



## Full wwPDB EM Validation Report ⓘ

Jun 12, 2024 – 05:10 PM EDT

PDB ID : 8UGD  
EMDB ID : EMD-42221  
Title : In-situ complex III, state I  
Authors : Zheng, W.; Zhang, K.; Zhu, J.  
Deposited on : 2023-10-05  
Resolution : 3.50 Å (reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

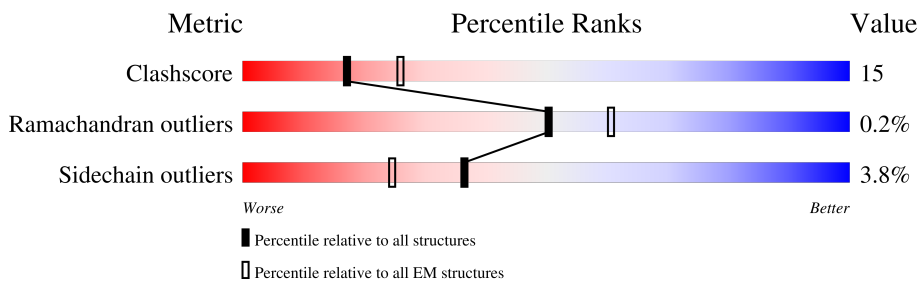
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	3A	480	6% (red), 66% (green), 24% (yellow), 8% (grey)
1	3N	480	67% (green), 24% (yellow), 7% (grey)
2	3B	453	8% (red), 68% (green), 23% (yellow), 8% (grey)
2	3O	453	5% (red), 68% (green), 23% (yellow), 8% (grey)
3	3C	379	71% (green), 27% (yellow), 2% (grey)
3	3P	379	67% (green), 32% (yellow), 1% (grey)
4	3D	326	50% (green), 22% (yellow), 27% (grey)
4	3Q	326	48% (green), 24% (yellow), 27% (grey)

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Mol	Chain	Length	Quality of chain
5	3E	274	
5	3I	274	
5	3R	274	
5	3V	274	
6	3F	111	
6	3S	111	
7	3G	82	
7	3T	82	
8	3H	91	
8	3U	91	
9	3J	64	
9	3W	64	
10	3X	56	
10	3Y	56	

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
16	FES	3E	301	-	-	X	-

## 2 Entry composition [i](#)

There are 17 unique types of molecules in this entry. The entry contains 33543 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 b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	3A	440	Total	C	N	O	S	0	0
			3411	2131	599	662	19		
1	3N	445	Total	C	N	O	S	1	0
			3424	2162	606	637	19		

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	3B	418	Total	C	N	O	S	0	0
			3138	1965	555	610	8		
2	3O	417	Total	C	N	O	S	0	0
			3124	1960	554	602	8		

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3C	379	Total	C	N	O	S	0	0
			3025	2031	471	502	21		
3	3P	379	Total	C	N	O	S	0	0
			3024	2031	471	501	21		

- Molecule 4 is a protein called Cytochrome c1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3D	237	Total	C	N	O	S	0	0
			1888	1205	325	342	16		
4	3Q	239	Total	C	N	O	S	0	0
			1904	1215	327	346	16		

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	3E	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		
5	3I	47	Total	C	N	O	S	0	0
			337	210	62	64	1		
5	3R	196	Total	C	N	O	S	0	0
			1518	955	265	291	7		
5	3V	31	Total	C	N	O	S	0	0
			223	137	45	40	1		

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	3F	98	Total	C	N	O	S	0	0
			868	557	152	157	2		
6	3S	98	Total	C	N	O	S	0	0
			868	557	152	157	2		

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	3G	74	Total	C	N	O	S	0	0
			628	411	116	99	2		
7	3T	74	Total	C	N	O	S	0	0
			628	411	116	99	2		

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	3H	65	Total	C	N	O	S	0	0
			533	325	97	106	5		
8	3U	65	Total	C	N	O	S	0	0
			533	325	97	106	5		

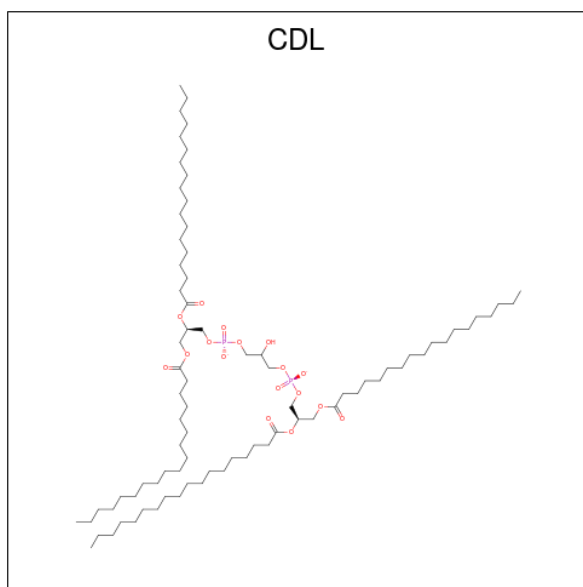
- Molecule 9 is a protein called Ubiquinol-cytochrome c reductase complex 7.2 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	3J	56	Total	C	N	O	0	0
			464	305	82	77		
9	3W	56	Total	C	N	O	0	0
			464	305	82	77		

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	3X	52	Total	C	N	O	S	0	0
			429	286	75	66	2		
10	3Y	51	Total	C	N	O	S	0	0
			421	281	74	65	1		

- Molecule 11 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



Mol	Chain	Residues	Atoms				AltConf
11	3A	1	Total	C	O	P	0
			58	39	17	2	
11	3C	1	Total	C	O	P	0
			52	33	17	2	
11	3D	1	Total	C	O	P	0
			56	37	17	2	
11	3P	1	Total	C	O	P	0
			56	37	17	2	
11	3P	1	Total	C	O	P	0
			43	24	17	2	
11	3Q	1	Total	C	O	P	0
			57	38	17	2	

- Molecule 12 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula:  $C_{41}H_{82}NO_8P$ ).



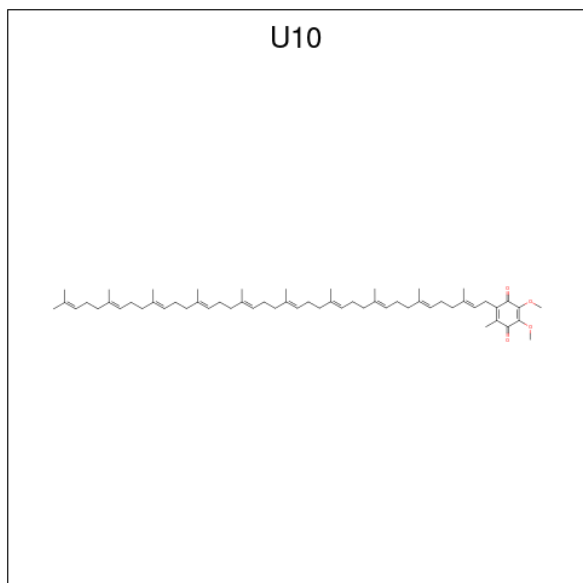
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
12	3A	1	27	17	1	8	1	0
12	3A	1	32	22	1	8	1	0
12	3C	1	35	25	1	8	1	0
12	3D	1	33	23	1	8	1	0
12	3G	1	29	19	1	8	1	0
12	3N	1	33	23	1	8	1	0
12	3N	1	25	15	1	8	1	0
12	3P	1	33	23	1	8	1	0
12	3Q	1	47	37	1	8	1	0
12	3R	1	34	24	1	8	1	0
12	3Y	1	30	20	1	8	1	0

- Molecule 13 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Fe	N		O
13	3C	1	43	34	1	4	4	0
13	3C	1	43	34	1	4	4	0
13	3P	1	43	34	1	4	4	0
13	3P	1	43	34	1	4	4	0

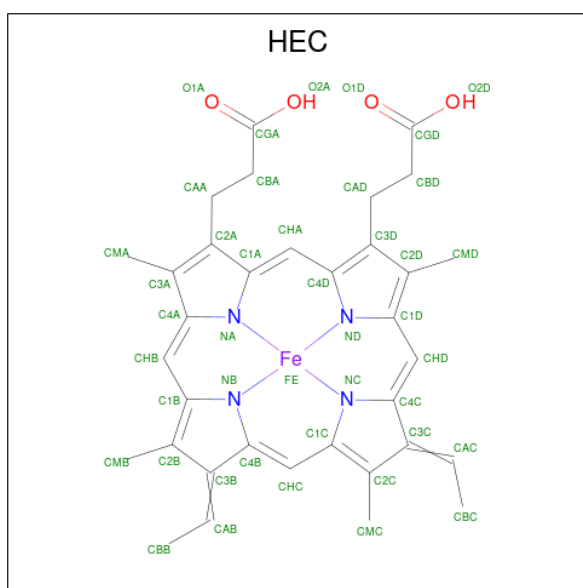
- Molecule 14 is UBIQUINONE-10 (three-letter code: U10) (formula:  $C_{59}H_{90}O_4$ ).





Mol	Chain	Residues	Atoms			AltConf
14	3C	1	Total	C	O	0
			28	24	4	
14	3C	1	Total	C	O	0
			28	24	4	
14	3P	1	Total	C	O	0
			23	19	4	
14	3P	1	Total	C	O	0
			28	24	4	

- Molecule 15 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



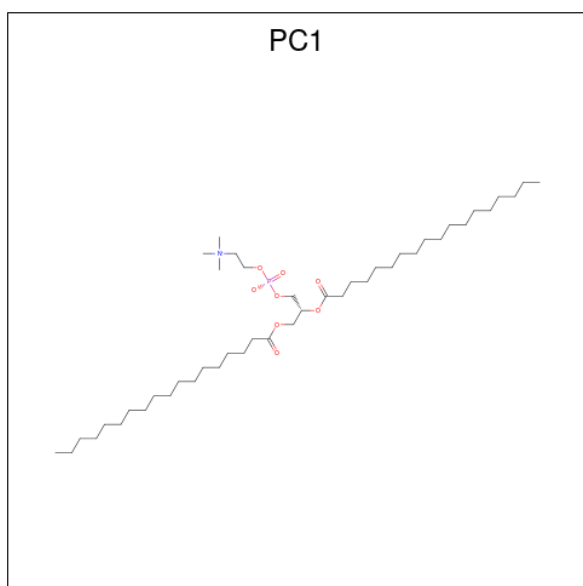
Mol	Chain	Residues	Atoms				AltConf	
15	3D	1	Total	C	Fe	N	O	0
			42	34	1	4	3	
15	3Q	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $Fe_2S_2$ ).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
16	3E	1	4	2	2	0
16	3R	1	4	2	2	0

- Molecule 17 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: C<sub>44</sub>H<sub>88</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		P
17	3E	1	47	37	1	8	1	0

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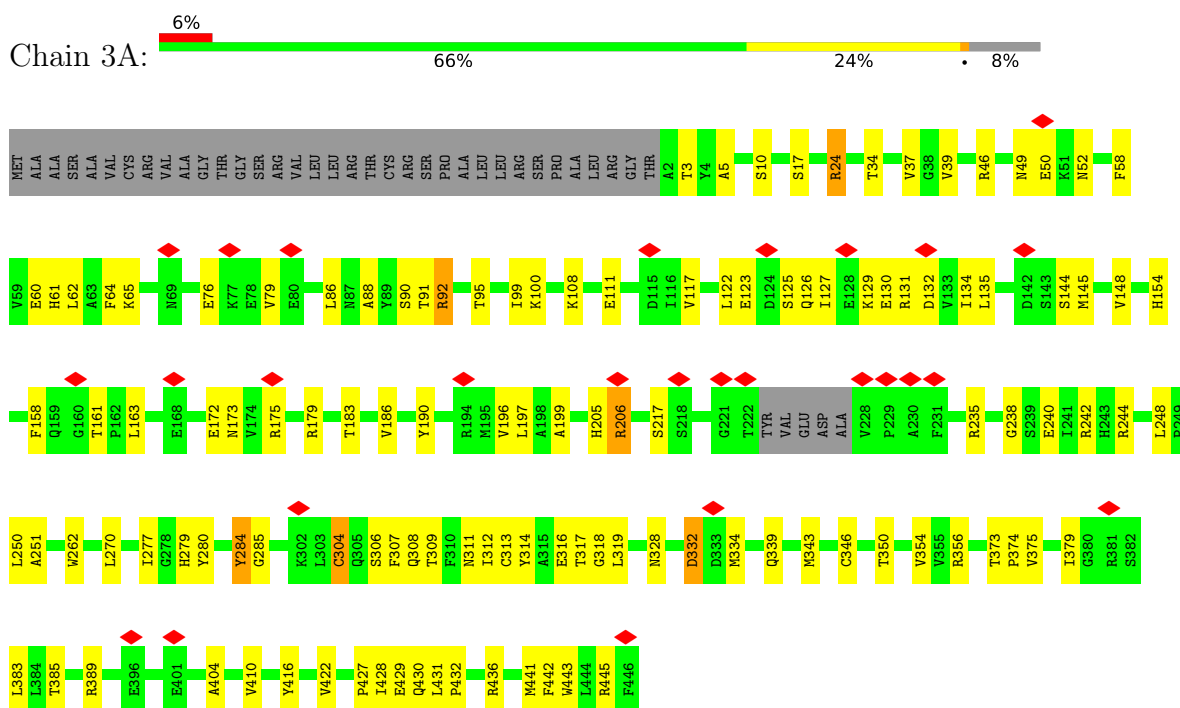
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
17	3R	1	45	35	1	8	1	0
17	3X	1	29	19	1	8	1	0

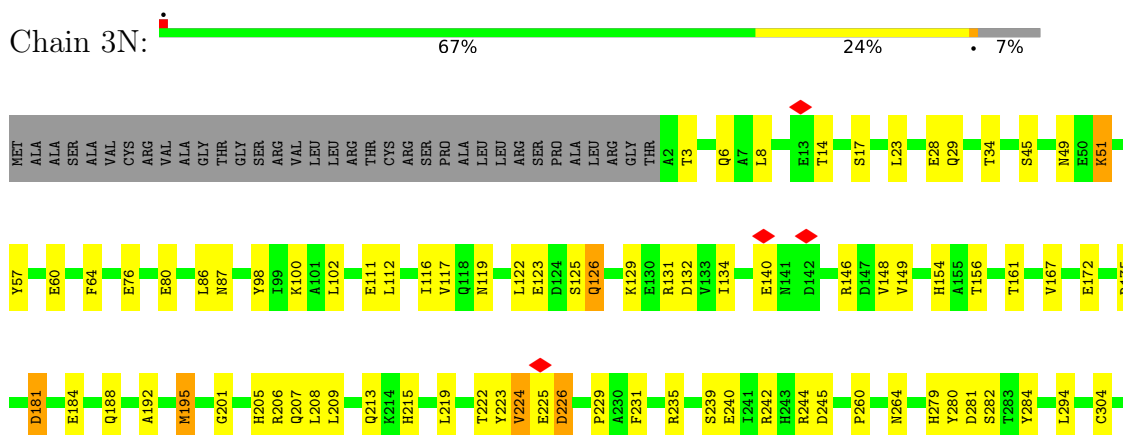
### 3 Residue-property plots

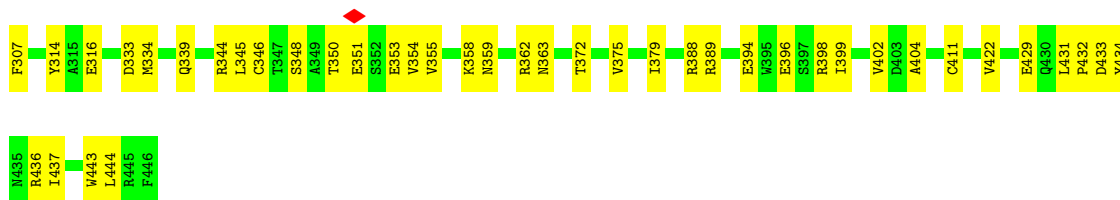
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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 b-c1 complex subunit 1, mitochondrial

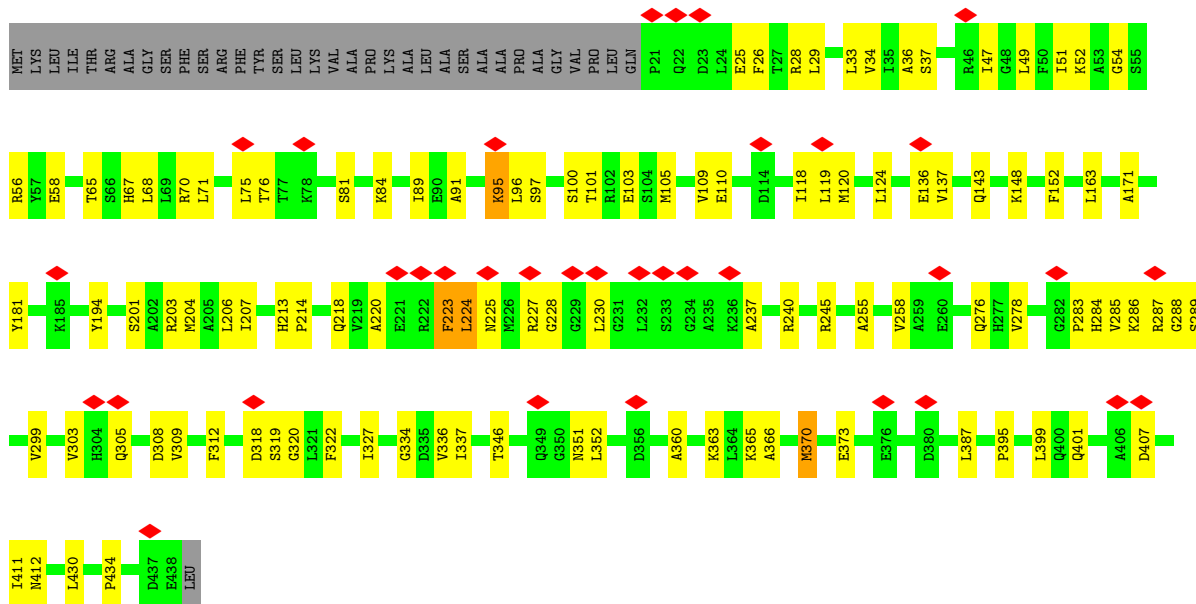


- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

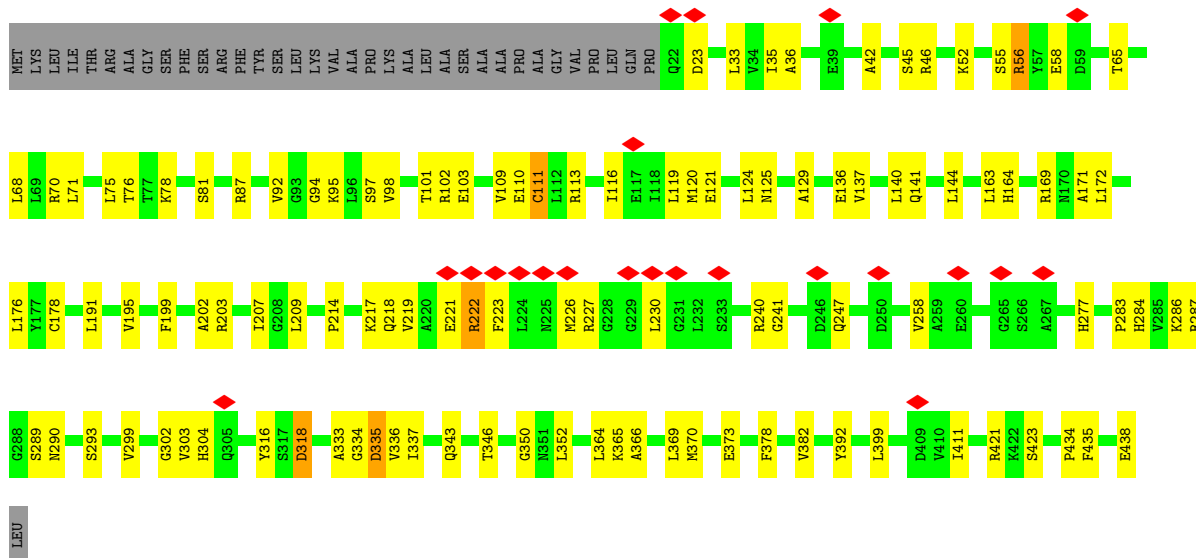




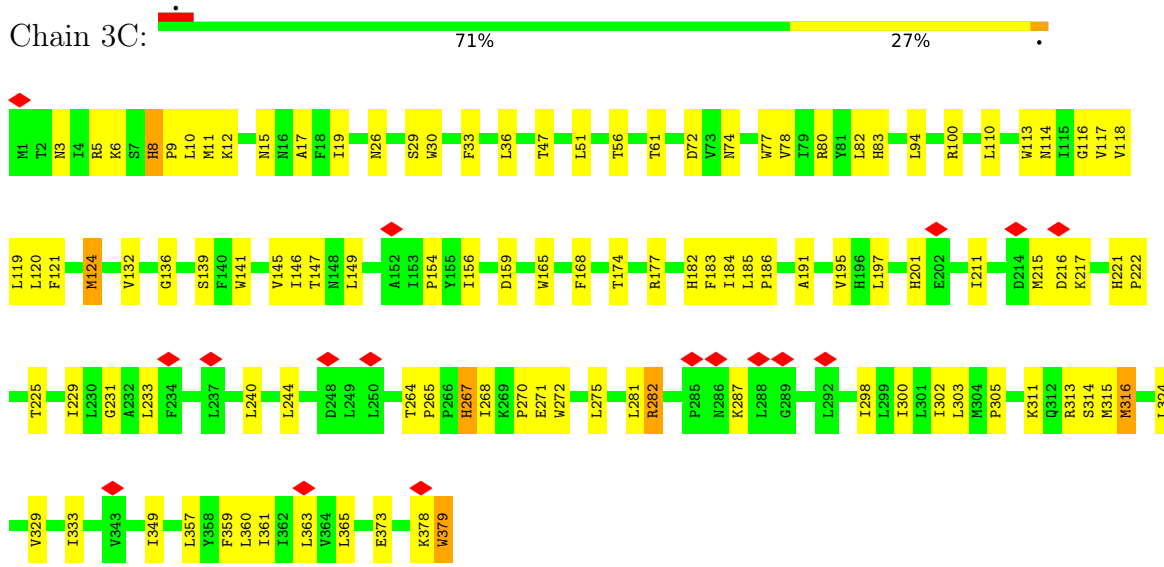
• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



