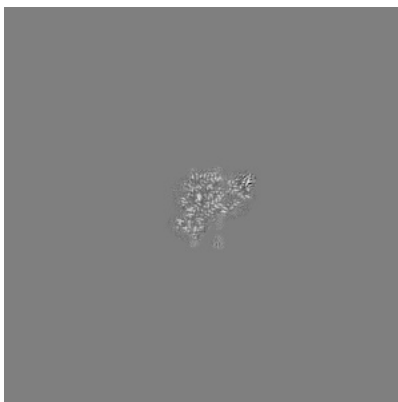


Z Index: 256

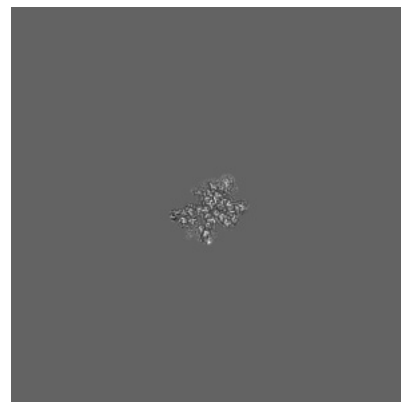
6.2.2 Raw map



X Index: 256



Y Index: 256

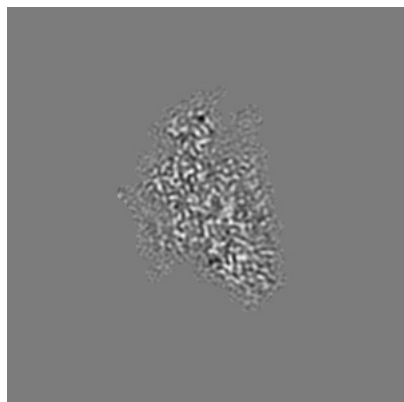


Z Index: 256

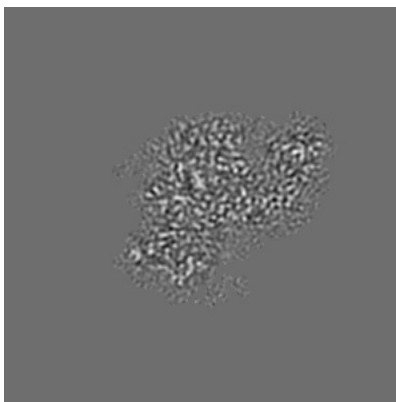
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

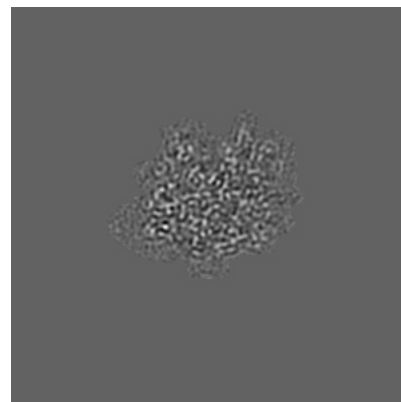
6.3.1 Primary map



X Index: 268

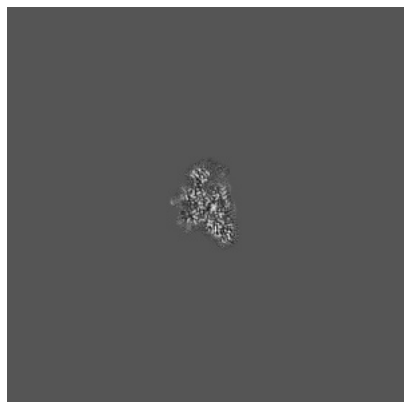


Y Index: 255

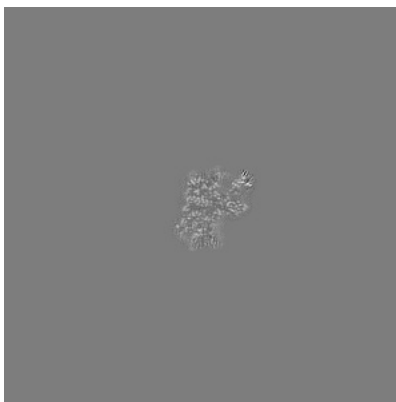


Z Index: 207

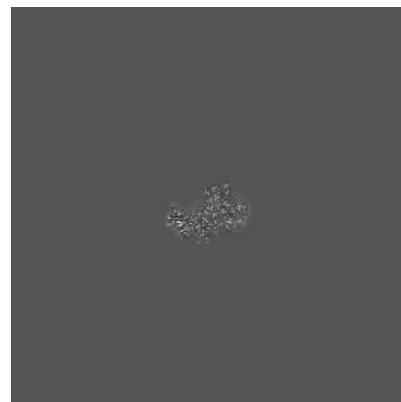
6.3.2 Raw map



X Index: 261



Y Index: 250

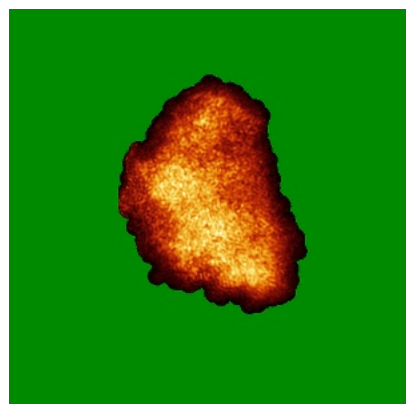


Z Index: 270

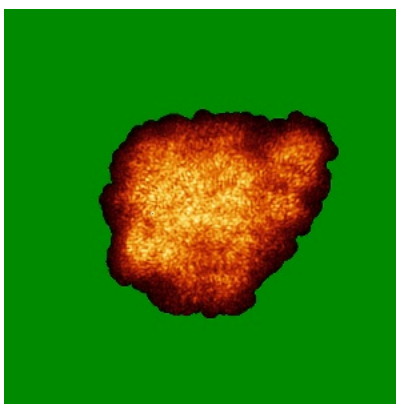
The images above show the largest variance slices of the map in three orthogonal directions.

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

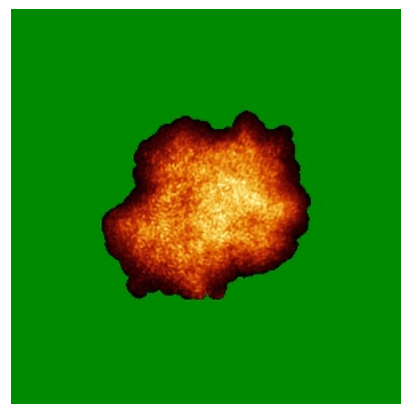
6.4.1 Primary map



X

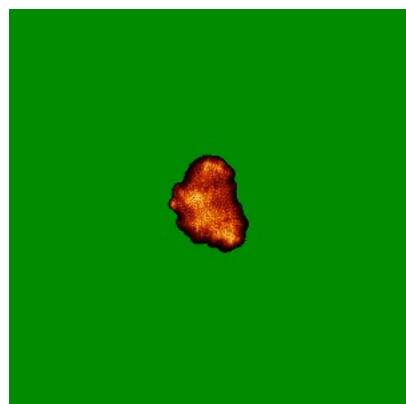


Y

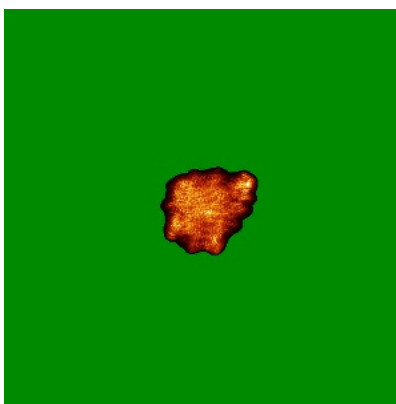


Z

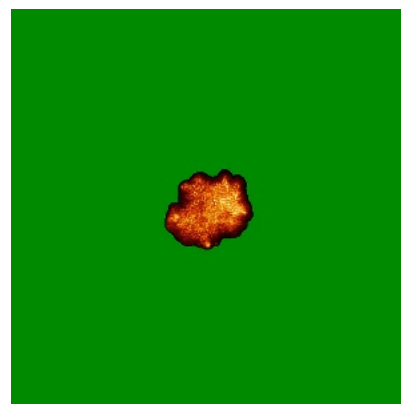
6.4.2 Raw map



X



Y

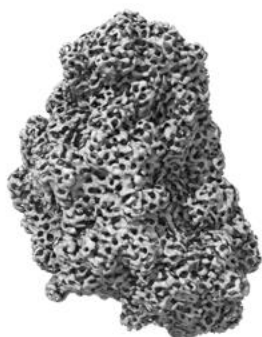


Z

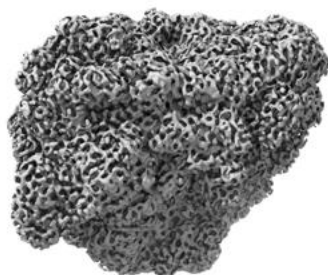
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