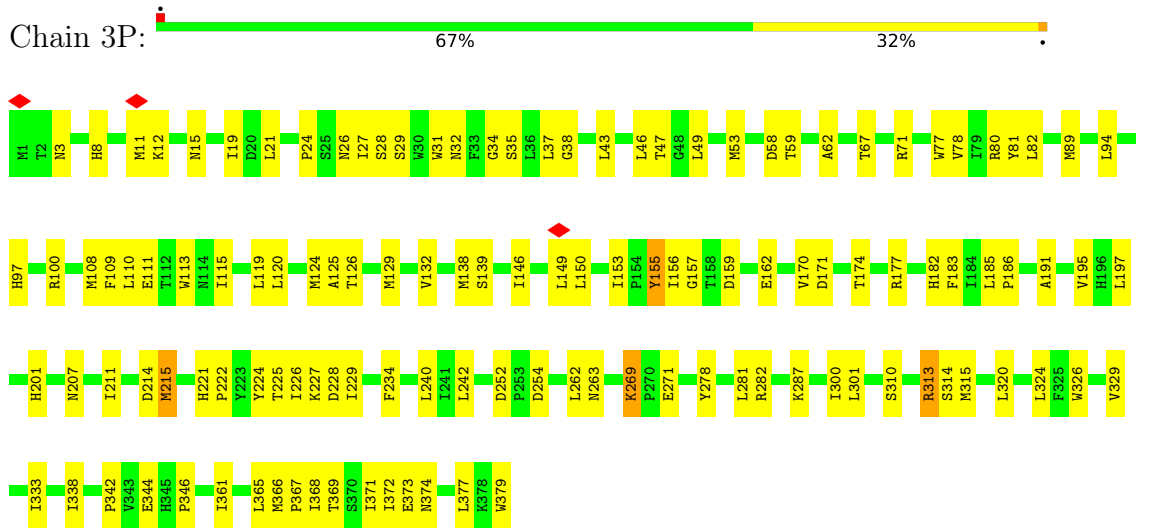
• Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



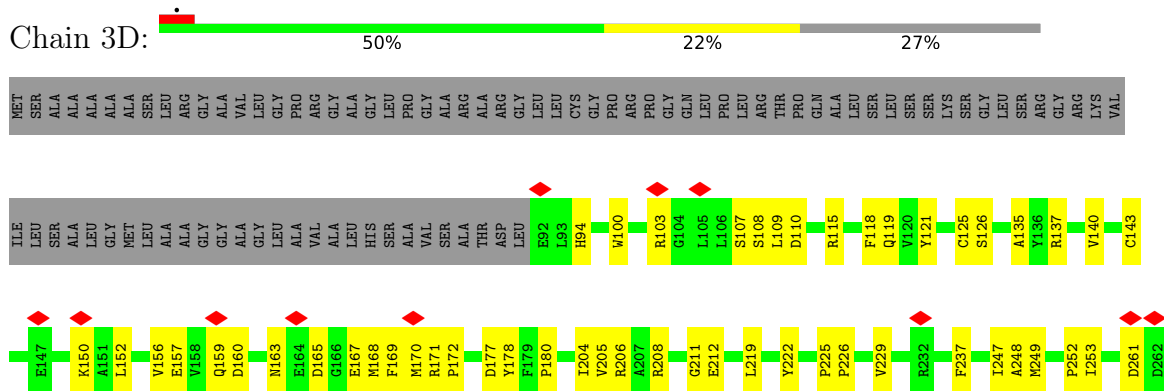
• Molecule 3: Cytochrome b



• Molecule 3: Cytochrome b



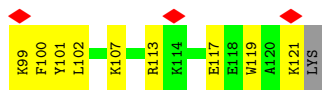
• Molecule 4: Cytochrome c1



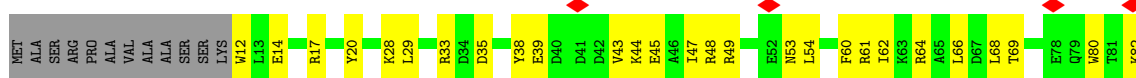




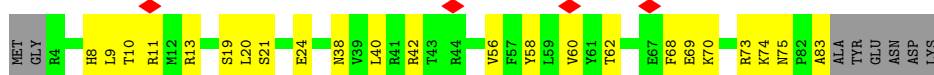




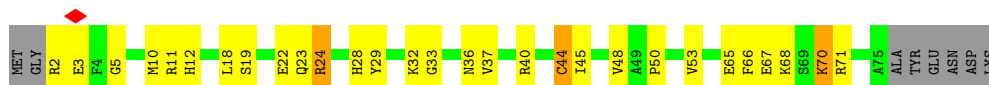
• Molecule 6: Cytochrome b-c1 complex subunit 7



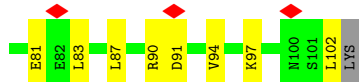
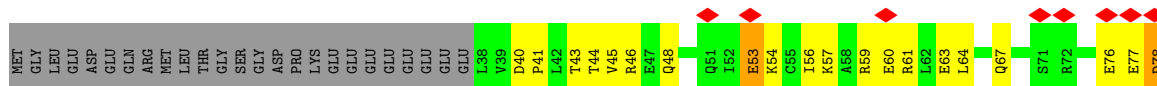
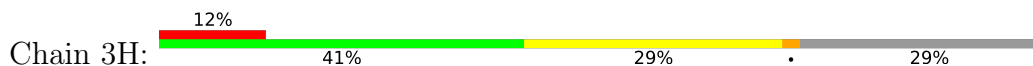
• Molecule 7: Cytochrome b-c1 complex subunit 8



• Molecule 7: Cytochrome b-c1 complex subunit 8

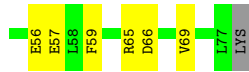


• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial

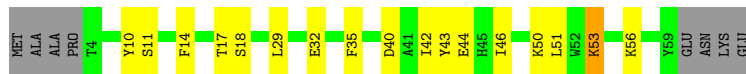




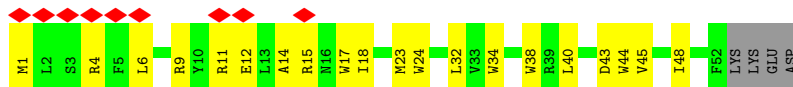
● Molecule 9: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein



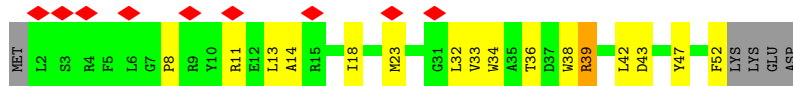
● Molecule 9: Ubiquinol-cytochrome c reductase complex 7.2 kDa protein



● Molecule 10: Cytochrome b-c1 complex subunit 10



● Molecule 10: Cytochrome b-c1 complex subunit 10



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	90000	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	0.481	Depositor
Minimum map value	-0.210	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.12	Depositor
Map size ( $\text{\AA}$ )	425.6, 425.6, 425.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.33, 1.33, 1.33	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: HEC, 3PE, FES, HEM, PC1, U10, CDL

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	3A	0.29	0/3481	0.51	1/4722 (0.0%)
1	3N	0.29	0/3496	0.50	0/4723
2	3B	0.28	0/3190	0.49	0/4317
2	3O	0.28	0/3175	0.48	0/4292
3	3C	0.31	0/3123	0.45	0/4269
3	3P	0.30	0/3122	0.47	0/4269
4	3D	0.31	0/1946	0.51	0/2641
4	3Q	0.30	0/1962	0.53	1/2663 (0.0%)
5	3E	0.29	0/1551	0.56	0/2098
5	3I	1.63	2/342 (0.6%)	1.54	6/465 (1.3%)
5	3R	0.31	0/1551	0.63	2/2098 (0.1%)
5	3V	0.26	0/225	0.67	0/303
6	3F	0.31	0/888	0.58	0/1193
6	3S	0.28	0/888	0.53	0/1193
7	3G	0.30	0/648	0.57	0/874
7	3T	0.31	0/649	0.63	1/878 (0.1%)
8	3H	0.30	0/538	0.57	0/721
8	3U	0.37	0/539	0.70	1/724 (0.1%)
9	3J	0.28	0/476	0.55	0/641
9	3W	0.29	0/476	0.58	0/641
10	3X	0.29	0/445	0.57	0/608
10	3Y	0.28	0/437	0.57	0/598
All	All	0.34	2/33148 (0.0%)	0.54	12/44931 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
5	3R	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	3I	49	PHE	C-N	27.39	1.97	1.34
5	3I	48	SER	C-N	11.13	1.59	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	3I	49	PHE	CA-C-N	-17.88	77.87	117.20
5	3I	48	SER	O-C-N	14.96	146.63	122.70
5	3I	48	SER	CA-C-N	-11.87	91.10	117.20
5	3R	160	PRO	CA-N-CD	-11.37	95.58	111.50
5	3I	49	PHE	C-N-CA	-10.60	95.20	121.70
5	3I	49	PHE	O-C-N	8.70	136.62	122.70
5	3I	48	SER	C-N-CA	-8.27	101.02	121.70
4	3Q	3	LEU	CA-CB-CG	6.80	130.94	115.30
5	3R	160	PRO	N-CD-CG	-5.78	94.53	103.20
1	3A	332	ASP	CB-CG-OD1	5.38	123.14	118.30
7	3T	70	LYS	CA-CB-CG	5.29	125.05	113.40
8	3U	17	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	3R	163	LYS	Peptide

## 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	3A	3411	0	3309	85	0
1	3N	3424	0	3350	87	0
2	3B	3138	0	3116	82	0
2	3O	3124	0	3108	77	0
3	3C	3025	0	3090	97	0
3	3P	3024	0	3090	93	0
4	3D	1888	0	1834	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	3Q	1904	0	1848	68	0
5	3E	1518	0	1498	85	0
5	3I	337	0	346	32	0
5	3R	1518	0	1499	98	0
5	3V	223	0	233	9	0
6	3F	868	0	857	32	0
6	3S	868	0	857	23	0
7	3G	628	0	634	19	0
7	3T	628	0	634	36	0
8	3H	533	0	512	20	0
8	3U	533	0	513	28	0
9	3J	464	0	467	59	0
9	3W	464	0	467	20	0
10	3X	429	0	430	13	0
10	3Y	421	0	418	17	0
11	3A	58	0	60	5	0
11	3C	52	0	48	4	0
11	3D	56	0	56	4	0
11	3P	99	0	86	9	0
11	3Q	57	0	58	10	0
12	3A	59	0	66	7	0
12	3C	35	0	44	4	0
12	3D	33	0	40	4	0
12	3G	29	0	32	1	0
12	3N	58	0	62	6	0
12	3P	33	0	40	1	0
12	3Q	47	0	71	7	0
12	3R	34	0	42	3	0
12	3Y	30	0	34	6	0
13	3C	86	0	60	6	0
13	3P	86	0	60	6	0
14	3C	56	0	62	9	0
14	3P	51	0	54	10	0
15	3D	42	0	32	4	0
15	3Q	43	0	32	2	0
16	3E	4	0	0	2	0
16	3R	4	0	0	0	0
17	3E	47	0	68	8	0
17	3R	45	0	64	4	0
17	3X	29	0	32	3	0
All	All	33543	0	33313	1025	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 15.

All (1025) 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)
9:3J:53:TRP:CG	9:3J:57:LYS:CE	1.88	1.55
9:3J:53:TRP:CG	9:3J:57:LYS:HE3	1.47	1.45
9:3J:53:TRP:HD1	9:3J:57:LYS:NZ	1.10	1.44
9:3J:53:TRP:CG	9:3J:57:LYS:HE2	1.57	1.27
9:3J:53:TRP:NE1	9:3J:57:LYS:HE2	0.94	1.27
9:3J:53:TRP:CE2	9:3J:57:LYS:HG2	1.75	1.21
9:3J:53:TRP:CD1	9:3J:57:LYS:NZ	1.89	1.20
5:3I:49:PHE:C	5:3I:50:LEU:N	1.97	1.18
9:3J:53:TRP:CD1	9:3J:57:LYS:CD	2.25	1.18
4:3D:115:ARG:NE	9:3J:60:TYR:CE1	2.17	1.11
9:3J:53:TRP:CE2	9:3J:57:LYS:HE2	1.89	1.06
5:3I:49:PHE:CA	5:3I:50:LEU:N	2.22	1.03
9:3J:53:TRP:NE1	9:3J:57:LYS:CD	2.23	0.97
14:3P:503:U10:H4M3	14:3P:503:U10:H3M3	1.47	0.96
14:3C:504:U10:H4M3	14:3C:504:U10:H3M3	1.47	0.96
2:3B:283:PRO:HD3	5:3I:57:GLY:HA3	1.45	0.95
9:3J:53:TRP:O	9:3J:57:LYS:HE3	1.68	0.94
4:3D:115:ARG:HD3	9:3J:60:TYR:CZ	2.05	0.92
4:3D:115:ARG:CZ	9:3J:60:TYR:CE1	2.54	0.91
9:3J:53:TRP:HD1	9:3J:57:LYS:HZ1	1.12	0.90
4:3D:115:ARG:HD3	9:3J:60:TYR:OH	1.70	0.90
9:3J:53:TRP:CD2	9:3J:57:LYS:HG2	2.06	0.89
9:3J:53:TRP:CE2	9:3J:57:LYS:CG	2.56	0.89
9:3J:53:TRP:CB	9:3J:57:LYS:HE3	2.04	0.87
5:3E:238:CYS:SG	4:3Q:144:ARG:NH2	2.47	0.87
9:3J:53:TRP:NE1	9:3J:57:LYS:CE	1.72	0.86
9:3J:53:TRP:CD1	9:3J:57:LYS:HE2	0.45	0.86
4:3D:115:ARG:CD	9:3J:60:TYR:CZ	2.59	0.85
9:3J:53:TRP:CD1	9:3J:57:LYS:CE	0.91	0.85
7:3T:18:LEU:HB3	7:3T:23:GLN:HE21	1.41	0.83
9:3J:53:TRP:CD2	9:3J:57:LYS:HE2	2.14	0.82
2:3O:92:VAL:HG21	2:3O:119:LEU:HD11	1.63	0.80
11:3P:506:CDL:HB31	7:3T:40:ARG:HB3	1.64	0.79
5:3I:49:PHE:HA	5:3I:50:LEU:N	1.97	0.78
8:3U:25:GLU:OE1	8:3U:26:GLN:NE2	2.16	0.78
4:3Q:164:ILE:HG22	4:3Q:179:MET:HG2	1.67	0.77
5:3E:237:PRO:HG2	4:3Q:144:ARG:HD3	1.67	0.76
9:3J:53:TRP:CD2	9:3J:57:LYS:CG	2.69	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3B:220:ALA:HA	2:3B:224:LEU:HD12	1.67	0.76
2:3B:95:LYS:HE2	5:3I:32:ALA:HA	1.67	0.76
5:3I:55:LEU:HA	5:3I:58:GLN:HE21	1.51	0.75
1:3A:172:GLU:OE1	1:3A:175:ARG:NH2	2.19	0.75
2:3B:96:LEU:HB3	5:3I:70:LEU:HB3	1.69	0.75
11:3Q:502:CDL:HA62	7:3T:33:GLY:HA3	1.68	0.75
9:3J:53:TRP:CD1	9:3J:57:LYS:HE3	1.28	0.75
5:3R:194:GLN:HG3	5:3R:196:ARG:H	1.52	0.74
9:3J:53:TRP:O	9:3J:57:LYS:CE	2.34	0.74
5:3E:178:HIS:ND1	5:3E:178:HIS:O	2.19	0.74
11:3C:505:CDL:H111	12:3C:506:3PE:H322	1.69	0.73
5:3I:49:PHE:C	5:3I:50:LEU:CA	2.55	0.73
5:3I:42:VAL:HG13	5:3I:43:LEU:HD12	1.70	0.73
5:3E:162:GLY:H	5:3E:178:HIS:HB3	1.54	0.72
5:3E:242:HIS:HB2	5:3E:250:ARG:HB2	1.71	0.72
3:3P:310:SER:HA	3:3P:374:ASN:HD21	1.55	0.72
10:3Y:33:VAL:HG23	10:3Y:38:TRP:HB3	1.71	0.71
1:3N:422:VAL:HG21	1:3N:437:ILE:HD13	1.72	0.71
1:3A:131:ARG:HD3	1:3A:175:ARG:HA	1.72	0.71
12:3C:506:3PE:H292	12:3C:506:3PE:H242	1.71	0.71
1:3N:60:GLU:OE2	2:3O:287:ARG:NH2	2.24	0.71
1:3A:279:HIS:CG	5:3I:35:PRO:HB3	2.25	0.71
2:3B:51:ILE:HG23	2:3B:204:MET:HG2	1.73	0.71
4:3D:159:GLN:NE2	4:3D:169:PHE:O	2.24	0.71
5:3R:222:CYS:SG	5:3R:223:VAL:N	2.64	0.71
3:3P:252:ASP:OD2	3:3P:269:LYS:NZ	2.24	0.70
1:3A:445:ARG:NH2	12:3A:503:3PE:O14	2.16	0.69
8:3H:45:VAL:HG13	8:3H:97:LYS:HE3	1.72	0.69
3:3P:81:TYR:OH	4:3Q:118:ARG:NH1	2.26	0.69
3:3C:216:ASP:HB2	6:3F:75:LYS:HD2	1.73	0.69
3:3C:379:TRP:HB3	6:3F:45:ARG:HH21	1.58	0.69
4:3D:115:ARG:NE	9:3J:60:TYR:CZ	2.61	0.69
5:3R:200:HIS:HE1	5:3R:202:LEU:HB2	1.58	0.69
3:3C:82:LEU:HD21	12:3D:502:3PE:H272	1.75	0.68
9:3W:53:LYS:HA	9:3W:56:LYS:HD3	1.76	0.68
9:3J:10:LEU:O	9:3J:14:LEU:HB2	1.94	0.68
11:3Q:502:CDL:OA4	7:3T:36:ASN:ND2	2.27	0.68
3:3C:229:ILE:HD12	17:3E:302:PC1:H382	1.76	0.68
4:3D:306:PRO:HB3	12:3G:101:3PE:H361	1.76	0.68
7:3T:67:GLU:N	7:3T:67:GLU:OE2	2.26	0.68
3:3P:377:LEU:HD12	6:3S:20:TYR:HE2	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3R:159:ILE:O	5:3R:159:ILE:HD12	1.94	0.67
5:3R:214:ILE:HD12	5:3R:216:VAL:H	1.59	0.67
1:3A:445:ARG:HH21	12:3A:503:3PE:H222	1.59	0.67
3:3C:149:LEU:HD21	14:3C:504:U10:H1M3	1.77	0.67
5:3E:159:ILE:HD11	5:3E:165:MET:HB3	1.77	0.66
5:3E:179:ARG:HH21	5:3E:208:PRO:HA	1.61	0.66
5:3E:222:CYS:N	16:3E:301:FES:S2	2.62	0.66
5:3R:234:TYR:HB2	5:3R:243:TYR:HB2	1.77	0.66
1:3A:285:GLY:HA3	5:3I:70:LEU:HA	1.77	0.66
3:3P:38:GLY:HA3	14:3P:503:U10:H121	1.77	0.66
9:3W:10:TYR:HA	9:3W:14:PHE:HB2	1.77	0.66
2:3B:346:THR:O	2:3B:351:ASN:ND2	2.27	0.66
1:3A:65:LYS:NZ	2:3B:287:ARG:O	2.29	0.65
8:3U:35:GLU:HA	8:3U:38:GLU:OE1	1.97	0.65
2:3B:124:LEU:HD11	2:3B:224:LEU:HG	1.79	0.65
4:3D:115:ARG:CZ	9:3J:60:TYR:CD1	2.80	0.65
3:3P:207:ASN:ND2	3:3P:211:ILE:O	2.29	0.65
2:3B:366:ALA:O	2:3B:370:MET:HG3	1.97	0.65
3:3C:15:ASN:HA	3:3C:19:ILE:HB	1.78	0.64
5:3E:160:PRO:HG2	5:3E:163:LYS:HG3	1.79	0.64
1:3A:17:SER:OG	1:3A:205:HIS:NE2	2.29	0.64
11:3Q:502:CDL:H311	7:3T:37:VAL:HG21	1.80	0.64
5:3E:217:CYS:HB3	5:3E:221:GLY:HA2	1.78	0.64
8:3H:45:VAL:HG12	8:3H:94:VAL:HG22	1.80	0.64
4:3Q:9:SER:HB2	4:3Q:15:ARG:HH22	1.61	0.64
7:3T:3:GLU:N	7:3T:3:GLU:OE1	2.31	0.64
8:3U:50:THR:HG22	8:3U:52:GLU:H	1.62	0.64
12:3Q:503:3PE:N	5:3R:131:ASN:OD1	2.24	0.64
1:3N:192:ALA:HB2	1:3N:219:LEU:HB3	1.79	0.64
3:3P:8:HIS:HB3	3:3P:11:MET:HB2	1.80	0.64
11:3A:501:CDL:H511	11:3A:501:CDL:H141	1.80	0.64
8:3H:77:GLU:O	8:3H:78:ASP:N	2.31	0.64
5:3R:231:PHE:HB2	5:3R:250:ARG:HH22	1.63	0.64
3:3C:119:LEU:HD22	13:3C:502:HEM:HBB2	1.80	0.63
4:3Q:116:ILE:HG12	15:3Q:501:HEC:HMA3	1.81	0.63
5:3E:200:HIS:HB3	5:3E:203:GLU:HG2	1.80	0.63
9:3J:33:GLU:OE1	10:3Y:34:TRP:NE1	2.31	0.63
5:3R:159:ILE:HD13	5:3R:178:HIS:HB2	1.79	0.63
5:3E:194:GLN:HE22	5:3E:250:ARG:HD2	1.62	0.63
1:3N:184:GLU:OE1	1:3N:184:GLU:N	2.31	0.63
4:3Q:181:GLN:NE2	4:3Q:185:ASP:OD1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:3F:45:ARG:NH1	6:3F:100:PHE:HD2	1.97	0.63
6:3F:45:ARG:NH1	6:3F:46:ASP:OD1	2.31	0.63
1:3N:281:ASP:OD1	1:3N:282:SER:N	2.32	0.63
1:3N:156:THR:OG1	1:3N:239:SER:OG	2.15	0.63
5:3E:223:VAL:HB	4:3Q:144:ARG:HH22	1.63	0.63
5:3E:155:LYS:HE3	5:3E:176:VAL:HG21	1.81	0.63
6:3F:47:ASP:OD1	6:3F:101:TYR:OH	2.16	0.63
6:3F:97:GLU:N	6:3F:97:GLU:OE1	2.32	0.62
9:3J:53:TRP:CZ2	9:3J:57:LYS:HG2	2.30	0.62
1:3N:358:LYS:NZ	1:3N:399:ILE:O	2.31	0.62
2:3O:352:LEU:HB3	2:3O:411:ILE:HD11	1.81	0.62
17:3R:302:PC1:H152	9:3W:17:THR:HG22	1.80	0.62
3:3P:234:PHE:HB3	11:3Q:502:CDL:H771	1.80	0.62
2:3B:109:VAL:HB	2:3B:119:LEU:HD12	1.79	0.62
3:3C:72:ASP:OD1	4:3D:137:ARG:NH2	2.27	0.62
6:3S:39:GLU:O	6:3S:44:LYS:NZ	2.32	0.62
2:3O:164:HIS:HE2	2:3O:316:TYR:HH	1.44	0.62
5:3R:196:ARG:HE	5:3R:255:PRO:HA	1.65	0.62
5:3R:242:HIS:NE2	5:3R:251:LYS:HB3	2.14	0.62
3:3P:329:VAL:O	3:3P:333:ILE:HD12	1.99	0.62
13:3P:502:HEM:HBA1	14:3P:503:U10:H4M2	1.82	0.62
4:3Q:28:ARG:NE	4:3Q:185:ASP:OD2	2.30	0.62
5:3V:49:PHE:HD1	5:3V:54:SER:HB3	1.65	0.62
1:3N:14:THR:HG21	1:3N:389:ARG:HB3	1.82	0.62
7:3G:70:LYS:HE3	7:3G:70:LYS:HA	1.82	0.61
5:3E:125:VAL:HG21	17:3E:302:PC1:H362	1.82	0.61
5:3R:234:TYR:O	5:3R:243:TYR:N	2.25	0.61
2:3O:334:GLY:HA2	2:3O:434:PRO:HD3	1.82	0.61
3:3C:233:LEU:HG	17:3E:302:PC1:H3A2	1.81	0.61
7:3G:73:ARG:NH1	8:3H:81:GLU:OE1	2.29	0.61
3:3C:5:ARG:HD2	3:3C:19:ILE:HG21	1.83	0.61
4:3Q:232:SER:OG	7:3T:23:GLN:NE2	2.34	0.61
5:3R:159:ILE:HD11	5:3R:210:TRP:HD1	1.65	0.61
4:3D:163:ASN:HD21	4:3D:167:GLU:HB2	1.66	0.60
5:3E:173:PRO:O	5:3E:215:GLY:N	2.34	0.60
3:3P:119:LEU:HD22	13:3P:502:HEM:HBB2	1.83	0.60
5:3R:208:PRO:HD2	5:3R:210:TRP:HZ3	1.66	0.60
4:3D:115:ARG:NE	9:3J:60:TYR:HE1	1.93	0.60
5:3R:177:ARG:NH1	5:3R:178:HIS:O	2.34	0.60
7:3G:58:TYR:O	7:3G:62:THR:HG23	2.02	0.60
3:3C:215:MET:SD	3:3C:215:MET:N	2.72	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3A:60:GLU:OE2	2:3B:287:ARG:NH2	2.34	0.60
1:3A:379:ILE:HG12	1:3A:389:ARG:HD3	1.84	0.60
5:3R:176:VAL:HA	5:3R:212:ILE:HG22	1.83	0.60
5:3E:125:VAL:HG11	17:3E:302:PC1:H371	1.82	0.60
5:3E:217:CYS:SG	5:3E:243:TYR:OH	2.53	0.60
4:3Q:97:ASN:OD1	4:3Q:100:ALA:N	2.34	0.60
4:3D:273:LYS:HD2	8:3H:102:LEU:HD23	1.84	0.60
4:3Q:31:GLN:OE1	4:3Q:35:GLN:NE2	2.34	0.60
3:3C:264:THR:HG21	5:3R:222:CYS:SG	2.42	0.60
3:3C:314:SER:OG	3:3C:315:MET:N	2.33	0.60
11:3C:505:CDL:O1	11:3C:505:CDL:OA7	2.20	0.60
1:3N:172:GLU:OE1	1:3N:175:ARG:NH2	2.35	0.60
2:3O:56:ARG:NH1	2:3O:318:ASP:OD1	2.34	0.59
11:3Q:502:CDL:OA3	7:3T:40:ARG:NH1	2.35	0.59
3:3C:267:HIS:O	3:3C:267:HIS:ND1	2.36	0.59
4:3D:109:LEU:HD11	4:3D:287:HIS:HB3	1.85	0.59
4:3Q:68:VAL:HG21	4:3Q:92:PRO:HG2	1.85	0.59
9:3J:46:HIS:HA	9:3J:49:GLN:OE1	2.02	0.59
4:3Q:203:ARG:NH1	9:3W:40:ASP:OD1	2.35	0.59
5:3R:163:LYS:HB3	5:3R:165:MET:CE	2.33	0.59
5:3R:248:ARG:HD2	5:3R:257:ASN:HD21	1.68	0.59
12:3Q:503:3PE:H261	12:3Q:503:3PE:H381	1.85	0.59
3:3C:361:ILE:HA	3:3C:365:LEU:HB2	1.84	0.59
2:3B:75:LEU:HD22	2:3B:136:GLU:HB3	1.84	0.58
1:3A:126:GLN:NE2	1:3A:130:GLU:OE1	2.36	0.58
9:3J:53:TRP:CD2	9:3J:57:LYS:CE	2.74	0.58
1:3A:123:GLU:HB3	1:3A:126:GLN:HB3	1.86	0.58
5:3E:205:VAL:HG21	5:3E:211:VAL:HA	1.86	0.58
5:3E:225:ILE:N	5:3E:235:TYR:O	2.25	0.58
1:3N:76:GLU:OE2	2:3O:290:ASN:N	2.36	0.58
5:3R:206:LYS:HE2	5:3R:263:TYR:CE1	2.38	0.58
6:3F:25:LEU:HD21	6:3F:29:ARG:HE	1.67	0.58
3:3P:170:VAL:HG12	3:3P:174:THR:HG21	1.84	0.58
2:3B:303:VAL:HG22	2:3B:305:GLN:H	1.68	0.58
5:3E:237:PRO:HD2	4:3Q:144:ARG:HH11	1.68	0.58
2:3O:350:GLY:HA2	2:3O:411:ILE:HD12	1.85	0.58
8:3U:28:GLU:HB2	8:3U:32:LYS:HZ1	1.68	0.58
2:3B:171:ALA:HB3	2:3B:237:ALA:HB2	1.86	0.58
2:3B:327:ILE:HD12	5:3I:58:GLN:HB2	1.86	0.58
5:3I:62:ARG:HB2	5:3I:77:ARG:HH22	1.67	0.58
1:3N:394:GLU:O	1:3N:398:ARG:HG3	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:3N:502:3PE:H32	3:3P:221:HIS:HE1	1.68	0.58
1:3A:238:GLY:O	7:3G:21:SER:OG	2.22	0.58
12:3D:502:3PE:H372	5:3E:128:ALA:HB1	1.85	0.58
1:3N:354:VAL:HG21	1:3N:404:ALA:HA	1.86	0.58
2:3O:207:ILE:HG21	2:3O:382:VAL:CG1	2.34	0.58
3:3C:244:LEU:HD23	4:3D:294:GLY:HA2	1.86	0.57
3:3C:147:THR:OG1	3:3C:165:TRP:NE1	2.35	0.57
1:3A:154:HIS:NE2	1:3A:314:TYR:OH	2.32	0.57
3:3C:74:ASN:ND2	5:3E:142:ALA:O	2.38	0.57
3:3C:360:LEU:HG	3:3C:365:LEU:HD23	1.86	0.57
8:3H:40:ASP:HB3	8:3H:43:THR:HG23	1.85	0.57
3:3C:270:PRO:HD3	14:3C:504:U10:H3M2	1.85	0.57
5:3E:248:ARG:HA	5:3E:257:ASN:HB3	1.86	0.57
1:3N:339:GLN:HE22	1:3N:437:ILE:HG23	1.69	0.57
4:3Q:19:SER:O	4:3Q:202:LYS:NZ	2.38	0.57
2:3O:56:ARG:NH1	2:3O:103:GLU:OE2	2.36	0.57
3:3P:35:SER:OG	3:3P:228:ASP:OD2	2.16	0.57
5:3R:224:PRO:HA	5:3R:236:CYS:HA	1.86	0.57
7:3T:67:GLU:O	7:3T:71:ARG:N	2.38	0.57
2:3B:287:ARG:HG2	5:3I:53:GLU:HB3	1.85	0.57
3:3C:379:TRP:HB3	6:3F:45:ARG:NH2	2.19	0.57
11:3P:506:CDL:H121	11:3Q:502:CDL:H521	1.87	0.57
5:3R:268:ASP:OD1	5:3R:269:ASP:N	2.38	0.57
5:3E:140:MET:O	3:3P:177:ARG:NH2	2.25	0.57
2:3O:46:ARG:NE	2:3O:110:GLU:OE1	2.34	0.57
3:3P:229:ILE:HG23	17:3R:302:PC1:H3B1	1.85	0.57
6:3S:84:GLU:N	6:3S:84:GLU:OE2	2.38	0.57
7:3T:18:LEU:HB3	7:3T:23:GLN:NE2	2.14	0.57
1:3A:304:CYS:HB3	1:3A:334:MET:SD	2.45	0.57
3:3C:270:PRO:HB3	14:3C:504:U10:O4	2.05	0.57
1:3N:362:ARG:NH2	1:3N:396:GLU:OE2	2.38	0.57
3:3C:29:SER:HB2	11:3D:503:CDL:H732	1.86	0.56
8:3H:76:GLU:O	8:3H:78:ASP:N	2.38	0.56
5:3R:241:SER:HA	5:3R:252:GLY:HA3	1.87	0.56
1:3A:354:VAL:HG21	1:3A:404:ALA:HA	1.87	0.56
7:3G:73:ARG:NH1	7:3G:74:LYS:O	2.38	0.56
3:3C:244:LEU:O	4:3D:290:ARG:NE	2.39	0.56
5:3E:131:ASN:O	5:3E:135:GLN:HG2	2.05	0.56
1:3N:444:LEU:HD13	12:3N:502:3PE:H122	1.86	0.56
2:3O:365:LYS:HG2	2:3O:399:LEU:HD22	1.87	0.56
3:3P:125:ALA:O	3:3P:129:MET:HG3	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3Q:20:SER:OG	9:3W:43:TYR:OH	2.22	0.56
5:3R:200:HIS:CE1	5:3R:202:LEU:H	2.23	0.56
5:3R:214:ILE:HG23	5:3R:261:PRO:HD3	1.86	0.56
10:3Y:14:ALA:O	10:3Y:18:ILE:HG12	2.04	0.56
1:3A:34:THR:OG1	2:3B:373:GLU:OE1	2.17	0.56
4:3D:137:ARG:HG3	4:3D:137:ARG:HH11	1.71	0.56
5:3E:152:ILE:HB	5:3E:272:ILE:HG23	1.87	0.56
5:3E:195:LEU:HD22	5:3E:248:ARG:HB3	1.88	0.56
5:3E:264:GLU:OE2	5:3E:264:GLU:N	2.36	0.56
1:3N:344:ARG:NH2	1:3N:353:GLU:OE1	2.36	0.56
6:3S:45:GLU:OE1	6:3S:48:ARG:NH2	2.38	0.56
4:3D:156:VAL:HG11	4:3D:180:PRO:HG3	1.88	0.56
4:3D:248:ALA:HB3	15:3D:501:HEC:HBD2	1.87	0.56
8:3H:83:LEU:O	8:3H:87:LEU:HG	2.06	0.56
10:3Y:36:THR:HG21	12:3Y:101:3PE:H222	1.88	0.56
1:3A:235:ARG:NH1	5:3E:92:ARG:HH22	2.04	0.56
4:3Q:23:HIS:NE2	4:3Q:199:ASP:OD2	2.38	0.56
4:3Q:77:ASP:N	4:3Q:77:ASP:OD1	2.34	0.56
3:3C:316:MET:HG3	12:3C:506:3PE:H111	1.88	0.55
2:3O:36:ALA:HB3	2:3O:207:ILE:HD12	1.88	0.55
2:3O:42:ALA:O	2:3O:113:ARG:NH1	2.39	0.55
2:3O:382:VAL:HG23	2:3O:392:TYR:CD1	2.41	0.55
1:3A:250:LEU:HD12	5:3I:44:ASP:HB2	1.87	0.55
1:3N:429:GLU:HG2	7:3T:5:GLY:H	1.71	0.55
4:3D:107:SER:O	4:3D:291:LYS:NZ	2.40	0.55
4:3D:108:SER:HB3	9:3J:48:ASN:HD22	1.70	0.55
3:3C:282:ARG:HG3	3:3C:282:ARG:HH11	1.70	0.55
5:3E:175:PHE:CD2	5:3E:215:GLY:HA2	2.41	0.55
9:3J:9:ARG:H	9:3J:9:ARG:HD2	1.72	0.55
1:3N:372:THR:N	2:3O:373:GLU:OE2	2.36	0.55
1:3N:304:CYS:HB3	1:3N:334:MET:SD	2.47	0.55
5:3R:224:PRO:HA	5:3R:237:PRO:HD3	1.88	0.55
5:3E:265:PHE:HD1	5:3E:271:VAL:HB	1.72	0.55
8:3H:90:ARG:HH11	8:3H:90:ARG:HB3	1.72	0.55
2:3O:78:LYS:HE2	2:3O:129:ALA:HB1	1.87	0.55
4:3Q:180:SER:HB3	8:3U:17:LEU:HB2	1.88	0.55
1:3A:61:HIS:CG	1:3A:134:ILE:HD11	2.41	0.55
4:3Q:223:LYS:NZ	11:3Q:502:CDL:OB4	2.30	0.55
17:3E:302:PC1:H111	17:3E:302:PC1:H11	1.89	0.55
2:3O:55:SER:HA	2:3O:58:GLU:HG3	1.89	0.55
5:3R:141:SER:OG	5:3R:142:ALA:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3O:222:ARG:HH21	2:3O:223:PHE:HE1	1.55	0.54
3:3P:34:GLY:HA3	13:3P:502:HEM:HBA2	1.90	0.54
2:3B:312:PHE:HA	5:3I:61:GLY:HA2	1.88	0.54
3:3C:116:GLY:C	13:3C:502:HEM:HBC2	2.28	0.54
9:3J:48:ASN:HB2	9:3J:51:LYS:HE2	1.87	0.54
1:3A:91:THR:HG22	1:3A:92:ARG:H	1.71	0.54
7:3G:20:LEU:HD21	7:3G:24:GLU:HB2	1.89	0.54
10:3X:14:ALA:O	10:3X:18:ILE:HG12	2.07	0.54
12:3N:502:3PE:H11	17:3R:302:PC1:H11	1.89	0.54
2:3O:70:ARG:O	2:3O:98:VAL:HG21	2.07	0.54
3:3P:37:LEU:HD11	3:3P:94:LEU:HA	1.90	0.54
5:3E:192:VAL:HA	5:3E:195:LEU:HD12	1.89	0.54
2:3O:45:SER:HB2	2:3O:116:ILE:HG13	1.89	0.54
2:3O:75:LEU:HD12	2:3O:136:GLU:HB3	1.89	0.54
3:3P:171:ASP:N	3:3P:171:ASP:OD1	2.41	0.54
7:3T:19:SER:HB3	7:3T:22:GLU:HG3	1.90	0.54
3:3C:136:GLY:N	3:3C:139:SER:OG	2.41	0.54
1:3A:39:VAL:HG12	1:3A:197:LEU:HD13	1.90	0.53
4:3D:219:LEU:HB3	4:3D:253:ILE:HD12	1.90	0.53
6:3F:96:GLU:HG2	6:3F:97:GLU:OE1	2.08	0.53
1:3N:60:GLU:OE2	2:3O:286:LYS:NZ	2.40	0.53
3:3C:282:ARG:HG3	3:3C:282:ARG:NH1	2.23	0.53
2:3O:299:VAL:HG11	2:3O:336:VAL:HG13	1.90	0.53
5:3R:219:HIS:HB2	5:3R:254:ALA:HA	1.89	0.53
8:3U:28:GLU:OE1	8:3U:28:GLU:N	2.41	0.53
10:3Y:38:TRP:CD2	12:3Y:101:3PE:H221	2.44	0.53
2:3B:29:LEU:N	2:3B:33:LEU:O	2.36	0.53
4:3D:125:CYS:O	4:3D:126:SER:OG	2.27	0.53
3:3P:197:LEU:O	3:3P:201:HIS:ND1	2.35	0.53
11:3P:506:CDL:HA32	11:3Q:502:CDL:HB61	1.90	0.53
4:3Q:144:ARG:HE	4:3Q:147:LEU:HD22	1.73	0.53
5:3R:204:ARG:HG3	5:3R:205:VAL:HG13	1.90	0.53
1:3A:62:LEU:HD21	1:3A:127:ILE:HG12	1.90	0.53
1:3N:359:ASN:O	1:3N:363:ASN:ND2	2.40	0.53
3:3P:326:TRP:HZ2	12:3P:505:3PE:H31	1.74	0.53
12:3A:502:3PE:H2	17:3E:302:PC1:H31	1.90	0.53
8:3U:24:CYS:O	8:3U:27:ILE:HG22	2.08	0.53
2:3B:97:SER:HA	5:3I:69:GLY:HA3	1.90	0.53
4:3D:115:ARG:CD	9:3J:60:TYR:CE1	2.88	0.53
5:3E:249:ILE:HG23	5:3E:257:ASN:HA	1.90	0.53
2:3O:120:MET:SD	2:3O:219:VAL:HG21	2.49	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3P:186:PRO:HG2	13:3P:501:HEM:HMC3	1.91	0.53
1:3A:339:GLN:O	1:3A:343:MET:HG2	2.09	0.53
2:3O:137:VAL:O	2:3O:141:GLN:HG2	2.09	0.53
5:3R:115:TYR:CD1	17:3R:302:PC1:H143	2.43	0.53
3:3C:329:VAL:O	3:3C:333:ILE:HG12	2.09	0.53
3:3C:373:GLU:OE2	6:3F:32:TYR:OH	2.25	0.53
5:3E:219:HIS:O	5:3E:219:HIS:ND1	2.42	0.53
1:3N:375:VAL:O	1:3N:379:ILE:HG13	2.09	0.53
2:3B:214:PRO:O	2:3B:218:GLN:HG2	2.09	0.52
11:3D:503:CDL:H541	11:3D:503:CDL:H752	1.90	0.52
6:3S:35:ASP:OD1	6:3S:89:TYR:OH	2.17	0.52
11:3A:501:CDL:H121	11:3A:501:CDL:H321	1.92	0.52
2:3B:28:ARG:HB2	2:3B:34:VAL:HG12	1.91	0.52
11:3C:505:CDL:OB7	7:3G:42:ARG:NH2	2.41	0.52
1:3A:125:SER:O	1:3A:129:LYS:HG3	2.10	0.52
4:3D:110:ASP:HA	9:3J:51:LYS:HB3	1.91	0.52
9:3J:53:TRP:CG	9:3J:57:LYS:CG	2.92	0.52
1:3A:3:THR:O	1:3A:5:ALA:N	2.38	0.52
3:3C:33:PHE:HA	3:3C:36:LEU:HD12	1.91	0.52
3:3C:282:ARG:HH12	5:3R:220:LEU:HD11	1.73	0.52
3:3C:324:LEU:HD12	3:3C:361:ILE:HG23	1.90	0.52
1:3A:244:ARG:CZ	1:3A:429:GLU:HB2	2.39	0.52
3:3P:361:ILE:HA	3:3P:365:LEU:HB2	1.90	0.52
5:3R:207:LYS:HB3	5:3R:210:TRP:HE3	1.74	0.52
1:3A:356:ARG:HG3	2:3B:91:ALA:HA	1.91	0.52
2:3B:163:LEU:HD21	2:3B:258:VAL:HG21	1.92	0.52
4:3Q:126:TYR:OH	15:3Q:501:HEC:O2A	2.22	0.52
1:3A:242:ARG:HB3	1:3A:428:ILE:HD11	1.92	0.52
1:3A:306:SER:OG	5:3I:39:GLU:OE1	2.24	0.52
3:3C:313:ARG:HB2	6:3F:50:TYR:CD1	2.45	0.52
1:3N:244:ARG:NH2	1:3N:429:GLU:OE2	2.27	0.52
11:3P:506:CDL:H522	11:3P:506:CDL:HA4	1.91	0.52
4:3Q:113:LEU:HD12	4:3Q:116:ILE:HG21	1.92	0.52
7:3T:71:ARG:NE	8:3U:56:GLU:OE2	2.28	0.52
9:3W:11:SER:O	9:3W:11:SER:OG	2.25	0.52
10:3Y:39:ARG:O	10:3Y:42:LEU:N	2.42	0.52
4:3Q:62:LYS:HD2	4:3Q:63:ALA:N	2.25	0.52
1:3A:76:GLU:OE1	2:3B:289:SER:N	2.42	0.52
5:3I:49:PHE:CB	5:3I:50:LEU:N	2.73	0.52
1:3N:444:LEU:HA	9:3W:17:THR:HG21	1.92	0.52
2:3O:121:GLU:O	2:3O:125:ASN:ND2	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3O:304:HIS:HA	5:3V:52:ARG:HH22	1.74	0.52
3:3P:320:LEU:HB2	3:3P:373:GLU:OE2	2.10	0.52
3:3P:29:SER:O	3:3P:32:ASN:HB2	2.10	0.51
6:3S:53:ASN:OD1	6:3S:54:LEU:N	2.44	0.51
8:3U:34:ARG:NH1	8:3U:37:LEU:HD23	2.25	0.51
1:3A:39:VAL:HG21	1:3A:117:VAL:HG11	1.91	0.51
3:3C:8:HIS:HB3	3:3C:11:MET:HG2	1.92	0.51
4:3D:121:TYR:HA	4:3D:125:CYS:SG	2.50	0.51
4:3D:222:TYR:OH	4:3D:249:MET:SD	2.67	0.51
5:3E:156:LEU:HD12	5:3E:157:SER:H	1.75	0.51
9:3J:53:TRP:CD1	9:3J:57:LYS:CG	2.92	0.51
4:3Q:3:LEU:HB3	7:3T:70:LYS:HE2	1.92	0.51
1:3A:86:LEU:HD12	1:3A:99:ILE:HB	1.93	0.51
2:3B:223:PHE:O	2:3B:225:ASN:ND2	2.42	0.51
4:3D:100:TRP:NE1	4:3D:212:GLU:HB2	2.25	0.51
5:3E:149:MET:SD	5:3E:150:SER:HB2	2.50	0.51
1:3N:3:THR:OG1	1:3N:6:GLN:OE1	2.23	0.51
2:3O:102:ARG:HG2	2:3O:176:LEU:HD21	1.92	0.51
8:3U:32:LYS:HD3	8:3U:32:LYS:N	2.26	0.51
2:3B:47:ILE:HD13	2:3B:120:MET:HG3	1.93	0.51
4:3D:165:ASP:N	4:3D:165:ASP:OD1	2.43	0.51
8:3U:35:GLU:O	8:3U:39:LEU:HD23	2.09	0.51
10:3Y:39:ARG:CZ	12:3Y:101:3PE:H12	2.40	0.51
6:3F:87:LEU:HB3	6:3F:91:GLN:HG3	1.92	0.51
8:3H:76:GLU:N	8:3H:76:GLU:OE1	2.44	0.51
2:3O:56:ARG:HD2	2:3O:103:GLU:HG2	1.93	0.51
8:3H:57:LYS:O	8:3H:60:GLU:HG3	2.11	0.51
1:3N:350:THR:OG1	1:3N:353:GLU:HG2	2.11	0.51
3:3C:165:TRP:O	3:3C:174:THR:OG1	2.27	0.51
12:3N:501:3PE:O12	12:3N:501:3PE:N	2.32	0.51
2:3O:71:LEU:HD22	2:3O:144:LEU:HD23	1.92	0.51
5:3R:180:THR:N	5:3R:183:GLU:OE2	2.40	0.51
1:3A:50:GLU:O	1:3A:173:ASN:ND2	2.38	0.51
2:3O:195:VAL:O	2:3O:199:PHE:HB2	2.11	0.51
5:3R:231:PHE:HB2	5:3R:250:ARG:NH2	2.25	0.51
3:3P:77:TRP:CD2	4:3Q:197:GLU:HG3	2.47	0.50
4:3Q:207:LYS:NZ	12:3Q:503:3PE:O12	2.43	0.50
1:3N:224:VAL:HG13	1:3N:225:GLU:N	2.26	0.50
5:3R:205:VAL:HG21	5:3R:211:VAL:HA	1.92	0.50
4:3D:135:ALA:HA	4:3D:178:TYR:HA	1.94	0.50
4:3D:157:GLU:HB3	4:3D:170:MET:HE2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3P:367:PRO:O	3:3P:371:ILE:HG12	2.12	0.50
2:3B:54:GLY:O	2:3B:194:TYR:OH	2.30	0.50
3:3C:146:ILE:HD11	14:3C:504:U10:C6	2.42	0.50
7:3G:56:VAL:O	7:3G:60:VAL:HG13	2.12	0.50
2:3O:58:GLU:OE1	2:3O:65:THR:N	2.45	0.50
2:3O:68:LEU:HD23	2:3O:191:LEU:HD21	1.93	0.50
8:3U:57:GLU:OE1	8:3U:57:GLU:N	2.41	0.50
10:3X:6:LEU:HD13	10:3X:11:ARG:HH12	1.76	0.50
1:3N:154:HIS:NE2	1:3N:314:TYR:OH	2.44	0.50
1:3N:399:ILE:O	1:3N:402:VAL:HG12	2.12	0.50
8:3U:18:THR:O	8:3U:22:GLU:HG2	2.12	0.50
4:3D:252:PRO:HB3	15:3D:501:HEC:HHC	1.92	0.50
5:3E:223:VAL:HB	4:3Q:144:ARG:NH2	2.26	0.50
3:3C:378:LYS:HG3	6:3F:29:ARG:NH1	2.26	0.50
5:3E:157:SER:N	5:3E:269:ASP:HB3	2.26	0.50
2:3O:214:PRO:O	2:3O:218:GLN:HG2	2.12	0.50
5:3R:220:LEU:HD12	5:3R:239:HIS:CE1	2.47	0.50
2:3B:96:LEU:O	5:3I:70:LEU:N	2.45	0.50
5:3I:55:LEU:HA	5:3I:58:GLN:NE2	2.25	0.50
3:3P:314:SER:OG	3:3P:315:MET:N	2.44	0.50
7:3T:50:PRO:HA	7:3T:53:VAL:HG12	1.94	0.50
1:3A:144:SER:HA	5:3I:47:ARG:HD2	1.94	0.50
1:3N:444:LEU:O	9:3W:17:THR:OG1	2.29	0.50
5:3E:225:ILE:HB	5:3E:235:TYR:HB3	1.93	0.49
13:3C:501:HEM:O1D	13:3C:501:HEM:HHA	2.11	0.49
8:3U:20:VAL:HG12	8:3U:69:VAL:HG22	1.94	0.49
2:3B:58:GLU:OE2	2:3B:65:THR:N	2.44	0.49
6:3F:92:TRP:O	6:3F:94:LYS:HD3	2.12	0.49
6:3F:121:LYS:O	10:3X:9:ARG:NH1	2.45	0.49
2:3O:76:THR:HG23	2:3O:81:SER:HA	1.94	0.49
2:3O:101:THR:HG22	5:3V:65:VAL:HG23	1.94	0.49
4:3D:280:ARG:O	4:3D:280:ARG:HD3	2.11	0.49
9:3J:5:THR:OG1	9:3J:9:ARG:NH1	2.46	0.49
3:3P:35:SER:OG	14:3P:503:U10:O5	2.29	0.49
1:3A:158:PHE:O	1:3A:161:THR:OG1	2.25	0.49
2:3B:278:VAL:HG11	2:3B:352:LEU:HD11	1.94	0.49
2:3O:209:LEU:HD11	2:3O:378:PHE:HD2	1.77	0.49
4:3Q:178:THR:OG1	8:3U:15:ASP:OD1	2.30	0.49
1:3A:79:VAL:HG11	1:3A:86:LEU:HB2	1.94	0.49
5:3R:225:ILE:HG13	5:3R:235:TYR:O	2.12	0.49
1:3A:304:CYS:SG	1:3A:306:SER:N	2.86	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:3H:46:ARG:NE	8:3H:90:ARG:HH21	2.10	0.49
9:3J:21:PHE:O	9:3J:25:ILE:HG12	2.13	0.49
2:3B:201:SER:HB2	2:3B:228:GLY:HA2	1.93	0.49
3:3C:51:LEU:HD13	13:3C:501:HEM:HBD1	1.93	0.49
5:3E:157:SER:H	5:3E:269:ASP:HB3	1.77	0.49
6:3F:25:LEU:O	6:3F:28:ILE:HG22	2.13	0.49
9:3J:53:TRP:CE2	9:3J:57:LYS:CE	2.66	0.49
1:3N:131:ARG:HD3	1:3N:175:ARG:HA	1.94	0.49
3:3P:369:THR:O	3:3P:373:GLU:HG3	2.12	0.49
4:3D:208:ARG:HH21	15:3D:501:HEC:CGA	2.24	0.49
1:3N:161:THR:HG21	1:3N:235:ARG:H	1.78	0.49
4:3D:159:GLN:NE2	4:3D:168:MET:O	2.45	0.49
7:3G:10:THR:OG1	7:3G:11:ARG:N	2.45	0.49
5:3I:49:PHE:C	5:3I:50:LEU:CB	2.82	0.49
6:3F:113:ARG:O	6:3F:117:GLU:HG2	2.13	0.48
2:3O:303:VAL:HG11	2:3O:336:VAL:HG22	1.94	0.48
3:3P:221:HIS:O	3:3P:225:THR:OG1	2.17	0.48
5:3R:150:SER:HA	5:3R:169:TRP:HE1	1.78	0.48
5:3R:175:PHE:HE2	5:3R:224:PRO:HG2	1.78	0.48
1:3A:3:THR:O	1:3A:3:THR:OG1	2.30	0.48
3:3C:229:ILE:HG23	17:3E:302:PC1:H3A1	1.95	0.48
4:3D:119:GLN:NE2	4:3D:261:ASP:OD2	2.44	0.48
14:3P:503:U10:H3M3	14:3P:503:U10:C4M	2.32	0.48
3:3C:184:ILE:HD13	3:3P:49:LEU:HD12	1.94	0.48
3:3C:233:LEU:HD12	4:3D:308:VAL:HG21	1.95	0.48
1:3N:80:GLU:HG2	2:3O:284:HIS:HB2	1.95	0.48
2:3O:169:ARG:HG3	2:3O:240:ARG:HB3	1.95	0.48
3:3P:313:ARG:N	6:3S:38:TYR:HB2	2.29	0.48
5:3R:152:ILE:HG12	5:3R:154:ILE:HG12	1.96	0.48
1:3A:90:SER:HB3	1:3A:95:THR:HG23	1.96	0.48
1:3A:373:THR:HB	1:3A:374:PRO:HD3	1.95	0.48
3:3C:145:VAL:O	3:3C:149:LEU:HD13	2.14	0.48
4:3D:226:PRO:O	4:3D:229:VAL:HG22	2.14	0.48
1:3N:100:LYS:HG2	2:3O:370:MET:CE	2.43	0.48
2:3O:202:ALA:HB3	2:3O:230:LEU:HA	1.93	0.48
2:3O:302:GLY:O	2:3O:304:HIS:ND1	2.45	0.48
5:3I:41:PRO:O	5:3I:44:ASP:HB3	2.13	0.48
9:3J:53:TRP:NE1	9:3J:57:LYS:HD3	2.20	0.48
2:3O:207:ILE:HG21	2:3O:382:VAL:HG11	1.95	0.48
2:3B:276:GLN:HB2	2:3B:322:PHE:HE1	1.78	0.48
1:3N:140:GLU:OE2	5:3V:50:LEU:HD23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3O:366:ALA:O	2:3O:370:MET:HB2	2.13	0.48
4:3Q:31:GLN:O	4:3Q:35:GLN:HG2	2.14	0.48
5:3R:225:ILE:HG23	5:3R:237:PRO:HG3	1.96	0.48
8:3U:17:LEU:HD13	8:3U:21:ARG:HD2	1.95	0.48
1:3A:183:THR:HA	1:3A:186:VAL:HG12	1.95	0.48
2:3B:95:LYS:CE	5:3I:32:ALA:HA	2.42	0.48
2:3B:101:THR:HG23	2:3B:103:GLU:H	1.77	0.48
2:3B:352:LEU:HD12	2:3B:352:LEU:HA	1.72	0.48
4:3D:204:ILE:HD12	15:3D:501:HEC:HMA3	1.96	0.48
1:3N:244:ARG:HE	7:3T:10:MET:HB2	1.78	0.48
10:3Y:32:LEU:O	10:3Y:36:THR:HG22	2.12	0.48
1:3A:108:LYS:O	1:3A:111:GLU:HB3	2.13	0.48
2:3B:319:SER:OG	2:3B:320:GLY:N	2.47	0.48
2:3B:334:GLY:HA2	2:3B:434:PRO:HD3	1.95	0.48
4:3D:137:ARG:HG3	4:3D:137:ARG:NH1	2.27	0.48
6:3F:99:LYS:N	6:3F:99:LYS:HD2	2.28	0.48
5:3R:154:ILE:HG21	5:3R:167:PHE:CD2	2.49	0.48
10:3X:45:VAL:HG13	10:3X:48:ILE:HB	1.95	0.48
5:3E:205:VAL:HG22	5:3E:207:LYS:H	1.79	0.48
8:3H:44:THR:O	8:3H:48:GLN:HG2	2.14	0.48
1:3N:244:ARG:HH12	1:3N:429:GLU:CD	2.17	0.48
5:3R:163:LYS:HB3	5:3R:165:MET:HE1	1.96	0.48
1:3N:6:GLN:OE1	1:3N:6:GLN:N	2.47	0.47
7:3T:67:GLU:HA	7:3T:70:LYS:HB3	1.96	0.47
1:3A:46:ARG:NH2	1:3A:316:GLU:OE1	2.45	0.47
1:3A:308:GLN:HE21	5:3I:35:PRO:HB2	1.79	0.47
2:3B:365:LYS:HG2	2:3B:399:LEU:HD22	1.96	0.47
4:3D:160:ASP:OD2	4:3D:171:ARG:NE	2.45	0.47
5:3E:152:ILE:HD12	5:3E:152:ILE:O	2.14	0.47
1:3N:209:LEU:HA	1:3N:209:LEU:HD23	1.75	0.47
5:3R:130:LYS:NZ	9:3W:32:GLU:OE1	2.40	0.47
5:3E:232:GLY:HA3	5:3E:245:ALA:HA	1.95	0.47
1:3A:46:ARG:HH22	1:3A:316:GLU:CD	2.18	0.47
3:3P:46:LEU:HD11	12:3Q:503:3PE:H2C1	1.96	0.47
5:3R:159:ILE:CD1	5:3R:178:HIS:HB2	2.44	0.47
5:3R:160:PRO:HD2	5:3R:160:PRO:O	2.12	0.47