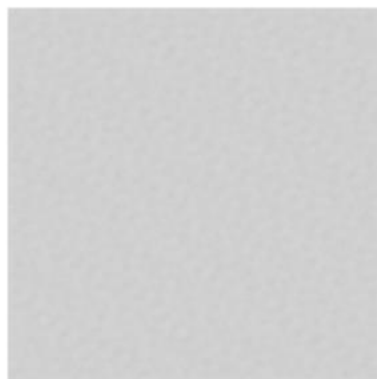
Z

The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

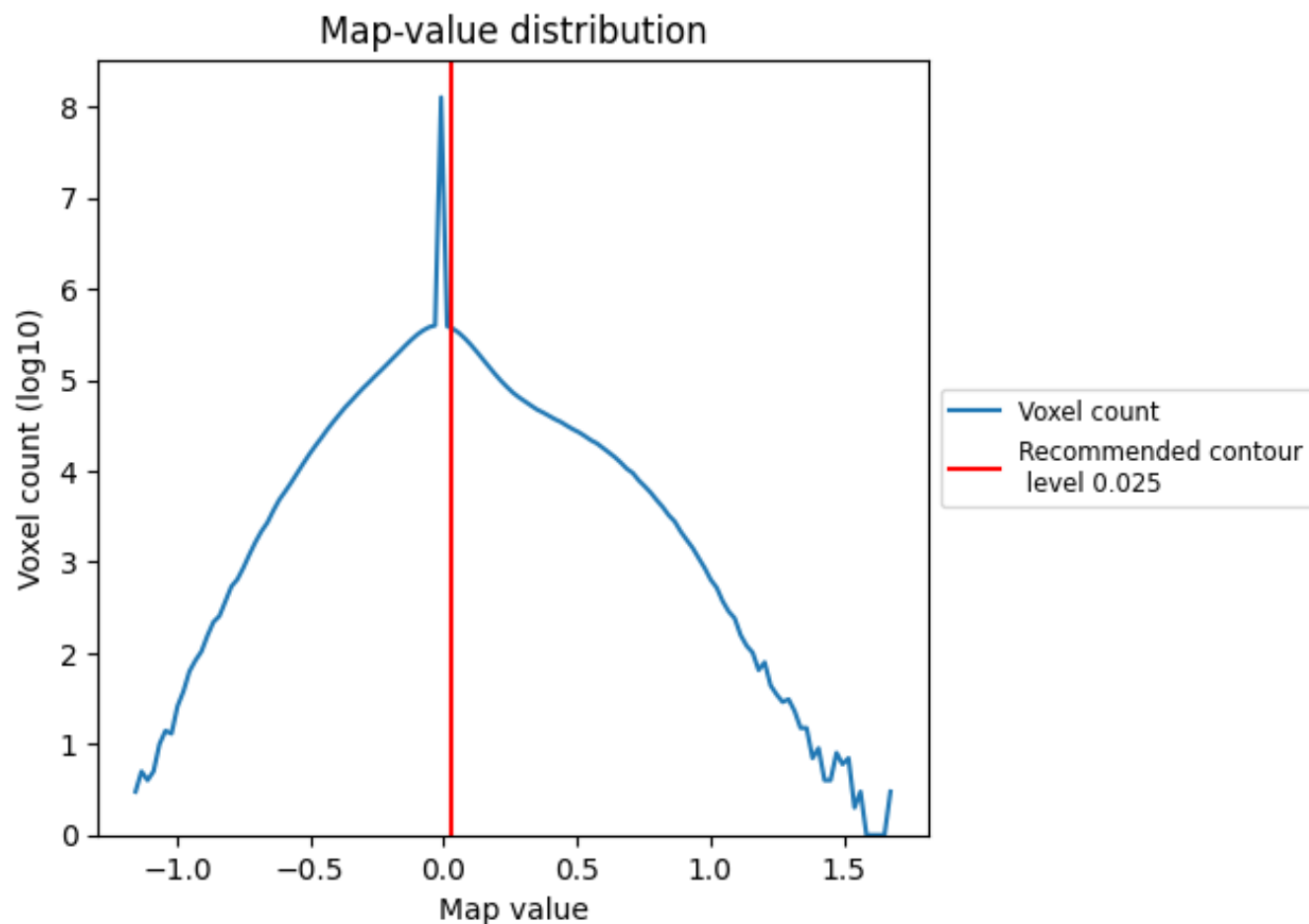
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