1:3A:279:HIS:ND1	1:3A:284:TYR:OH	2.39	0.47
2:3B:285:VAL:HG13	2:3B:288:GLY:HA3	1.95	0.47
2:3O:36:ALA:O	2:3O:207:ILE:HA	2.14	0.47
3:3P:146:ILE:O	3:3P:149:LEU:HB2	2.15	0.47
5:3R:205:VAL:HA	5:3R:263:TYR:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3C:29:SER:OG	11:3C:505:CDL:OA9	2.25	0.47
5:3R:235:TYR:HE1	5:3R:240:GLY:HA2	1.78	0.47
3:3C:8:HIS:O	3:3C:12:LYS:N	2.41	0.47
3:3C:78:VAL:O	3:3C:82:LEU:HB2	2.15	0.47
5:3E:241:SER:HA	5:3E:251:LYS:O	2.15	0.47
8:3H:59:ARG:O	8:3H:63:GLU:HG2	2.13	0.47
1:3N:45:SER:HB2	1:3N:167:VAL:HA	1.96	0.47
3:3P:215:MET:HB2	7:3T:10:MET:HE2	1.97	0.47
4:3Q:134:TYR:OH	4:3Q:160:MET:HB2	2.15	0.47
5:3R:256:LEU:HD23	5:3R:257:ASN:H	1.79	0.47
8:3U:28:GLU:O	8:3U:32:LYS:NZ	2.40	0.47
3:3C:77:TRP:CZ3	4:3D:290:ARG:HG3	2.50	0.47
6:3F:57:GLU:OE1	6:3F:60:ARG:NH1	2.48	0.47
1:3N:245:ASP:OD1	7:3T:11:ARG:NH1	2.48	0.47
2:3O:52:LYS:HB2	2:3O:203:ARG:HB2	1.97	0.47
1:3A:240:GLU:HG2	7:3G:19:SER:HB3	1.97	0.47
3:3C:30:TRP:NE1	12:3C:506:3PE:H221	2.30	0.47
3:3C:221:HIS:O	3:3C:225:THR:OG1	2.20	0.47
1:3N:231:PHE:HZ	1:3N:316:GLU:HB3	1.79	0.47
5:3R:226:ALA:HA	5:3R:234:TYR:HD1	1.79	0.47
2:3B:49:LEU:HD11	2:3B:204:MET:HE3	1.96	0.47
2:3B:56:ARG:NH1	2:3B:318:ASP:OD1	2.48	0.47
2:3B:411:ILE:C	2:3B:412:ASN:HB2	2.35	0.47
4:3Q:42:SER:HB3	4:3Q:94:PRO:HD2	1.97	0.47
2:3B:220:ALA:O	2:3B:224:LEU:HB2	2.15	0.46
3:3C:120:LEU:O	3:3C:124:MET:HG3	2.15	0.46
6:3F:52:ASP:O	6:3F:56:LYS:HG3	2.15	0.46
5:3I:32:ALA:N	5:3I:71:ASN:OD1	2.48	0.46
3:3P:67:THR:HG22	4:3Q:115:TYR:HE2	1.79	0.46
3:3P:346:PRO:HB3	7:3T:65:GLU:HG3	1.96	0.46
5:3R:158:ASP:OD1	5:3R:159:ILE:HG23	2.16	0.46
5:3R:195:LEU:HD11	5:3R:250:ARG:HG2	1.98	0.46
6:3S:29:LEU:HD21	6:3S:69:THR:HG23	1.97	0.46
1:3A:37:VAL:HG23	1:3A:199:ALA:HB2	1.96	0.46
11:3A:501:CDL:H151	12:3A:502:3PE:H241	1.97	0.46
2:3O:97:SER:HA	5:3V:69:GLY:HA2	1.96	0.46
5:3R:216:VAL:HA	5:3R:222:CYS:O	2.15	0.46
2:3B:76:THR:HG23	2:3B:81:SER:HA	1.98	0.46
1:3N:17:SER:OG	1:3N:205:HIS:NE2	2.39	0.46
3:3P:15:ASN:HA	3:3P:19:ILE:HD12	1.98	0.46
3:3P:211:ILE:HG21	6:3S:62:ILE:HD13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3P:342:PRO:HB2	3:3P:344:GLU:OE1	2.15	0.46
5:3R:160:PRO:CD	5:3R:163:LYS:HB2	2.45	0.46
3:3P:8:HIS:O	3:3P:12:LYS:N	2.40	0.46
1:3A:346:CYS:SG	1:3A:416:TYR:HB2	2.56	0.46
8:3H:64:LEU:O	8:3H:67:GLN:HG2	2.15	0.46
5:3I:49:PHE:HB3	5:3I:50:LEU:N	2.31	0.46
4:3Q:62:LYS:HB3	4:3Q:87:LEU:HD11	1.98	0.46
1:3A:163:LEU:HD23	1:3A:163:LEU:HA	1.76	0.46
6:3F:119:TRP:CZ2	2:3O:87:ARG:HB3	2.51	0.46
4:3Q:56:TYR:HD2	4:3Q:60:GLU:HB3	1.79	0.46
4:3Q:206:LEU:HD23	9:3W:43:TYR:HB2	1.98	0.46
12:3D:502:3PE:H31	5:3E:131:ASN:OD1	2.16	0.46
5:3E:265:PHE:CD1	5:3E:271:VAL:HB	2.51	0.46
12:3N:501:3PE:H2	12:3N:501:3PE:H221	1.55	0.46
3:3P:138:MET:HE3	3:3P:254:ASP:HB2	1.98	0.46
4:3Q:211:MET:HG2	12:3Q:503:3PE:H332	1.96	0.46
6:3S:12:TRP:CD1	6:3S:14:GLU:HB2	2.51	0.46
7:3T:71:ARG:HD2	7:3T:71:ARG:HA	1.72	0.46
10:3X:38:TRP:NE1	10:3X:40:LEU:HB3	2.31	0.46
2:3B:52:LYS:HB2	2:3B:387:LEU:HD22	1.96	0.46
3:3C:373:GLU:OE2	6:3F:32:TYR:CZ	2.69	0.46
4:3D:307:LEU:O	4:3D:311:MET:HG3	2.15	0.46
5:3E:237:PRO:HD2	4:3Q:144:ARG:NH1	2.30	0.46
3:3P:156:ILE:HG13	3:3P:157:GLY:H	1.81	0.46
4:3Q:12:TRP:NE1	4:3Q:125:ASP:OD1	2.46	0.46
4:3Q:72:ASP:OD2	4:3Q:83:ARG:NH1	2.49	0.46
5:3R:228:ALA:HB3	5:3R:235:TYR:HB3	1.97	0.46
6:3S:64:ARG:O	6:3S:68:LEU:HD23	2.15	0.46
3:3C:311:LYS:HA	3:3C:311:LYS:HD2	1.79	0.46
1:3N:17:SER:HG	1:3N:205:HIS:CE1	2.33	0.46
4:3Q:49:ARG:O	4:3Q:52:VAL:HG22	2.15	0.46
9:3W:42:ILE:O	9:3W:46:ILE:HG13	2.16	0.46
2:3B:26:PHE:CD2	2:3B:36:ALA:HB2	2.51	0.46
3:3P:346:PRO:HG3	7:3T:66:PHE:HA	1.97	0.46
5:3R:225:ILE:HD11	5:3R:235:TYR:HD2	1.81	0.46
9:3W:18:SER:HB2	10:3X:23:MET:SD	2.56	0.46
1:3A:186:VAL:HG23	1:3A:190:TYR:CD2	2.51	0.45
1:3A:280:TYR:HB3	1:3A:307:PHE:CE1	2.51	0.45
4:3D:108:SER:HB3	9:3J:48:ASN:ND2	2.31	0.45
14:3P:504:U10:H1M1	14:3P:504:U10:H103	1.97	0.45
5:3R:256:LEU:HD23	5:3R:257:ASN:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:3S:85:GLU:O	6:3S:85:GLU:HG2	2.14	0.45
7:3T:11:ARG:HG2	7:3T:11:ARG:HH11	1.80	0.45
5:3E:152:ILE:HA	5:3E:274:GLY:HA2	1.98	0.45
3:3P:377:LEU:HD22	6:3S:33:ARG:HG3	1.98	0.45
5:3R:121:THR:O	5:3R:125:VAL:HG23	2.17	0.45
3:3C:168:PHE:CE2	5:3R:149:MET:HG3	2.51	0.45
3:3C:357:LEU:O	3:3C:361:ILE:HG13	2.16	0.45
7:3G:69:GLU:OE2	7:3G:70:LYS:HD2	2.17	0.45
1:3N:34:THR:HA	1:3N:102:LEU:HA	1.98	0.45
1:3N:348:SER:OG	10:3X:17:TRP:NE1	2.48	0.45
3:3P:28:SER:HB2	11:3P:506:CDL:HA22	1.98	0.45
3:3P:324:LEU:HD23	3:3P:324:LEU:HA	1.84	0.45
4:3Q:8:PRO:HG3	8:3U:66:ASP:HB3	1.99	0.45
1:3A:145:MET:SD	1:3A:248:LEU:HD13	2.57	0.45
2:3B:255:ALA:HB3	2:3B:337:ILE:HD11	1.97	0.45
3:3C:177:ARG:NH1	5:3R:140:MET:O	2.46	0.45
6:3F:96:GLU:N	6:3F:96:GLU:OE1	2.49	0.45
1:3N:223:TYR:CD2	1:3N:229:PRO:HD2	2.52	0.45
1:3N:181:ASP:OD1	1:3N:181:ASP:N	2.48	0.45
1:3N:339:GLN:NE2	1:3N:437:ILE:HG23	2.30	0.45
3:3P:78:VAL:O	3:3P:82:LEU:HB2	2.17	0.45
3:3P:185:LEU:HD23	3:3P:185:LEU:HA	1.82	0.45
3:3P:377:LEU:CD2	6:3S:33:ARG:HG3	2.47	0.45
4:3Q:3:LEU:HD12	8:3U:59:PHE:CD2	2.52	0.45
5:3R:248:ARG:HA	5:3R:257:ASN:ND2	2.32	0.45
8:3U:38:GLU:HA	8:3U:41:ASP:HB2	1.99	0.45
12:3A:503:3PE:H341	3:3C:5:ARG:HB2	1.98	0.45
2:3B:203:ARG:HD2	2:3B:230:LEU:O	2.16	0.45
2:3O:369:LEU:HD11	2:3O:399:LEU:HD11	1.98	0.45
5:3R:206:LYS:HE2	5:3R:263:TYR:CD1	2.52	0.45
1:3A:61:HIS:CE1	2:3B:287:ARG:HD2	2.52	0.45
2:3B:286:LYS:HE3	2:3B:287:ARG:NH2	2.32	0.45
2:3B:305:GLN:O	5:3I:52:ARG:NH1	2.47	0.45
3:3C:186:PRO:HG2	13:3C:501:HEM:HMC3	1.99	0.45
2:3O:56:ARG:HB2	2:3O:172:LEU:HD23	1.98	0.45
3:3P:159:ASP:O	3:3P:162:GLU:HG3	2.17	0.45
5:3R:131:ASN:O	5:3R:135:GLN:HG2	2.17	0.45
5:3R:187:GLU:OE2	5:3R:246:SER:OG	2.28	0.45
5:3R:200:HIS:CE1	5:3R:202:LEU:HB2	2.47	0.45
7:3T:65:GLU:HA	7:3T:68:LYS:NZ	2.32	0.45
2:3B:118:ILE:HD12	2:3B:118:ILE:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3I:40:SER:OG	5:3I:40:SER:O	2.33	0.45
2:3O:75:LEU:HD21	2:3O:140:LEU:HD13	1.98	0.45
2:3O:163:LEU:HD21	2:3O:258:VAL:HG21	1.98	0.45
3:3P:24:PRO:HB2	3:3P:27:ILE:HG23	1.97	0.45
5:3V:62:ARG:HH21	5:3V:77:ARG:NH1	2.14	0.45
4:3D:225:PRO:HG3	4:3D:237:PHE:HB2	1.99	0.45
6:3F:63:PRO:HG2	6:3F:66:LEU:HB2	1.99	0.45
2:3O:111:CYS:SG	2:3O:119:LEU:HD13	2.57	0.45
2:3O:164:HIS:NE2	2:3O:316:TYR:OH	2.38	0.45
4:3Q:41:HIS:HE1	4:3Q:111:PRO:HD2	1.82	0.45
5:3R:155:LYS:HB3	5:3R:270:LEU:HD13	1.99	0.45
5:3R:195:LEU:C	5:3R:197:ASP:H	2.20	0.45
8:3U:42:GLN:N	8:3U:42:GLN:OE1	2.50	0.45
1:3A:436:ARG:HD3	3:3C:222:PRO:HD3	1.99	0.45
3:3C:146:ILE:HD13	3:3C:146:ILE:HA	1.83	0.45
3:3C:268:ILE:HG13	14:3C:504:U10:H3M1	1.98	0.45
4:3D:115:ARG:HE	9:3J:60:TYR:HE1	1.58	0.45
5:3E:266:THR:HB	5:3E:270:LEU:HB2	1.97	0.45
5:3E:269:ASP:O	5:3E:270:LEU:HD23	2.17	0.45
3:3P:226:ILE:HD12	3:3P:226:ILE:HA	1.81	0.45
3:3C:9:PRO:HA	3:3C:12:LYS:HE2	1.99	0.44
3:3P:58:ASP:OD1	3:3P:59:THR:N	2.51	0.44
12:3Y:101:3PE:H32	12:3Y:101:3PE:H321	1.63	0.44
2:3B:67:HIS:O	2:3B:71:LEU:HD12	2.17	0.44
3:3C:26:ASN:ND2	6:3F:78:LEU:HG	2.32	0.44
3:3C:141:TRP:CD1	3:3C:265:PRO:HD3	2.52	0.44
4:3D:171:ARG:HD2	4:3D:172:PRO:O	2.16	0.44
11:3D:503:CDL:H112	11:3D:503:CDL:HA4	1.35	0.44
6:3F:85:GLN:HG3	7:3G:38:ASN:HD21	1.82	0.44
14:3P:503:U10:H72	14:3P:503:U10:H1M1	1.80	0.44
6:3S:35:ASP:OD2	6:3S:61:ARG:NH1	2.50	0.44
7:3T:65:GLU:HA	7:3T:68:LYS:HZ2	1.82	0.44
2:3B:89:ILE:HD13	2:3B:119:LEU:HD13	1.99	0.44
3:3C:47:THR:OG1	3:3C:83:HIS:ND1	2.41	0.44
4:3D:288:ASP:OD1	4:3D:288:ASP:N	2.49	0.44
5:3E:216:VAL:HG11	3:3P:262:LEU:HD22	1.99	0.44
3:3P:26:ASN:ND2	6:3S:69:THR:OG1	2.37	0.44
3:3P:150:LEU:O	3:3P:153:ILE:HG22	2.17	0.44
5:3R:161:GLU:HG2	5:3R:181:LYS:H	1.83	0.44
8:3U:15:ASP:OD2	8:3U:17:LEU:HB3	2.17	0.44
3:3C:182:HIS:HE1	13:3C:501:HEM:NB	2.10	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3E:212:ILE:O	5:3E:213:LEU:HD23	2.17	0.44
9:3J:34:ARG:NE	9:3J:38:GLN:HE21	2.16	0.44
4:3Q:240:PRO:HD3	7:3T:12:HIS:CD2	2.53	0.44
5:3R:130:LYS:HA	12:3R:303:3PE:H2B2	1.98	0.44
1:3A:262:TRP:CG	1:3A:385:THR:HB	2.52	0.44
4:3D:247:ILE:HD12	4:3D:247:ILE:HA	1.84	0.44
6:3F:28:ILE:HD12	6:3F:28:ILE:HA	1.83	0.44
1:3N:125:SER:O	1:3N:129:LYS:HG3	2.18	0.44
1:3N:345:LEU:HD23	1:3N:345:LEU:HA	1.77	0.44
3:3P:113:TRP:NE1	3:3P:301:LEU:O	2.41	0.44
3:3P:197:LEU:HD22	14:3P:503:U10:H1M3	2.00	0.44
5:3V:53:GLU:CD	5:3V:53:GLU:H	2.21	0.44
1:3A:64:PHE:CZ	1:3A:88:ALA:HB2	2.53	0.44
1:3A:375:VAL:O	1:3A:379:ILE:HG13	2.17	0.44
4:3D:206:ARG:HD2	4:3D:283:SER:HB3	1.98	0.44
1:3N:219:LEU:HD23	1:3N:219:LEU:HA	1.78	0.44
5:3R:164:ASN:ND2	5:3R:226:ALA:HB1	2.32	0.44
3:3C:185:LEU:HA	3:3C:185:LEU:HD23	1.81	0.44
5:3E:155:LYS:HB2	5:3E:271:VAL:HG13	2.00	0.44
5:3E:163:LYS:O	5:3E:177:ARG:HA	2.17	0.44
5:3E:179:ARG:NH2	5:3E:208:PRO:HA	2.29	0.44
1:3N:346:CYS:SG	1:3N:411:CYS:HB3	2.58	0.44
5:3R:186:GLN:O	5:3R:190:VAL:HG23	2.17	0.44
7:3T:45:ILE:HD12	7:3T:45:ILE:HA	1.90	0.44
10:3Y:8:PRO:O	10:3Y:11:ARG:HG2	2.17	0.44
1:3A:100:LYS:HD3	1:3A:373:THR:OG1	2.17	0.44
1:3A:332:ASP:H	1:3A:430:GLN:HG2	1.83	0.44
1:3A:379:ILE:O	1:3A:383:LEU:HD12	2.18	0.44
3:3C:94:LEU:HD23	3:3C:94:LEU:HA	1.81	0.44
3:3C:146:ILE:O	3:3C:149:LEU:HB2	2.18	0.44
4:3D:115:ARG:CD	9:3J:60:TYR:OH	2.54	0.44
3:3P:149:LEU:HD21	3:3P:281:LEU:HD11	1.99	0.44
4:3Q:172:ASP:OD1	4:3Q:173:ASP:N	2.51	0.44
1:3A:350:THR:HG22	10:3Y:13:LEU:HD21	1.99	0.44
2:3B:148:LYS:HE3	2:3B:152:PHE:HE2	1.83	0.44
3:3C:10:LEU:HD23	3:3C:10:LEU:HA	1.85	0.44
5:3E:213:LEU:HD12	5:3E:234:TYR:CE2	2.53	0.44
3:3P:3:ASN:ND2	11:3P:507:CDL:OA3	2.38	0.44
5:3R:180:THR:HB	5:3R:182:LYS:HE3	2.00	0.44
5:3R:248:ARG:HA	5:3R:257:ASN:HD21	1.83	0.44
3:3P:21:LEU:HD13	3:3P:201:HIS:HD2	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3P:132:VAL:HA	3:3P:139:SER:HB3	2.00	0.43
5:3R:159:ILE:HD11	5:3R:210:TRP:CD1	2.48	0.43
1:3A:148:VAL:HG22	5:3E:80:HIS:CG	2.53	0.43
1:3A:206:ARG:HD2	1:3A:206:ARG:N	2.33	0.43
2:3B:407:ASP:O	2:3B:411:ILE:HD13	2.17	0.43
5:3E:95:GLU:OE1	5:3E:95:GLU:N	2.47	0.43
5:3E:220:LEU:HD13	3:3P:263:ASN:ND2	2.33	0.43
3:3P:214:ASP:OD1	7:3T:2:ARG:NH1	2.50	0.43
4:3Q:35:GLN:HG2	4:3Q:35:GLN:H	1.73	0.43
6:3S:45:GLU:O	6:3S:49:ARG:HG3	2.18	0.43
3:3C:56:THR:OG1	3:3C:61:THR:O	2.35	0.43
1:3N:148:VAL:HG12	5:3R:80:HIS:CD2	2.52	0.43
1:3N:240:GLU:HA	1:3N:422:VAL:O	2.18	0.43
3:3P:71:ARG:NH2	4:3Q:193:ALA:O	2.45	0.43
3:3P:149:LEU:HD11	3:3P:281:LEU:HD11	2.00	0.43
4:3Q:223:LYS:HE2	4:3Q:227:TRP:CD1	2.53	0.43
2:3B:148:LYS:HE3	2:3B:152:PHE:CE2	2.53	0.43
5:3E:156:LEU:HD12	5:3E:157:SER:N	2.31	0.43
9:3J:34:ARG:HG3	10:3Y:47:TYR:HE1	1.82	0.43
1:3N:100:LYS:HG2	2:3O:370:MET:HE1	2.00	0.43
12:3N:502:3PE:H32	3:3P:221:HIS:CE1	2.52	0.43
4:3Q:202:LYS:HZ2	4:3Q:202:LYS:HG3	1.56	0.43
1:3A:312:ILE:O	1:3A:319:LEU:N	2.42	0.43
2:3O:98:VAL:HG22	5:3V:68:VAL:O	2.19	0.43
11:3P:507:CDL:HB32	11:3P:507:CDL:H112	2.01	0.43
5:3R:195:LEU:HD12	5:3R:195:LEU:HA	1.85	0.43
5:3E:112:GLY:HA2	9:3J:11:TYR:HB2	2.01	0.43
9:3J:54:LYS:HE3	9:3J:54:LYS:HB3	1.83	0.43
2:3B:68:LEU:HD21	2:3B:137:VAL:HG13	2.00	0.43
1:3A:431:LEU:HD12	1:3A:432:PRO:HD2	2.00	0.43
2:3B:70:ARG:HD3	2:3B:100:SER:HB3	2.00	0.43
5:3E:88:PHE:O	5:3E:92:ARG:HG3	2.19	0.43
1:3N:436:ARG:HD3	3:3P:222:PRO:HD3	2.01	0.43
2:3O:94:GLY:HA3	2:3O:119:LEU:HD21	2.01	0.43
3:3P:26:ASN:HD21	6:3S:66:LEU:HD23	1.84	0.43
3:3P:31:TRP:HE3	3:3P:31:TRP:H	1.66	0.43
4:3Q:43:MET:HG2	4:3Q:46:VAL:HG12	1.99	0.43
9:3W:29:LEU:HD13	10:3X:34:TRP:HB2	2.00	0.43
2:3B:37:SER:HB3	2:3B:213:HIS:CD2	2.52	0.43
2:3B:181:TYR:CZ	2:3O:247:GLN:HG2	2.54	0.43
1:3N:64:PHE:CD1	1:3N:86:LEU:HD21	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:3O:241:GLY:HA2	2:3O:423:SER:OG	2.19	0.43
2:3O:335:ASP:N	2:3O:335:ASP:OD1	2.50	0.43
2:3O:438:GLU:N	2:3O:438:GLU:OE1	2.52	0.43
1:3A:132:ASP:HA	1:3A:135:LEU:HD12	2.01	0.43
3:3P:338:ILE:HD13	3:3P:338:ILE:HA	1.86	0.43
5:3R:160:PRO:O	5:3R:178:HIS:HB3	2.19	0.43
5:3R:264:GLU:O	5:3R:272:ILE:HB	2.19	0.43
2:3B:25:GLU:O	2:3B:36:ALA:HA	2.19	0.42
2:3B:206:LEU:HD12	2:3B:224:LEU:HD11	2.01	0.42
2:3B:401:GLN:HA	2:3B:401:GLN:OE1	2.19	0.42
3:3C:116:GLY:HA2	3:3C:119:LEU:HD12	2.00	0.42
3:3C:132:VAL:HA	3:3C:139:SER:HB2	2.01	0.42
3:3C:154:PRO:O	3:3C:156:ILE:N	2.46	0.42
3:3C:302:ILE:O	3:3C:305:PRO:HD2	2.18	0.42
5:3E:79:SER:N	5:3E:82:ASP:OD2	2.51	0.42
6:3F:79:ASP:O	6:3F:82:MET:HG2	2.19	0.42
7:3G:20:LEU:HD23	7:3G:21:SER:N	2.34	0.42
8:3H:53:GLU:HA	8:3H:56:ILE:HD12	2.01	0.42
1:3N:111:GLU:HB2	1:3N:215:HIS:CE1	2.54	0.42
4:3Q:7:ALA:HA	4:3Q:152:TYR:HE2	1.84	0.42
4:3Q:83:ARG:NH1	4:3Q:86:LYS:HE2	2.34	0.42
8:3U:15:ASP:HB3	8:3U:18:THR:HG23	2.01	0.42
9:3W:44:GLU:HG2	9:3W:53:LYS:HD3	2.01	0.42
9:3W:50:LYS:HB2	9:3W:50:LYS:HE3	1.84	0.42
1:3A:240:GLU:OE2	1:3A:242:ARG:HD2	2.19	0.42
11:3A:501:CDL:H312	3:3C:19:ILE:HD12	2.00	0.42
3:3C:349:ILE:H	3:3C:349:ILE:HD12	1.84	0.42
4:3Q:198:HIS:O	4:3Q:202:LYS:HG2	2.18	0.42
8:3U:39:LEU:HD13	8:3U:42:GLN:HE22	1.83	0.42
2:3B:245:ARG:HB3	2:3B:430:LEU:HD23	2.01	0.42
3:3C:272:TRP:HA	3:3C:275:LEU:HD12	2.01	0.42
1:3N:49:ASN:OD1	1:3N:51:LYS:N	2.52	0.42
4:3Q:23:HIS:HD2	9:3W:51:LEU:HA	1.84	0.42
5:3R:213:LEU:HD13	5:3R:213:LEU:HA	1.90	0.42
7:3T:28:HIS:HB2	7:3T:32:LYS:HE2	2.01	0.42
1:3A:270:LEU:HD13	1:3A:410:VAL:HG22	2.00	0.42
2:3B:36:ALA:HB3	2:3B:207:ILE:CD1	2.49	0.42
2:3B:395:PRO:O	2:3B:399:LEU:HG	2.18	0.42
12:3Q:503:3PE:H361	5:3R:128:ALA:HB1	2.01	0.42
3:3C:231:GLY:HA2	11:3D:503:CDL:H721	2.01	0.42
3:3C:240:LEU:HD23	3:3C:240:LEU:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3N:148:VAL:HG12	5:3R:80:HIS:CG	2.54	0.42
3:3P:300:ILE:HD12	3:3P:300:ILE:HA	1.92	0.42
5:3R:191:GLU:HB3	5:3R:195:LEU:HD13	2.01	0.42
7:3T:24:ARG:HD2	7:3T:24:ARG:HA	1.68	0.42
1:3A:240:GLU:HA	1:3A:422:VAL:O	2.18	0.42
4:3D:109:LEU:HD22	4:3D:281:TRP:HB2	2.00	0.42
4:3D:304:LEU:HD23	4:3D:304:LEU:HA	1.79	0.42
2:3O:283:PRO:HD3	5:3V:57:GLY:HA2	2.02	0.42
5:3R:187:GLU:HA	5:3R:190:VAL:HB	2.01	0.42
5:3R:212:ILE:HD12	5:3R:212:ILE:O	2.20	0.42
3:3C:191:ALA:O	3:3C:195:VAL:HG23	2.19	0.42
4:3D:205:VAL:O	4:3D:211:GLY:HA2	2.20	0.42
5:3E:241:SER:OG	16:3E:301:FES:S1	2.67	0.42
1:3N:260:PRO:HB2	1:3N:264:ASN:HB3	2.00	0.42
1:3N:294:LEU:HD23	1:3N:307:PHE:CZ	2.54	0.42
2:3O:218:GLN:O	2:3O:222:ARG:HB2	2.20	0.42
3:3P:89:MET:HE3	3:3P:89:MET:HB2	1.80	0.42
3:3P:109:PHE:O	3:3P:111:GLU:N	2.52	0.42
4:3Q:216:LEU:HD23	4:3Q:216:LEU:HA	1.90	0.42
1:3A:328:ASN:HB3	1:3A:427:PRO:HB2	2.02	0.42
1:3A:442:PHE:CE1	17:3E:302:PC1:H122	2.55	0.42
11:3A:501:CDL:H311	3:3C:221:HIS:CE1	2.55	0.42
5:3E:200:HIS:CE1	5:3E:202:LEU:HB2	2.55	0.42
5:3R:156:LEU:HD13	5:3R:210:TRP:NE1	2.35	0.42
12:3R:303:3PE:H222	12:3R:303:3PE:H261	2.00	0.42
3:3C:233:LEU:HA	3:3C:233:LEU:HD23	1.78	0.42
8:3H:59:ARG:HD3	8:3H:63:GLU:HG2	2.02	0.42
3:3P:182:HIS:HE1	13:3P:501:HEM:NA	2.18	0.42
1:3A:179:ARG:O	1:3A:183:THR:HG22	2.20	0.42
3:3C:211:ILE:HG21	6:3F:74:ILE:HG12	2.02	0.42
5:3E:130:LYS:HD3	10:3Y:34:TRP:CE2	2.55	0.42
5:3E:219:HIS:ND1	5:3E:239:HIS:CE1	2.88	0.42
9:3J:19:SER:HB2	10:3Y:23:MET:HB3	2.01	0.42
9:3J:53:TRP:O	9:3J:57:LYS:CD	2.68	0.42
1:3N:224:VAL:HG22	1:3N:225:GLU:H	1.85	0.42
1:3N:351:GLU:HG2	10:3X:12:GLU:OE2	2.20	0.42
1:3N:354:VAL:HG12	1:3N:358:LYS:HD2	2.02	0.42
1:3N:388:ARG:HG2	1:3N:388:ARG:HH11	1.85	0.42
1:3N:433:ASP:OD1	1:3N:434:TYR:N	2.53	0.42
1:3A:91:THR:HG22	1:3A:92:ARG:N	2.33	0.41
3:3C:94:LEU:HD13	3:3C:120:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3E:181:LYS:NZ	5:3E:185:ASP:HB3	2.34	0.41
1:3N:431:LEU:HD12	1:3N:432:PRO:HD2	2.02	0.41
2:3O:290:ASN:HB3	2:3O:293:SER:HB3	2.01	0.41
3:3P:126:THR:HG21	13:3P:501:HEM:HBB2	2.01	0.41
5:3R:160:PRO:HD2	5:3R:163:LYS:HB2	2.01	0.41
5:3R:212:ILE:O	5:3R:213:LEU:HD22	2.20	0.41
6:3S:43:VAL:O	6:3S:47:ILE:HG13	2.19	0.41
7:3T:44:CYS:O	7:3T:48:VAL:HG12	2.19	0.41
2:3B:95:LYS:HB2	2:3B:110:GLU:HB3	2.02	0.41
2:3B:411:ILE:O	2:3B:412:ASN:HB2	2.19	0.41
3:3C:17:ALA:HA	3:3C:201:HIS:CE1	2.55	0.41
3:3C:114:ASN:O	3:3C:118:VAL:HG23	2.20	0.41
4:3D:118:PHE:HE2	4:3D:152:LEU:HD13	1.84	0.41
5:3E:122:THR:HG22	9:3J:25:ILE:HG21	2.02	0.41
5:3E:256:LEU:HG	5:3E:257:ASN:H	1.85	0.41
6:3F:89:LYS:HA	6:3F:89:LYS:HD3	1.86	0.41
4:3Q:117:VAL:HG11	4:3Q:191:ARG:HE	1.85	0.41
11:3Q:502:CDL:HA61	7:3T:29:TYR:CE1	2.56	0.41
7:3G:20:LEU:CD2	7:3G:24:GLU:HB2	2.50	0.41
1:3N:29:GLN:HA	1:3N:201:GLY:O	2.21	0.41
1:3N:355:VAL:HA	1:3N:358:LYS:HD3	2.01	0.41
2:3O:68:LEU:HD13	2:3O:144:LEU:HD11	2.02	0.41
2:3O:124:LEU:HB3	2:3O:223:PHE:CD2	2.55	0.41
3:3P:227:LYS:HD2	4:3Q:223:LYS:HE3	2.02	0.41
3:3P:313:ARG:HB2	6:3S:38:TYR:CD1	2.55	0.41
5:3R:152:ILE:O	5:3R:272:ILE:HD13	2.20	0.41
5:3R:191:GLU:O	5:3R:195:LEU:HB2	2.20	0.41
5:3R:223:VAL:HG23	5:3R:223:VAL:O	2.21	0.41
5:3R:265:PHE:HD1	5:3R:271:VAL:HG12	1.84	0.41
1:3A:61:HIS:CD2	1:3A:134:ILE:HD11	2.56	0.41
2:3B:105:MET:HE3	2:3B:105:MET:HB3	1.96	0.41
3:3C:121:PHE:HE1	3:3C:298:ILE:HB	1.85	0.41
4:3D:100:TRP:HE1	4:3D:212:GLU:HB2	1.84	0.41
4:3D:293:MET:HG2	12:3D:502:3PE:H2	2.01	0.41
5:3E:237:PRO:CG	4:3Q:144:ARG:HD3	2.46	0.41
5:3E:242:HIS:O	5:3E:249:ILE:HA	2.21	0.41
5:3E:272:ILE:HD13	5:3E:272:ILE:HA	1.90	0.41
2:3O:95:LYS:O	2:3O:109:VAL:HA	2.20	0.41
3:3P:24:PRO:O	3:3P:224:TYR:OH	2.20	0.41
5:3R:167:PHE:H	5:3R:174:LEU:HD23	1.85	0.41
10:3Y:39:ARG:HB2	12:3Y:101:3PE:O13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3C:359:PHE:O	3:3C:363:LEU:HD12	2.20	0.41
1:3N:146:ARG:O	1:3N:149:VAL:HG12	2.20	0.41
1:3N:225:GLU:HG2	1:3N:226:ASP:N	2.34	0.41
1:3N:429:GLU:HG2	7:3T:5:GLY:N	2.34	0.41
4:3Q:150:ASN:HD22	4:3Q:150:ASN:HA	1.71	0.41
5:3R:161:GLU:HG2	5:3R:181:LYS:N	2.36	0.41
8:3U:28:GLU:HA	8:3U:31:ILE:HG12	2.01	0.41
1:3A:24:ARG:O	1:3A:196:VAL:HG23	2.21	0.41
1:3A:313:CYS:HA	1:3A:318:GLY:HA3	2.03	0.41
3:3C:217:LYS:HG3	7:3G:9:LEU:HD13	2.02	0.41
5:3E:207:LYS:HG3	5:3E:265:PHE:CD2	2.55	0.41
7:3G:74:LYS:HE3	7:3G:74:LYS:HB3	1.86	0.41
7:3G:75:ASN:O	7:3G:83:ALA:N	2.52	0.41
1:3N:122:LEU:HD23	1:3N:122:LEU:HA	1.83	0.41
1:3N:206:ARG:HE	1:3N:206:ARG:HA	1.85	0.41
2:3O:343:GLN:O	2:3O:346:THR:OG1	2.24	0.41
3:3P:120:LEU:O	3:3P:124:MET:HG3	2.20	0.41
5:3R:106:SER:O	5:3R:110:ARG:HG3	2.20	0.41
12:3R:303:3PE:H32	17:3X:101:PC1:H222	2.03	0.41
7:3T:68:LYS:HA	7:3T:71:ARG:HG2	2.01	0.41
10:3Y:39:ARG:H	10:3Y:39:ARG:HD3	1.84	0.41
12:3A:503:3PE:H371	12:3A:503:3PE:H331	2.03	0.41
2:3B:95:LYS:HB2	2:3B:95:LYS:HE3	1.85	0.41
4:3D:100:TRP:CZ3	4:3D:273:LYS:HG3	2.56	0.41
5:3E:154:ILE:HG13	5:3E:272:ILE:HD13	2.02	0.41
6:3F:102:LEU:HD12	6:3F:102:LEU:HA	1.89	0.41
2:3O:33:LEU:HD23	2:3O:35:ILE:HD11	2.02	0.41
3:3P:278:TYR:O	3:3P:281:LEU:HB3	2.20	0.41
4:3Q:209:LEU:HD23	4:3Q:209:LEU:HA	1.89	0.41
10:3X:11:ARG:O	10:3X:15:ARG:HG3	2.21	0.41
10:3X:32:LEU:HD11	17:3X:101:PC1:H342	2.03	0.41
1:3A:317:THR:OG1	1:3A:318:GLY:N	2.52	0.41
3:3C:3:ASN:HD22	3:3C:6:LYS:HD3	1.85	0.41
3:3C:146:ILE:HD13	3:3C:149:LEU:HD22	2.03	0.41
5:3E:162:GLY:N	5:3E:178:HIS:HB3	2.29	0.41
9:3J:9:ARG:HD2	9:3J:9:ARG:N	2.36	0.41
1:3N:76:GLU:CD	2:3O:289:SER:H	2.23	0.41
1:3N:224:VAL:HG13	1:3N:225:GLU:H	1.85	0.41
1:3N:280:TYR:HB3	1:3N:307:PHE:CE1	2.55	0.41
3:3P:43:LEU:O	3:3P:47:THR:OG1	2.23	0.41
3:3P:97:HIS:CE1	3:3P:100:ARG:HH22	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:3P:504:U10:O2	14:3P:504:U10:C3M	2.69	0.41
4:3Q:152:TYR:OH	8:3U:66:ASP:OD2	2.23	0.41
5:3R:235:TYR:HA	5:3R:242:HIS:HA	2.02	0.41
8:3U:31:ILE:O	8:3U:35:GLU:HG3	2.20	0.41
10:3X:38:TRP:HA	17:3X:101:PC1:H32	2.03	0.41
1:3A:251:ALA:HB1	1:3A:428:ILE:HG22	2.03	0.41
1:3A:280:TYR:HB3	1:3A:307:PHE:HE1	1.85	0.41
2:3B:95:LYS:HD3	5:3I:32:ALA:N	2.36	0.41
2:3B:207:ILE:HD13	2:3B:207:ILE:HA	1.92	0.41
2:3B:224:LEU:HD23	2:3B:224:LEU:HA	1.72	0.41
2:3B:240:ARG:HD2	2:3O:435:PHE:CE2	2.56	0.41
2:3B:299:VAL:HG21	2:3B:309:VAL:HG11	2.03	0.41
3:3C:113:TRP:O	3:3C:117:VAL:HG23	2.21	0.41
3:3C:159:ASP:N	3:3C:159:ASP:OD1	2.54	0.41
14:3C:503:U10:H72	14:3C:503:U10:H1M1	1.73	0.41
14:3C:504:U10:H72	14:3C:504:U10:H1M1	1.79	0.41
5:3E:234:TYR:HD2	5:3E:247:GLY:HA2	1.85	0.41
7:3G:40:LEU:HD13	7:3G:40:LEU:HA	1.88	0.41
1:3N:23:LEU:HD13	1:3N:195:MET:HB3	2.03	0.41
1:3N:280:TYR:HA	1:3N:284:TYR:CE2	2.56	0.41
1:3N:436:ARG:HD2	1:3N:436:ARG:HA	1.61	0.41
3:3P:49:LEU:O	3:3P:53:MET:HG3	2.21	0.41
3:3P:58:ASP:O	3:3P:62:ALA:N	2.53	0.41
3:3P:191:ALA:O	3:3P:195:VAL:HG23	2.20	0.41
3:3P:242:LEU:HD23	3:3P:242:LEU:HA	1.94	0.41
3:3P:368:ILE:O	3:3P:372:ILE:HG13	2.21	0.41
14:3P:504:U10:H1M1	14:3P:504:U10:H72	1.95	0.41
4:3Q:20:SER:H	9:3W:50:LYS:NZ	2.19	0.41
6:3S:28:LYS:HG2	6:3S:80:TRP:CZ2	2.56	0.41
6:3S:105:GLU:O	6:3S:109:LYS:HG2	2.21	0.41
8:3U:21:ARG:CZ	8:3U:65:ARG:HH12	2.34	0.41
9:3W:18:SER:HB3	10:3X:24:TRP:CE2	2.56	0.41
10:3Y:39:ARG:NH2	12:3Y:101:3PE:O14	2.54	0.41
2:3B:303:VAL:HG11	2:3B:336:VAL:HG22	2.03	0.41
2:3B:360:ALA:HA	2:3B:363:LYS:HD3	2.03	0.41
3:3C:281:LEU:HD22	14:3C:504:U10:H1M2	2.03	0.41
4:3D:160:ASP:N	4:3D:160:ASP:OD1	2.54	0.41
4:3D:291:LYS:HZ2	4:3D:291:LYS:HG3	1.65	0.41
4:3D:324:LEU:HD12	4:3D:324:LEU:H	1.86	0.41
5:3E:180:THR:O	5:3E:183:GLU:N	2.55	0.41
1:3N:87:ASN:HB3	1:3N:98:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3N:184:GLU:O	1:3N:188:GLN:HB2	2.21	0.41
2:3O:56:ARG:HA	2:3O:171:ALA:O	2.21	0.41
3:3P:111:GLU:O	3:3P:115:ILE:HG12	2.21	0.41
3:3P:240:LEU:HD11	12:3Q:503:3PE:H241	2.02	0.41
11:3P:506:CDL:H111	11:3Q:502:CDL:H132	2.03	0.41
4:3Q:210:MET:HB2	9:3W:35:PHE:HZ	1.86	0.41
4:3Q:230:LEU:O	4:3Q:233:ARG:HG2	2.21	0.41
5:3R:207:LYS:HA	5:3R:207:LYS:HD2	1.80	0.41
2:3B:308:ASP:OD2	5:3I:58:GLN:N	2.54	0.40
3:3C:300:ILE:HG13	3:3C:303:LEU:HD12	2.03	0.40
10:3Y:39:ARG:HG3	10:3Y:52:PHE:CE2	2.55	0.40
1:3A:49:ASN:ND2	1:3A:52:ASN:HB2	2.36	0.40
1:3A:62:LEU:HD23	1:3A:122:LEU:HA	2.04	0.40
12:3A:502:3PE:H321	12:3A:502:3PE:H32	1.83	0.40
2:3B:28:ARG:HA	2:3B:34:VAL:HA	2.02	0.40
5:3E:106:SER:O	5:3E:110:ARG:HG3	2.20	0.40
5:3E:182:LYS:HA	5:3E:185:ASP:OD2	2.21	0.40
5:3E:258:LEU:HD23	5:3E:258:LEU:HA	1.78	0.40
8:3H:53:GLU:H	8:3H:53:GLU:HG3	1.64	0.40
1:3N:242:ARG:NH2	1:3N:432:PRO:O	2.54	0.40
2:3O:217:LYS:O	2:3O:221:GLU:HG3	2.20	0.40
11:3P:506:CDL:HB61	7:3T:44:CYS:SG	2.61	0.40
4:3Q:237:TYR:HB2	6:3S:60:PHE:CE1	2.56	0.40
5:3R:218:THR:OG1	5:3R:256:LEU:O	2.39	0.40
3:3C:197:LEU:HD23	3:3C:197:LEU:HA	1.93	0.40
4:3D:137:ARG:O	4:3D:140:VAL:HG12	2.20	0.40
5:3E:207:LYS:HE2	5:3E:265:PHE:HE2	1.85	0.40
7:3G:13:ARG:HE	7:3G:13:ARG:HB3	1.71	0.40
1:3N:123:GLU:HG3	1:3N:126:GLN:H	1.86	0.40
2:3O:277:HIS:ND1	2:3O:364:LEU:HG	2.36	0.40
4:3Q:41:HIS:HB3	4:3Q:113:LEU:HD21	2.02	0.40
5:3R:127:TYR:CE1	9:3W:32:GLU:HG3	2.56	0.40
2:3B:56:ARG:HD2	2:3B:103:GLU:HG2	2.03	0.40
6:3F:51:GLU:O	6:3F:56:LYS:NZ	2.50	0.40
8:3H:61:ARG:HE	8:3H:61:ARG:HB3	1.70	0.40
3:3P:108:MET:HG2	3:3P:313:ARG:HD2	2.04	0.40
1:3A:65:LYS:HZ2	1:3A:65:LYS:HG2	1.70	0.40
1:3A:277:ILE:HB	1:3A:309:THR:HG21	2.03	0.40
4:3D:267:THR:HG21	8:3H:41:PRO:HD2	2.02	0.40
4:3D:296:LYS:HE3	9:3J:40:ALA:HB3	2.02	0.40
5:3E:119:ALA:HB2	9:3J:21:PHE:CE1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:3E:230:ASP:OD1	5:3E:231:PHE:N	2.54	0.40
1:3N:208:LEU:HD12	1:3N:208:LEU:HA	1.93	0.40
2:3O:333:ALA:O	2:3O:337:ILE:HD12	2.21	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	3A	436/480 (91%)	410 (94%)	26 (6%)	0	100	100
1	3N	444/480 (92%)	416 (94%)	27 (6%)	1 (0%)	47	81
2	3B	414/453 (91%)	394 (95%)	19 (5%)	1 (0%)	47	81
2	3O	413/453 (91%)	400 (97%)	13 (3%)	0	100	100
3	3C	377/379 (100%)	365 (97%)	12 (3%)	0	100	100
3	3P	377/379 (100%)	361 (96%)	14 (4%)	2 (0%)	29	68
4	3D	235/326 (72%)	214 (91%)	21 (9%)	0	100	100
4	3Q	237/326 (73%)	224 (94%)	12 (5%)	1 (0%)	34	72
5	3E	194/274 (71%)	164 (84%)	29 (15%)	1 (0%)	29	68
5	3I	45/274 (16%)	38 (84%)	6 (13%)	1 (2%)	6	37
5	3R	194/274 (71%)	172 (89%)	22 (11%)	0	100	100
5	3V	29/274 (11%)	29 (100%)	0	0	100	100
6	3F	96/111 (86%)	95 (99%)	1 (1%)	0	100	100
6	3S	96/111 (86%)	95 (99%)	1 (1%)	0	100	100
7	3G	70/82 (85%)	70 (100%)	0	0	100	100
7	3T	72/82 (88%)	72 (100%)	0	0	100	100
8	3H	61/91 (67%)	56 (92%)	5 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	3U	63/91 (69%)	59 (94%)	4 (6%)	0	100	100
9	3J	54/64 (84%)	51 (94%)	3 (6%)	0	100	100
9	3W	54/64 (84%)	49 (91%)	5 (9%)	0	100	100
10	3X	50/56 (89%)	48 (96%)	2 (4%)	0	100	100
10	3Y	49/56 (88%)	44 (90%)	5 (10%)	0	100	100
All	All	4060/5180 (78%)	3826 (94%)	227 (6%)	7 (0%)	50	81

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	3E	216	VAL
4	3Q	3	LEU
2	3B	224	LEU
5	3I	50	LEU
3	3P	110	LEU
1	3N	224	VAL
3	3P	155	TYR

### 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	3A	367/397 (92%)	356 (97%)	11 (3%)	41	71
1	3N	372/397 (94%)	351 (94%)	21 (6%)	21	54
2	3B	328/355 (92%)	321 (98%)	7 (2%)	53	79
2	3O	327/355 (92%)	317 (97%)	10 (3%)	40	70
3	3C	332/332 (100%)	320 (96%)	12 (4%)	35	66
3	3P	332/332 (100%)	321 (97%)	11 (3%)	38	68
4	3D	202/259 (78%)	194 (96%)	8 (4%)	31	64
4	3Q	204/259 (79%)	193 (95%)	11 (5%)	22	55
5	3E	166/225 (74%)	160 (96%)	6 (4%)	35	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	3I	36/225 (16%)	34 (94%)	2 (6%)	21	54
5	3R	166/225 (74%)	154 (93%)	12 (7%)	14	45
5	3V	24/225 (11%)	23 (96%)	1 (4%)	30	63
6	3F	90/99 (91%)	88 (98%)	2 (2%)	52	78
6	3S	90/99 (91%)	88 (98%)	2 (2%)	52	78
7	3G	67/73 (92%)	65 (97%)	2 (3%)	41	71
7	3T	67/73 (92%)	65 (97%)	2 (3%)	41	71
8	3H	62/85 (73%)	58 (94%)	4 (6%)	17	50
8	3U	62/85 (73%)	59 (95%)	3 (5%)	25	60
9	3J	46/52 (88%)	46 (100%)	0	100	100
9	3W	46/52 (88%)	45 (98%)	1 (2%)	52	78
10	3X	42/46 (91%)	38 (90%)	4 (10%)	8	34
10	3Y	41/46 (89%)	39 (95%)	2 (5%)	25	59
All	All	3469/4296 (81%)	3335 (96%)	134 (4%)	36	64