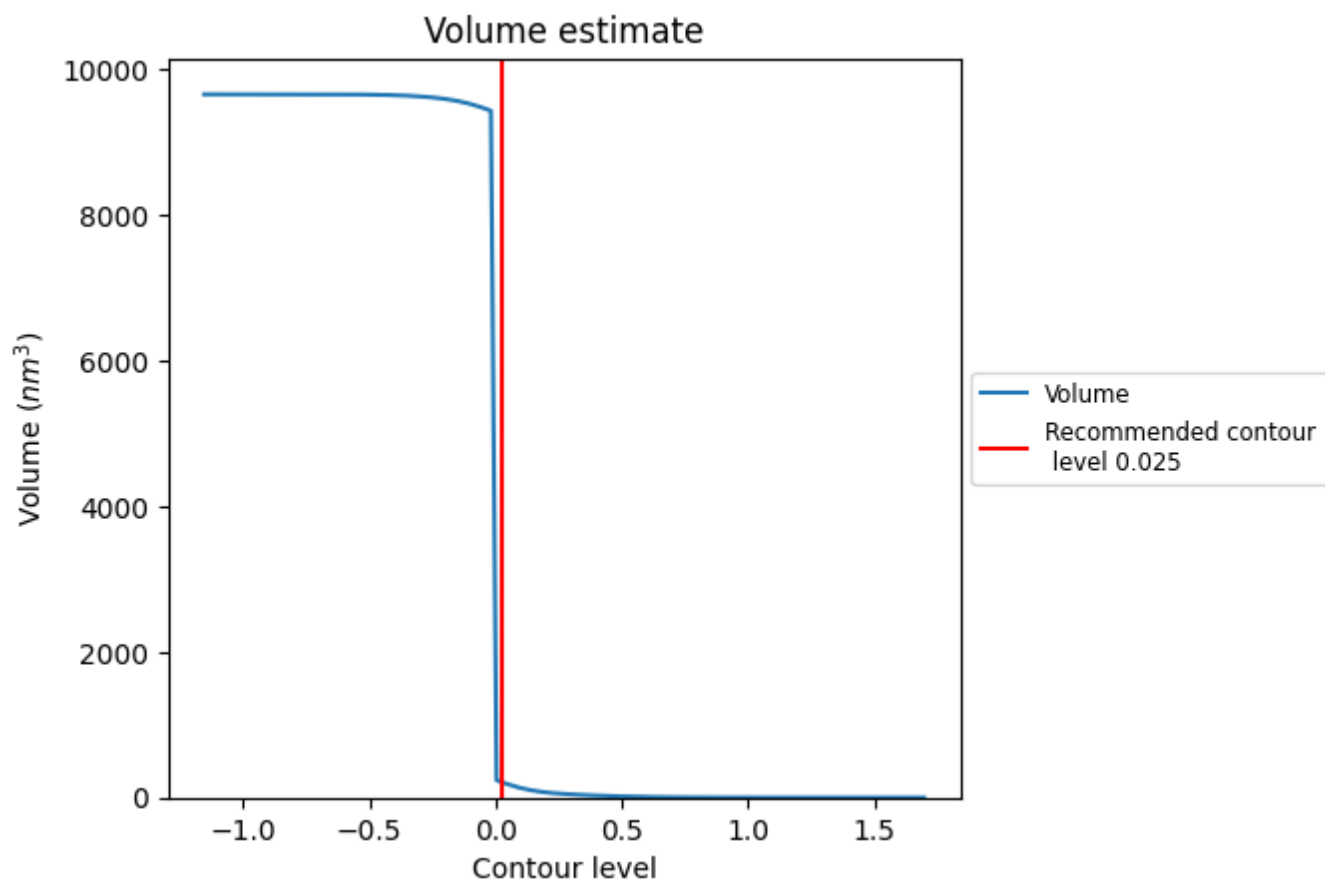
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