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	3A	10	SER
1	3A	24	ARG
1	3A	58	PHE
1	3A	92	ARG
1	3A	206	ARG
1	3A	217	SER
1	3A	284	TYR
1	3A	304	CYS
1	3A	311	ASN
1	3A	441	MET
1	3A	443	TRP
2	3B	84	LYS
2	3B	95	LYS
2	3B	143	GLN
2	3B	223	PHE
2	3B	227	ARG
2	3B	284	HIS
2	3B	370	MET
3	3C	8	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	3C	80	ARG
3	3C	100	ARG
3	3C	110	LEU
3	3C	124	MET
3	3C	183	PHE
3	3C	267	HIS
3	3C	271	GLU
3	3C	282	ARG
3	3C	287	LYS
3	3C	316	MET
3	3C	379	TRP
4	3D	94	HIS
4	3D	103	ARG
4	3D	143	CYS
4	3D	150	LYS
4	3D	177	ASP
4	3D	268	MET
4	3D	276	CYS
4	3D	312	LYS
5	3E	84	ARG
5	3E	150	SER
5	3E	163	LYS
5	3E	196	ARG
5	3E	234	TYR
5	3E	239	HIS
6	3F	90	GLU
6	3F	107	LYS
7	3G	8	HIS
7	3G	68	PHE
8	3H	53	GLU
8	3H	54	LYS
8	3H	78	ASP
8	3H	91	ASP
5	3I	54	SER
5	3I	78	TYR
1	3N	8	LEU
1	3N	28	GLU
1	3N	51	LYS
1	3N	57	TYR
1	3N	112	LEU
1	3N	116	ILE
1	3N	117	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	3N	119	ASN
1	3N	126	GLN
1	3N	132	ASP
1	3N	134	ILE
1	3N	181	ASP
1	3N	195	MET
1	3N	207[A]	GLN
1	3N	207[B]	GLN
1	3N	213	GLN
1	3N	222	THR
1	3N	226	ASP
1	3N	279	HIS
1	3N	333	ASP
1	3N	443	TRP
2	3O	23	ASP
2	3O	56	ARG
2	3O	111	CYS
2	3O	178	CYS
2	3O	222	ARG
2	3O	226	MET
2	3O	227	ARG
2	3O	318	ASP
2	3O	335	ASP
2	3O	421	ARG
3	3P	80	ARG
3	3P	155	TYR
3	3P	183	PHE
3	3P	215	MET
3	3P	269	LYS
3	3P	271	GLU
3	3P	282	ARG
3	3P	287	LYS
3	3P	313	ARG
3	3P	366	MET
3	3P	379	TRP
4	3Q	3	LEU
4	3Q	6	HIS
4	3Q	13	SER
4	3Q	55	CYS
4	3Q	62	LYS
4	3Q	135	CYS
4	3Q	156	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	3Q	170	GLU
4	3Q	184	LYS
4	3Q	187	CYS
4	3Q	233	ARG
5	3R	149	MET
5	3R	151	LYS
5	3R	155	LYS
5	3R	167	PHE
5	3R	174	LEU
5	3R	181	LYS
5	3R	201	ASP
5	3R	209	GLU
5	3R	235	TYR
5	3R	251	LYS
5	3R	263	TYR
5	3R	268	ASP
6	3S	17	ARG
6	3S	82	LYS
7	3T	24	ARG
7	3T	44	CYS
8	3U	29	LYS
8	3U	52	GLU
8	3U	53	ASP
5	3V	53	GLU
9	3W	53	LYS
10	3X	1	MET
10	3X	4	ARG
10	3X	43	ASP
10	3X	44	TRP
10	3Y	39	ARG
10	3Y	43	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	3A	52	ASN
1	3A	308	GLN
3	3C	44	GLN
4	3D	287	HIS
5	3E	194	GLN
5	3E	239	HIS
7	3G	25	GLN

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Mol	Chain	Res	Type
5	3I	58	GLN
9	3J	38	GLN
1	3N	9	GLN
1	3N	252	HIS
3	3P	374	ASN
4	3Q	150	ASN
4	3Q	198	HIS
7	3T	6	HIS
7	3T	23	GLN
8	3U	26	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

32 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	CDL	3A	501	-	57,57,99	0.34	0	63,69,111	0.43	0
14	U10	3P	503	-	23,23,63	0.98	2 (8%)	28,31,79	1.46	4 (14%)
13	HEM	3C	502	3	41,50,50	1.37	6 (14%)	45,82,82	1.79	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
11	CDL	3D	503	-	55,55,99	0.35	0	61,67,111	0.44	0
12	3PE	3P	505	-	32,32,50	0.34	0	35,37,55	0.51	0
11	CDL	3P	507	-	42,42,99	0.39	0	48,54,111	0.53	0
12	3PE	3Y	101	-	29,29,50	0.34	0	32,34,55	0.36	0
14	U10	3C	504	-	28,28,63	0.93	2 (7%)	34,37,79	1.29	5 (14%)
17	PC1	3X	101	-	28,28,53	0.37	0	34,36,61	0.39	0
13	HEM	3C	501	3	41,50,50	1.34	5 (12%)	45,82,82	1.85	11 (24%)
14	U10	3C	503	-	28,28,63	0.80	1 (3%)	34,37,79	1.10	4 (11%)
11	CDL	3C	505	-	51,51,99	0.36	0	57,63,111	0.49	0
13	HEM	3P	502	3	41,50,50	1.36	6 (14%)	45,82,82	1.75	9 (20%)
16	FES	3E	301	5	0,4,4	-	-	-	-	-
12	3PE	3A	503	-	31,31,50	0.33	0	34,36,55	0.64	1 (2%)
12	3PE	3D	502	-	32,32,50	0.34	0	35,37,55	0.43	0
11	CDL	3P	506	-	55,55,99	0.36	0	61,67,111	0.49	0
12	3PE	3C	506	-	34,34,50	0.32	0	37,39,55	0.44	0
16	FES	3R	301	5	0,4,4	-	-	-	-	-
12	3PE	3N	502	-	24,24,50	0.38	0	27,29,55	0.64	1 (3%)
14	U10	3P	504	-	28,28,63	0.83	1 (3%)	34,37,79	1.10	4 (11%)
12	3PE	3N	501	-	31,31,50	0.33	0	34,36,55	0.65	1 (2%)
17	PC1	3E	302	-	46,46,53	0.29	0	52,54,61	0.29	0
12	3PE	3R	303	-	33,33,50	0.32	0	36,38,55	0.36	0
11	CDL	3Q	502	-	56,56,99	0.35	0	62,68,111	0.47	0
12	3PE	3A	502	-	26,26,50	0.36	0	29,31,55	0.59	0
13	HEM	3P	501	3	41,50,50	1.35	6 (14%)	45,82,82	1.86	9 (20%)
17	PC1	3R	302	-	44,44,53	0.30	0	50,52,61	0.38	0
15	HEC	3Q	501	4	32,50,50	2.23	12 (37%)	24,82,82	2.26	6 (25%)
15	HEC	3D	501	4	31,49,50	2.46	12 (38%)	22,80,82	2.41	6 (27%)
12	3PE	3G	101	-	28,28,50	0.33	0	31,33,55	0.39	0
12	3PE	3Q	503	-	46,46,50	0.28	0	49,51,55	0.34	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
11	CDL	3A	501	-	-	10/68/68/110	-
14	U10	3P	503	-	-	1/15/39/87	0/1/1/1
13	HEM	3C	502	3	-	4/12/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CDL	3D	503	-	-	12/66/66/110	-
12	3PE	3P	505	-	-	10/36/36/54	-
11	CDL	3P	507	-	-	12/53/53/110	-
12	3PE	3Y	101	-	-	12/33/33/54	-
14	U10	3C	504	-	-	6/21/45/87	0/1/1/1
17	PC1	3X	101	-	-	13/32/32/57	-
13	HEM	3C	501	3	-	3/12/54/54	-
14	U10	3C	503	-	-	7/21/45/87	0/1/1/1
11	CDL	3C	505	-	-	7/62/62/110	-
13	HEM	3P	502	3	-	6/12/54/54	-
16	FES	3E	301	5	-	-	0/1/1/1
12	3PE	3A	503	-	-	5/35/35/54	-
12	3PE	3D	502	-	-	3/36/36/54	-
11	CDL	3P	506	-	-	11/66/66/110	-
12	3PE	3C	506	-	-	9/38/38/54	-
16	FES	3R	301	5	-	-	0/1/1/1
12	3PE	3N	502	-	-	9/28/28/54	-
14	U10	3P	504	-	-	3/21/45/87	0/1/1/1
12	3PE	3N	501	-	-	6/35/35/54	-
17	PC1	3E	302	-	-	3/50/50/57	-
12	3PE	3R	303	-	-	11/37/37/54	-
11	CDL	3Q	502	-	-	19/67/67/110	-
12	3PE	3A	502	-	-	12/30/30/54	-
13	HEM	3P	501	3	-	5/12/54/54	-
17	PC1	3R	302	-	-	7/48/48/57	-
15	HEC	3Q	501	4	-	3/10/54/54	-
15	HEC	3D	501	4	-	0/8/53/54	-
12	3PE	3G	101	-	-	8/32/32/54	-
12	3PE	3Q	503	-	-	4/50/50/54	-

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	3D	501	HEC	C3C-C2C	7.14	1.48	1.40
15	3D	501	HEC	C2B-C3B	7.07	1.48	1.40
15	3Q	501	HEC	C2B-C3B	6.73	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	3Q	501	HEC	C3C-C2C	5.42	1.46	1.40
13	3C	502	HEM	C1B-NB	-3.56	1.34	1.40
13	3P	501	HEM	C1B-NB	-3.56	1.34	1.40
13	3C	502	HEM	C4D-ND	-3.51	1.34	1.40
13	3P	502	HEM	C4D-ND	-3.51	1.34	1.40
13	3P	502	HEM	C1B-NB	-3.49	1.34	1.40
13	3P	501	HEM	C4D-ND	-3.47	1.34	1.40
13	3C	501	HEM	C4D-ND	-3.43	1.34	1.40
13	3C	501	HEM	C1B-NB	-3.42	1.34	1.40
15	3D	501	HEC	C2A-C3A	3.42	1.47	1.37
15	3Q	501	HEC	C3C-C4C	3.40	1.49	1.43
15	3D	501	HEC	C3D-C2D	3.37	1.47	1.37
15	3Q	501	HEC	C2A-C3A	3.26	1.47	1.37
15	3Q	501	HEC	C3D-C2D	3.19	1.47	1.37
15	3D	501	HEC	C4B-C3B	3.02	1.48	1.43
15	3D	501	HEC	C3C-C4C	2.81	1.48	1.43
13	3C	501	HEM	FE-NB	2.80	2.10	1.96
13	3C	502	HEM	FE-NB	2.75	2.10	1.96
13	3P	501	HEM	FE-NB	2.74	2.10	1.96
13	3P	502	HEM	FE-NB	2.74	2.10	1.96
14	3C	504	U10	C3-C2	-2.71	1.41	1.48
15	3Q	501	HEC	C2A-C1A	2.71	1.48	1.42
14	3P	504	U10	C4-C5	-2.65	1.41	1.48
15	3D	501	HEC	C3A-C4A	2.63	1.48	1.42
14	3P	503	U10	C3-C2	-2.61	1.41	1.48
15	3D	501	HEC	C2A-C1A	2.61	1.48	1.42
15	3Q	501	HEC	C4B-C3B	2.60	1.47	1.43
15	3Q	501	HEC	C3A-C4A	2.59	1.48	1.42
14	3C	503	U10	C4-C5	-2.57	1.41	1.48
14	3C	504	U10	C4-C5	-2.53	1.41	1.48
15	3D	501	HEC	C1B-CHB	2.52	1.48	1.41
15	3D	501	HEC	C1D-CHD	2.50	1.48	1.41
15	3D	501	HEC	C1C-CHC	2.47	1.47	1.41
15	3D	501	HEC	C4D-CHA	2.42	1.47	1.41
15	3Q	501	HEC	C4D-CHA	2.41	1.47	1.41
15	3Q	501	HEC	C1B-CHB	2.38	1.47	1.41
14	3P	503	U10	C4-C5	-2.35	1.42	1.48
15	3Q	501	HEC	C1D-CHD	2.25	1.47	1.41
15	3Q	501	HEC	C1C-CHC	2.24	1.47	1.41
13	3P	502	HEM	C1D-ND	-2.19	1.34	1.38
13	3C	501	HEM	C1D-ND	-2.17	1.34	1.38
13	3C	502	HEM	C1D-ND	-2.17	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	3P	501	HEM	C1D-ND	-2.13	1.34	1.38
13	3P	501	HEM	C4B-NB	-2.10	1.34	1.38
13	3P	502	HEM	C4B-NB	-2.09	1.34	1.38
13	3P	501	HEM	FE-ND	-2.06	1.86	1.96
13	3C	502	HEM	C4B-NB	-2.06	1.34	1.38
13	3P	502	HEM	FE-ND	-2.05	1.86	1.96
13	3C	502	HEM	FE-ND	-2.05	1.86	1.96
13	3C	501	HEM	FE-ND	-2.01	1.86	1.96

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	3Q	501	HEC	C1D-C2D-C3D	-6.30	102.62	107.00
15	3D	501	HEC	C1D-C2D-C3D	-5.96	102.85	107.00
15	3Q	501	HEC	CMB-C2B-C3B	5.69	132.51	125.82
15	3D	501	HEC	CMB-C2B-C3B	5.62	132.42	125.82
15	3D	501	HEC	CMC-C2C-C3C	5.16	131.88	125.82
13	3P	501	HEM	CHC-C4B-NB	5.11	129.98	124.43
13	3C	502	HEM	CHC-C4B-NB	5.07	129.94	124.43
13	3P	502	HEM	CHC-C4B-NB	4.97	129.83	124.43
13	3C	501	HEM	CHC-C4B-NB	4.96	129.82	124.43
13	3P	501	HEM	CHD-C1D-ND	4.54	129.37	124.43
13	3C	501	HEM	CHD-C1D-ND	4.51	129.33	124.43
13	3P	502	HEM	C1B-NB-C4B	4.05	109.25	105.07
13	3C	502	HEM	CHD-C1D-ND	4.05	128.83	124.43
13	3P	501	HEM	C1B-NB-C4B	4.01	109.21	105.07
13	3C	502	HEM	C1B-NB-C4B	3.94	109.15	105.07
13	3P	502	HEM	CHD-C1D-ND	3.89	128.66	124.43
13	3C	501	HEM	C1B-NB-C4B	3.79	108.99	105.07
13	3C	502	HEM	CHA-C4D-ND	3.63	128.86	124.38
13	3P	501	HEM	CHA-C4D-ND	3.60	128.83	124.38
13	3C	501	HEM	CHA-C4D-ND	3.60	128.83	124.38
13	3P	502	HEM	CHA-C4D-ND	3.47	128.66	124.38
13	3C	501	HEM	CHB-C1B-NB	3.45	128.64	124.38
14	3P	503	U10	O3-C3-C4	3.39	136.43	123.64
14	3P	503	U10	O4-C4-C3	3.37	136.36	123.64
14	3C	504	U10	O3-C3-C4	3.33	136.20	123.64
14	3C	504	U10	O4-C4-C3	3.32	136.17	123.64
13	3P	501	HEM	CHB-C1B-NB	3.31	128.47	124.38
14	3P	503	U10	O4-C4-C5	-3.28	105.46	116.56
14	3C	504	U10	O4-C4-C5	-3.26	105.53	116.56
14	3P	503	U10	O3-C3-C2	-3.09	106.10	116.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	3C	502	HEM	CHB-C1B-NB	3.09	128.20	124.38
13	3P	502	HEM	CHB-C1B-NB	3.04	128.14	124.38
14	3C	504	U10	O3-C3-C2	-2.90	106.75	116.56
14	3P	504	U10	O4-C4-C5	-2.88	106.82	116.56
15	3Q	501	HEC	CMC-C2C-C3C	2.85	129.18	125.82
13	3P	501	HEM	CHD-C1D-C2D	-2.77	120.65	124.98
14	3C	503	U10	O4-C4-C5	-2.77	107.19	116.56
14	3P	504	U10	O3-C3-C2	2.72	125.76	116.56
14	3C	503	U10	O3-C3-C2	2.71	125.73	116.56
13	3C	501	HEM	CHD-C1D-C2D	-2.67	120.81	124.98
12	3N	501	3PE	O21-C21-C22	2.62	117.14	111.50
13	3P	502	HEM	C4D-ND-C1D	2.54	107.69	105.07
13	3P	501	HEM	CAD-CBD-CGD	-2.49	108.25	113.60
13	3C	502	HEM	C4D-ND-C1D	2.47	107.63	105.07
12	3A	503	3PE	O21-C21-C22	2.47	116.82	111.50
15	3D	501	HEC	CAA-CBA-CGA	-2.41	107.00	113.76
13	3C	501	HEM	CBA-CAA-C2A	-2.40	108.52	112.62
13	3P	501	HEM	C4D-ND-C1D	2.37	107.53	105.07
13	3C	501	HEM	C4D-ND-C1D	2.35	107.50	105.07
13	3C	502	HEM	CHD-C1D-C2D	-2.34	121.32	124.98
14	3P	504	U10	O4-C4-C3	2.33	132.44	123.64
14	3C	503	U10	O4-C4-C3	2.31	132.37	123.64
12	3N	502	3PE	O21-C21-C22	2.31	116.48	111.50
15	3D	501	HEC	CMA-C3A-C2A	2.25	129.19	124.94
13	3P	502	HEM	CHD-C1D-C2D	-2.25	121.47	124.98
15	3Q	501	HEC	CMA-C3A-C2A	2.24	129.17	124.94
13	3C	501	HEM	CAD-CBD-CGD	-2.21	108.86	113.60
15	3Q	501	HEC	CMD-C2D-C3D	2.20	129.09	124.94
13	3C	502	HEM	CHA-C4D-C3D	-2.18	121.23	125.33
13	3C	501	HEM	CHA-C4D-C3D	-2.18	121.23	125.33
14	3C	504	U10	C4-C3-C2	-2.18	116.40	120.68
14	3P	504	U10	C4-C3-C2	-2.09	116.56	120.68
13	3P	501	HEM	CHA-C4D-C3D	-2.09	121.41	125.33
15	3Q	501	HEC	CAA-CBA-CGA	-2.06	107.99	113.76
14	3C	503	U10	C4-C3-C2	-2.05	116.64	120.68
13	3P	502	HEM	CHA-C4D-C3D	-2.01	121.55	125.33
15	3D	501	HEC	CMD-C2D-C3D	2.01	128.74	124.94
13	3C	501	HEM	CHB-C1B-C2B	-2.00	121.18	126.72
13	3P	502	HEM	CAD-CBD-CGD	-2.00	109.29	113.60

There are no chirality outliers.