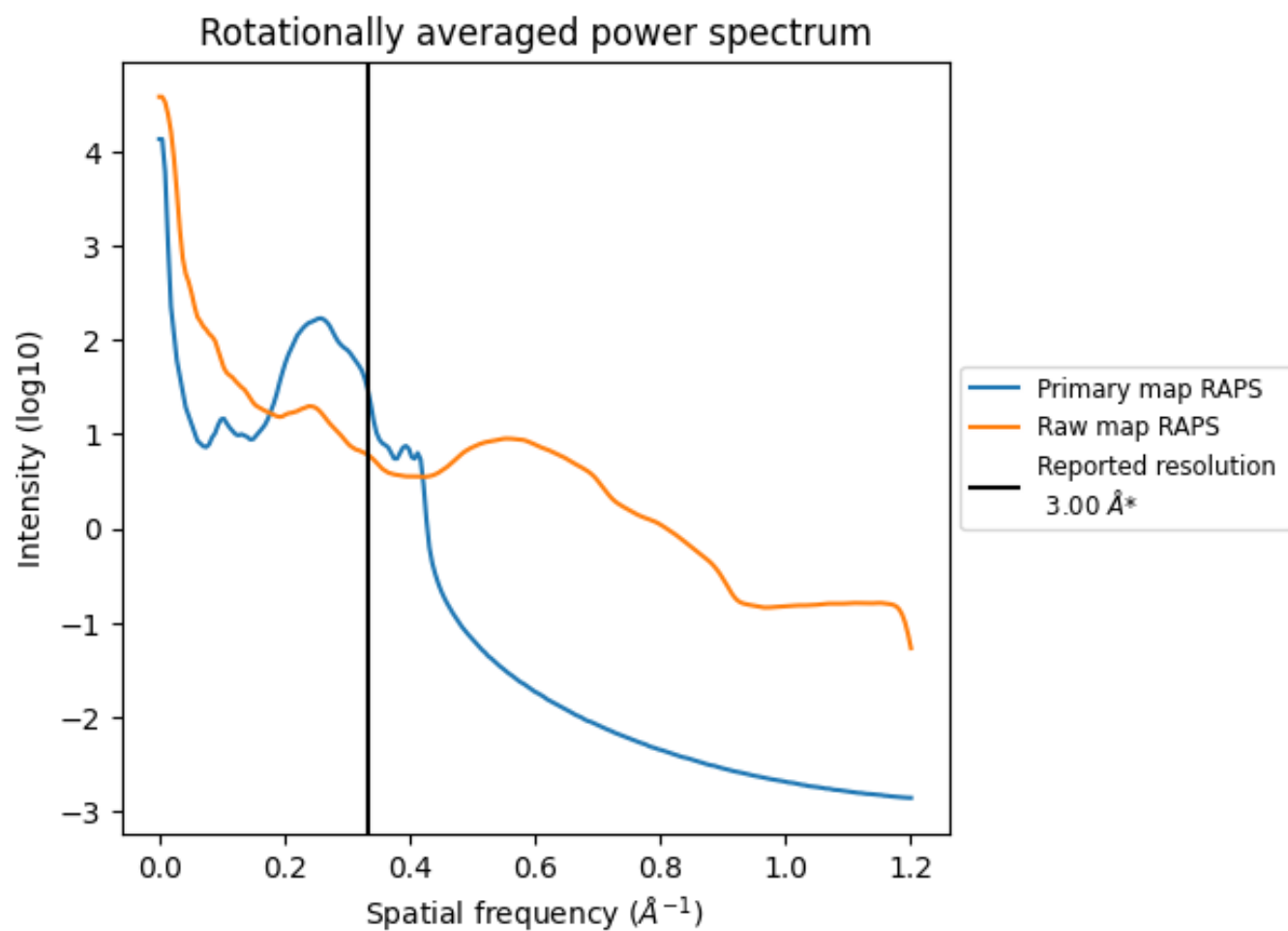
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 212 nm³; this corresponds to an approximate mass of 191 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

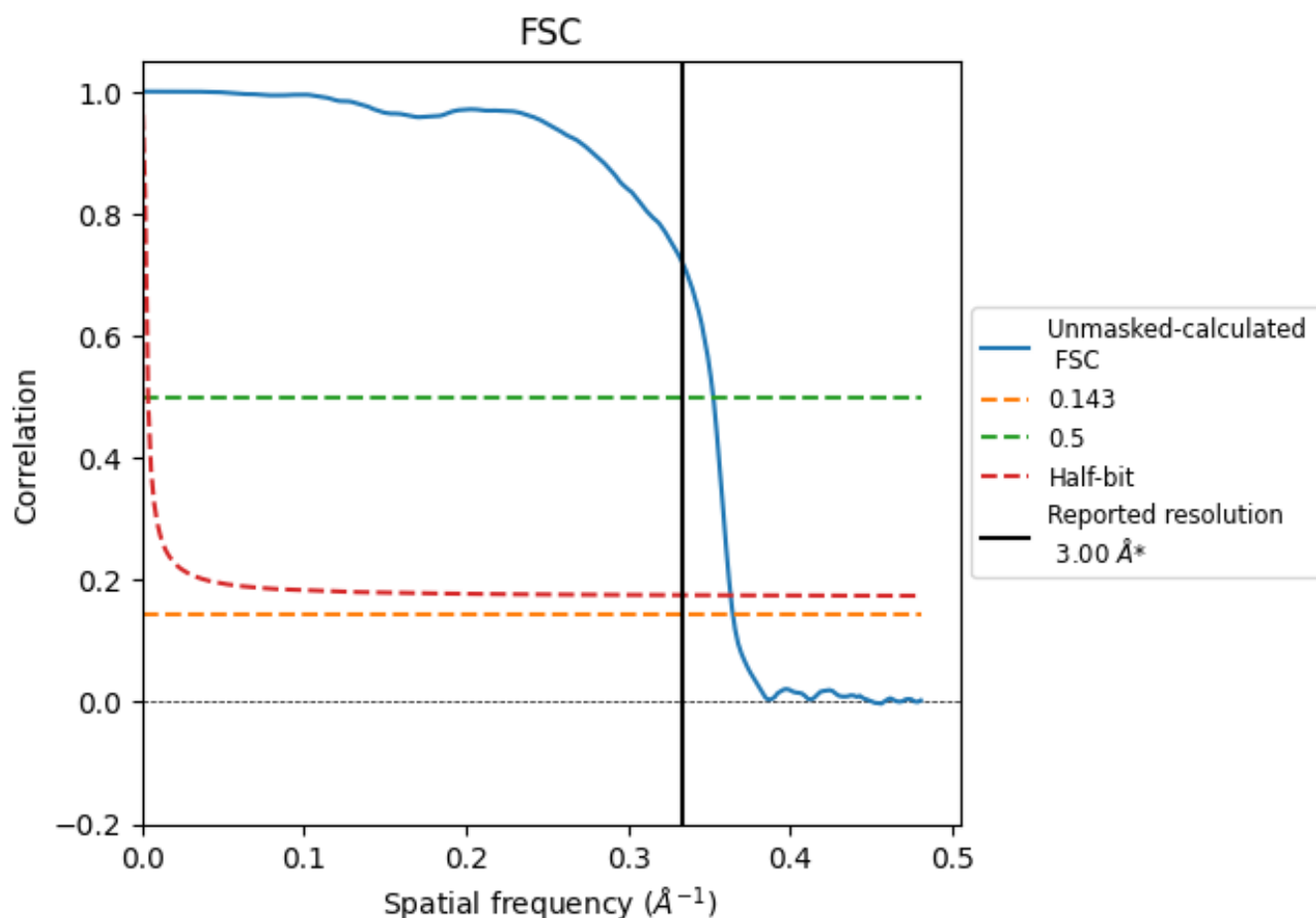


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

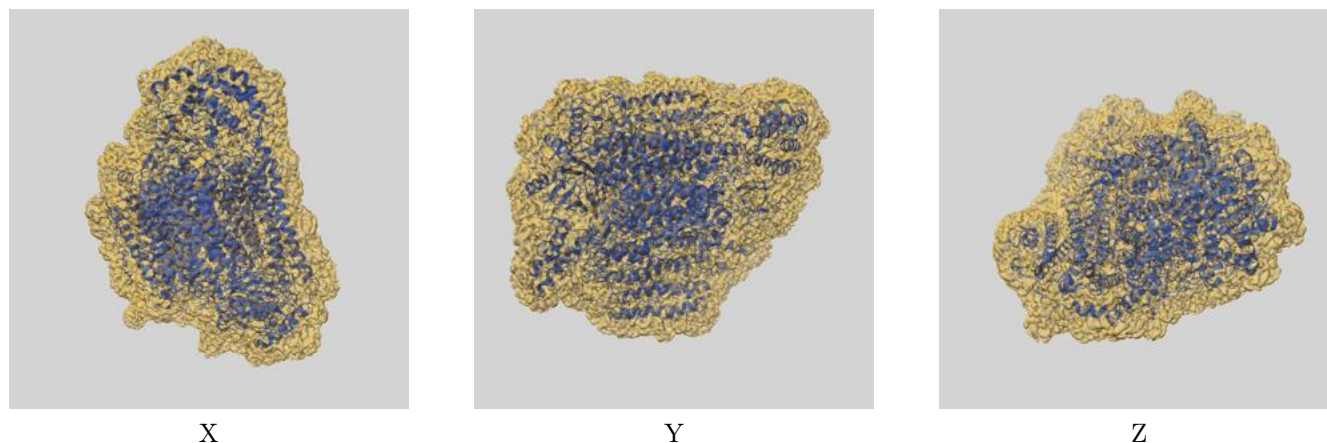
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.74	2.84	2.75

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

9 Map-model fit [i](#)

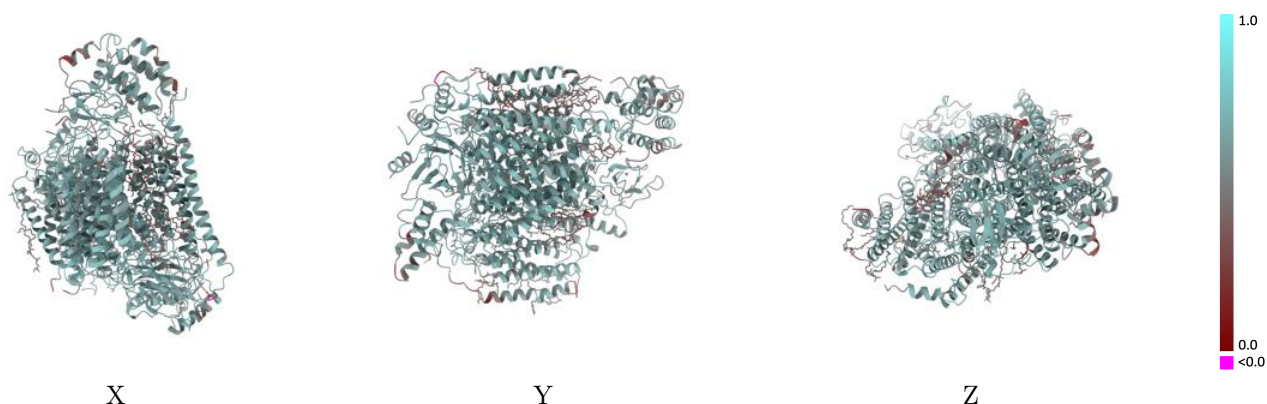
This section contains information regarding the fit between EMDB map EMD-42229 and PDB model 8UGL. Per-residue inclusion information can be found in section 3 on page 13.

9.1 Map-model overlay [i](#)



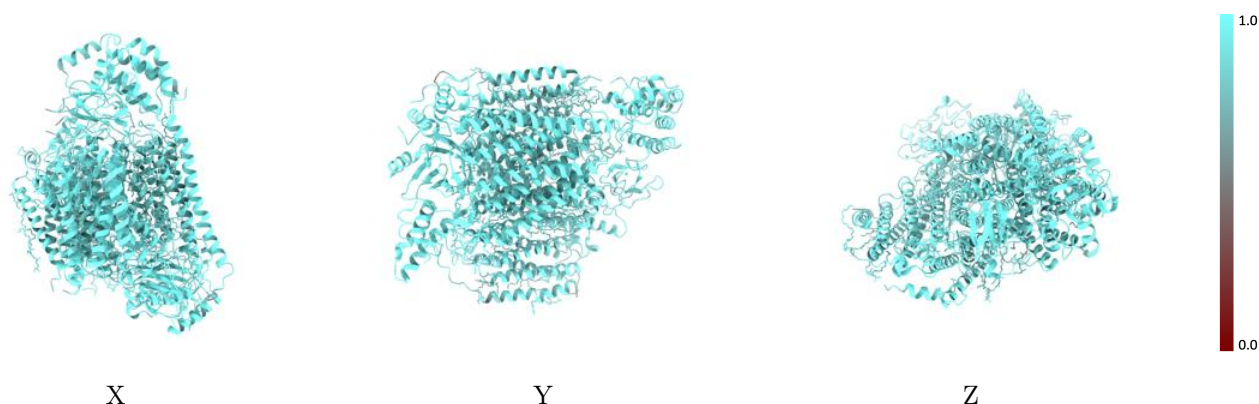
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



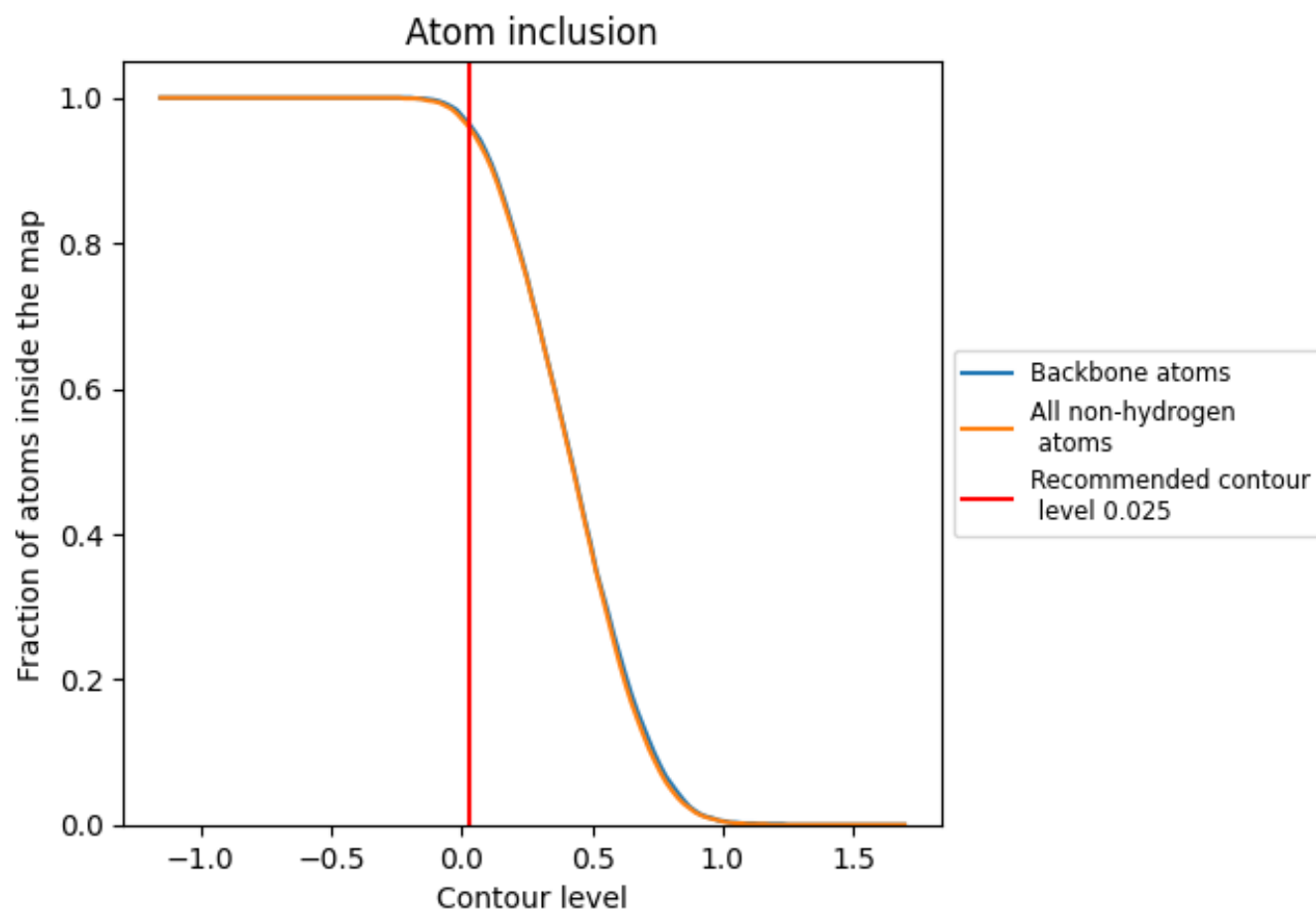
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.025).

9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9610	0.5920
4A	0.9900	0.6430
4B	0.9590	0.5920
4C	0.9700	0.6010
4D	0.9270	0.5440
4E	0.9340	0.5440
4F	0.9460	0.5720
4G	0.9230	0.5300
4H	0.9390	0.5660
4I	0.9700	0.5910
4J	0.9580	0.5780
4K	0.9320	0.5430
4L	0.9460	0.5810
4M	0.9400	0.5690
4N	0.9460	0.5580

1.0

0.0

<0.0