All (221) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	3A	501	CDL	OB9-CB7-OB8-CB6
11	3A	501	CDL	C71-CB7-OB8-CB6
11	3C	505	CDL	CB2-OB2-PB2-OB3
11	3D	503	CDL	CA3-OA5-PA1-OA3
11	3D	503	CDL	CA4-CA3-OA5-PA1
11	3D	503	CDL	OA7-CA5-OA6-CA4
11	3D	503	CDL	C11-CA5-OA6-CA4
11	3P	507	CDL	CA2-OA2-PA1-OA4
11	3Q	502	CDL	CA2-OA2-PA1-OA5
11	3Q	502	CDL	OA6-CA4-CA6-OA8
12	3A	502	3PE	O21-C2-C3-O31
12	3A	502	3PE	O32-C31-O31-C3
12	3A	502	3PE	C32-C31-O31-C3
12	3A	502	3PE	O22-C21-O21-C2
12	3A	502	3PE	C22-C21-O21-C2
12	3A	503	3PE	O22-C21-O21-C2
12	3A	503	3PE	C22-C21-O21-C2
12	3G	101	3PE	O32-C31-O31-C3
12	3G	101	3PE	C32-C31-O31-C3
12	3N	501	3PE	O11-C1-C2-O21
12	3N	501	3PE	O22-C21-O21-C2
12	3N	501	3PE	C22-C21-O21-C2
12	3N	502	3PE	C11-O13-P-O14
12	3N	502	3PE	O22-C21-O21-C2
12	3N	502	3PE	C22-C21-O21-C2
12	3P	505	3PE	C1-O11-P-O14
12	3P	505	3PE	C12-C11-O13-P
12	3R	303	3PE	C2-C1-O11-P
12	3Y	101	3PE	C1-O11-P-O13
12	3Y	101	3PE	C2-C1-O11-P
12	3Y	101	3PE	C12-C11-O13-P
12	3Y	101	3PE	O32-C31-O31-C3
12	3Y	101	3PE	C32-C31-O31-C3
13	3C	501	HEM	C2B-C3B-CAB-CBB
13	3C	501	HEM	C4B-C3B-CAB-CBB
13	3C	502	HEM	C2B-C3B-CAB-CBB
13	3P	501	HEM	C2B-C3B-CAB-CBB
13	3P	501	HEM	C4B-C3B-CAB-CBB
13	3P	502	HEM	C2B-C3B-CAB-CBB
17	3R	302	PC1	C2-C1-O11-P
17	3X	101	PC1	C11-O13-P-O12
17	3X	101	PC1	C11-O13-P-O14
17	3X	101	PC1	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
11	3Q	502	CDL	CB4-CB3-OB5-PB2
13	3P	501	HEM	C3D-CAD-CBD-CGD
14	3C	503	U10	C15-C14-C16-C17
14	3C	504	U10	C12-C11-C9-C10
14	3C	503	U10	C13-C14-C16-C17
14	3C	504	U10	C12-C11-C9-C8
14	3C	503	U10	C4-C3-O3-C3M
14	3P	504	U10	C4-C3-O3-C3M
14	3C	504	U10	C9-C11-C12-C13
11	3P	507	CDL	CA2-OA2-PA1-OA5
11	3P	507	CDL	CB3-OB5-PB2-OB2
11	3Q	502	CDL	CA3-OA5-PA1-OA2
12	3R	303	3PE	C1-O11-P-O13
17	3X	101	PC1	C11-O13-P-O11
12	3C	506	3PE	C29-C2A-C2B-C2C
12	3G	101	3PE	C33-C34-C35-C36
11	3A	501	CDL	C1-CA2-OA2-PA1
11	3D	503	CDL	O1-C1-CB2-OB2
11	3Q	502	CDL	CB5-C51-C52-C53
12	3P	505	3PE	C31-C32-C33-C34
12	3Y	101	3PE	C32-C33-C34-C35
14	3P	504	U10	C2-C3-O3-C3M
13	3C	502	HEM	C4B-C3B-CAB-CBB
13	3P	502	HEM	C4B-C3B-CAB-CBB
11	3D	503	CDL	C71-C72-C73-C74
11	3P	506	CDL	CA7-C31-C32-C33
11	3C	505	CDL	CB2-OB2-PB2-OB5
11	3P	506	CDL	C1-CA2-OA2-PA1
11	3Q	502	CDL	CA4-CA3-OA5-PA1
11	3Q	502	CDL	C1-CB2-OB2-PB2
12	3P	505	3PE	C2-C1-O11-P
12	3P	505	3PE	C33-C34-C35-C36
11	3P	506	CDL	OA5-CA3-CA4-CA6
12	3N	501	3PE	O11-C1-C2-C3
15	3Q	501	HEC	C3D-CAD-CBD-CGD
12	3C	506	3PE	C26-C27-C28-C29
11	3Q	502	CDL	CA3-CA4-CA6-OA8
11	3D	503	CDL	CB5-C51-C52-C53
11	3C	505	CDL	C72-C71-CB7-OB8
12	3G	101	3PE	O21-C21-C22-C23
12	3R	303	3PE	O31-C31-C32-C33
12	3R	303	3PE	O21-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
13	3C	501	HEM	C3D-CAD-CBD-CGD
17	3R	302	PC1	O21-C2-C3-O31
11	3A	501	CDL	C33-C34-C35-C36
17	3R	302	PC1	C3A-C3B-C3C-C3D
11	3D	503	CDL	C54-C55-C56-C57
12	3R	303	3PE	O11-C1-C2-C3
12	3N	502	3PE	C32-C33-C34-C35
17	3X	101	PC1	C21-C22-C23-C24
12	3A	502	3PE	C2-C1-O11-P
12	3A	503	3PE	C2-C1-O11-P
12	3P	505	3PE	C1-C2-C3-O31
12	3G	101	3PE	C1-O11-P-O13
17	3X	101	PC1	O21-C21-C22-C23
14	3C	503	U10	C2-C3-O3-C3M
11	3D	503	CDL	CA2-C1-CB2-OB2
17	3E	302	PC1	C35-C36-C37-C38
11	3Q	502	CDL	C31-C32-C33-C34
11	3Q	502	CDL	C11-C12-C13-C14
12	3Y	101	3PE	C24-C25-C26-C27
12	3R	303	3PE	C22-C23-C24-C25
12	3A	502	3PE	C1-C2-C3-O31
11	3P	506	CDL	OA5-CA3-CA4-OA6
12	3A	502	3PE	O11-C1-C2-O21
12	3R	303	3PE	O11-C1-C2-O21
17	3X	101	PC1	O11-C1-C2-O21
12	3C	506	3PE	C23-C24-C25-C26
12	3P	505	3PE	O21-C2-C3-O31
12	3Q	503	3PE	C27-C28-C29-C2A
12	3N	502	3PE	C11-O13-P-O11
12	3Y	101	3PE	C11-O13-P-O11
12	3C	506	3PE	C24-C25-C26-C27
11	3C	505	CDL	CB2-OB2-PB2-OB4
11	3P	507	CDL	CB3-OB5-PB2-OB3
11	3Q	502	CDL	CA2-OA2-PA1-OA4
11	3Q	502	CDL	CA3-OA5-PA1-OA3
11	3Q	502	CDL	CA3-OA5-PA1-OA4
12	3R	303	3PE	C1-O11-P-O14
12	3Y	101	3PE	C1-O11-P-O12
17	3X	101	PC1	O11-C1-C2-C3
12	3A	502	3PE	C12-C11-O13-P
12	3A	503	3PE	C12-C11-O13-P
12	3N	501	3PE	C12-C11-O13-P

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Mol	Chain	Res	Type	Atoms
12	3N	502	3PE	C12-C11-O13-P
17	3R	302	PC1	C12-C11-O13-P
12	3P	505	3PE	C21-C22-C23-C24
11	3P	506	CDL	C72-C71-CB7-OB8
17	3R	302	PC1	C32-C33-C34-C35
17	3E	302	PC1	C33-C34-C35-C36
17	3R	302	PC1	C1-C2-C3-O31
17	3X	101	PC1	O13-C11-C12-N
11	3P	506	CDL	C1-CB2-OB2-PB2
12	3Q	503	3PE	C21-C22-C23-C24
12	3D	502	3PE	C34-C35-C36-C37
11	3A	501	CDL	CA2-OA2-PA1-OA5
11	3A	501	CDL	CB2-OB2-PB2-OB5
11	3P	506	CDL	CA2-OA2-PA1-OA5
11	3P	506	CDL	CB3-OB5-PB2-OB2
11	3Q	502	CDL	CB3-OB5-PB2-OB2
12	3A	502	3PE	C1-O11-P-O13
12	3C	506	3PE	C1-O11-P-O13
12	3C	506	3PE	C11-O13-P-O11
12	3P	505	3PE	C1-O11-P-O13
12	3R	303	3PE	C11-O13-P-O11
17	3X	101	PC1	C1-O11-P-O13
12	3Q	503	3PE	C35-C36-C37-C38
17	3X	101	PC1	C2-C1-O11-P
13	3P	501	HEM	CAD-CBD-CGD-O2D
13	3P	502	HEM	CAA-CBA-CGA-O1A
17	3X	101	PC1	O22-C21-C22-C23
12	3A	502	3PE	O11-C1-C2-C3
12	3N	502	3PE	O21-C2-C3-O31
11	3C	505	CDL	C72-C71-CB7-OB9
12	3G	101	3PE	O22-C21-C22-C23
13	3P	502	HEM	CAD-CBD-CGD-O1D
11	3P	506	CDL	C33-C34-C35-C36
12	3A	503	3PE	C34-C35-C36-C37
13	3P	501	HEM	CAD-CBD-CGD-O1D
11	3P	506	CDL	CA5-C11-C12-C13
11	3D	503	CDL	CA3-CA4-CA6-OA8
13	3C	502	HEM	CAA-CBA-CGA-O2A
13	3P	502	HEM	CAA-CBA-CGA-O2A
15	3Q	501	HEC	CAD-CBD-CGD-O1D
11	3P	507	CDL	CB3-CB4-OB6-CB5
14	3C	503	U10	C12-C11-C9-C10

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Mol	Chain	Res	Type	Atoms
13	3C	502	HEM	CAA-CBA-CGA-O1A
13	3P	502	HEM	CAD-CBD-CGD-O2D
11	3Q	502	CDL	OB5-CB3-CB4-CB6
14	3C	503	U10	C5-C4-O4-C4M
14	3P	504	U10	C5-C4-O4-C4M
11	3D	503	CDL	C52-C53-C54-C55
12	3P	505	3PE	C23-C24-C25-C26
12	3R	303	3PE	O22-C21-C22-C23
11	3Q	502	CDL	C52-C53-C54-C55
11	3P	506	CDL	C12-C13-C14-C15
15	3Q	501	HEC	CAD-CBD-CGD-O2D
11	3P	507	CDL	C52-C51-CB5-OB6
11	3P	507	CDL	C72-C71-CB7-OB8
11	3A	501	CDL	C52-C51-CB5-OB6
12	3D	502	3PE	C32-C33-C34-C35
11	3D	503	CDL	CA3-OA5-PA1-OA2
12	3C	506	3PE	C1-C2-O21-C21
14	3C	503	U10	C12-C11-C9-C8
12	3G	101	3PE	C32-C33-C34-C35
12	3Q	503	3PE	C33-C34-C35-C36
11	3A	501	CDL	C12-C11-CA5-OA6
14	3C	504	U10	C11-C12-C13-C14
11	3P	507	CDL	OA6-CA4-CA6-OA8
12	3R	303	3PE	O32-C31-C32-C33
11	3C	505	CDL	C52-C51-CB5-OB6
11	3A	501	CDL	C52-C51-CB5-OB7
11	3P	507	CDL	C72-C71-CB7-OB9
12	3N	502	3PE	C1-C2-C3-O31
12	3Y	101	3PE	C1-C2-C3-O31
11	3P	507	CDL	CA4-CA6-OA8-CA7
11	3A	501	CDL	C12-C11-CA5-OA7
11	3Q	502	CDL	CB3-OB5-PB2-OB3
12	3A	502	3PE	C11-O13-P-O14
12	3C	506	3PE	C11-O13-P-O14
17	3R	302	PC1	C1-O11-P-O14
14	3C	504	U10	C2-C3-O3-C3M
14	3P	503	U10	C2-C3-O3-C3M
17	3E	302	PC1	C12-C11-O13-P
17	3X	101	PC1	C12-C11-O13-P
12	3N	501	3PE	O31-C31-C32-C33
14	3C	504	U10	C16-C17-C18-C19
11	3Q	502	CDL	C32-C31-CA7-OA8

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Mol	Chain	Res	Type	Atoms
12	3Y	101	3PE	O31-C31-C32-C33
12	3D	502	3PE	C21-C22-C23-C24
11	3P	507	CDL	C12-C11-CA5-OA6
12	3C	506	3PE	O21-C21-C22-C23
12	3G	101	3PE	O31-C31-C32-C33
11	3C	505	CDL	C52-C51-CB5-OB7
11	3Q	502	CDL	C32-C31-CA7-OA9
11	3P	507	CDL	C12-C11-CA5-OA7
12	3Y	101	3PE	O32-C31-C32-C33
12	3N	502	3PE	O21-C21-C22-C23

There are no ring outliers.

31 monomers are involved in 116 short contacts:

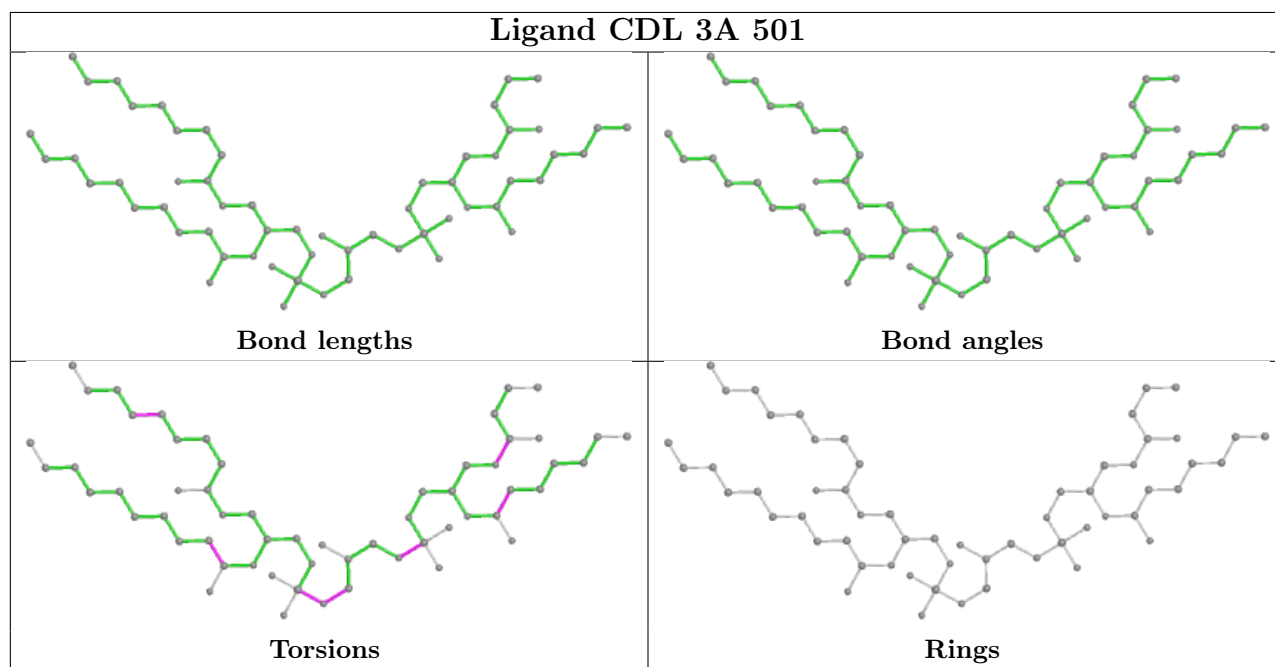
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	3A	501	CDL	5	0
14	3P	503	U10	7	0
13	3C	502	HEM	2	0
11	3D	503	CDL	4	0
12	3P	505	3PE	1	0
11	3P	507	CDL	2	0
12	3Y	101	3PE	6	0
14	3C	504	U10	8	0
17	3X	101	PC1	3	0
13	3C	501	HEM	4	0
14	3C	503	U10	1	0
11	3C	505	CDL	4	0
13	3P	502	HEM	3	0
16	3E	301	FES	2	0
12	3A	503	3PE	4	0
12	3D	502	3PE	4	0
11	3P	506	CDL	7	0
12	3C	506	3PE	4	0
12	3N	502	3PE	4	0
14	3P	504	U10	3	0
12	3N	501	3PE	2	0
17	3E	302	PC1	8	0
12	3R	303	3PE	3	0
11	3Q	502	CDL	10	0
12	3A	502	3PE	3	0
13	3P	501	HEM	3	0
17	3R	302	PC1	4	0

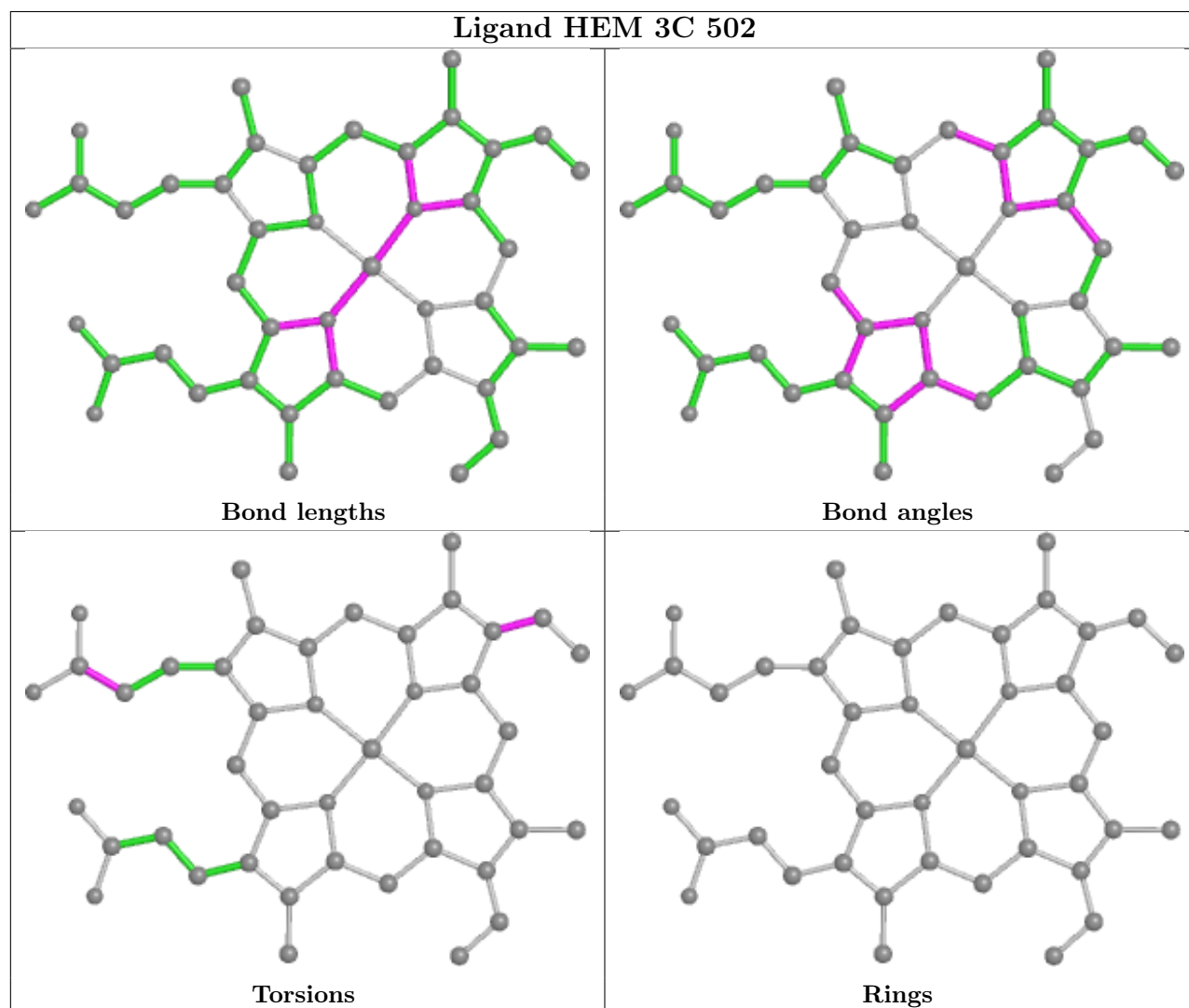
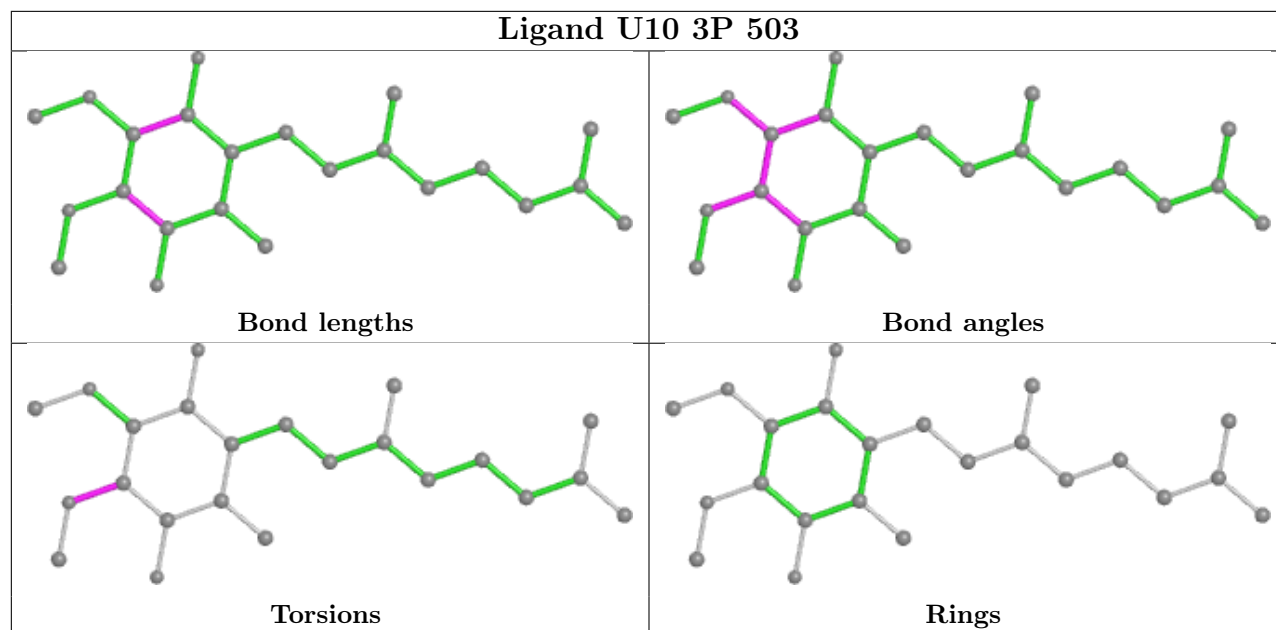
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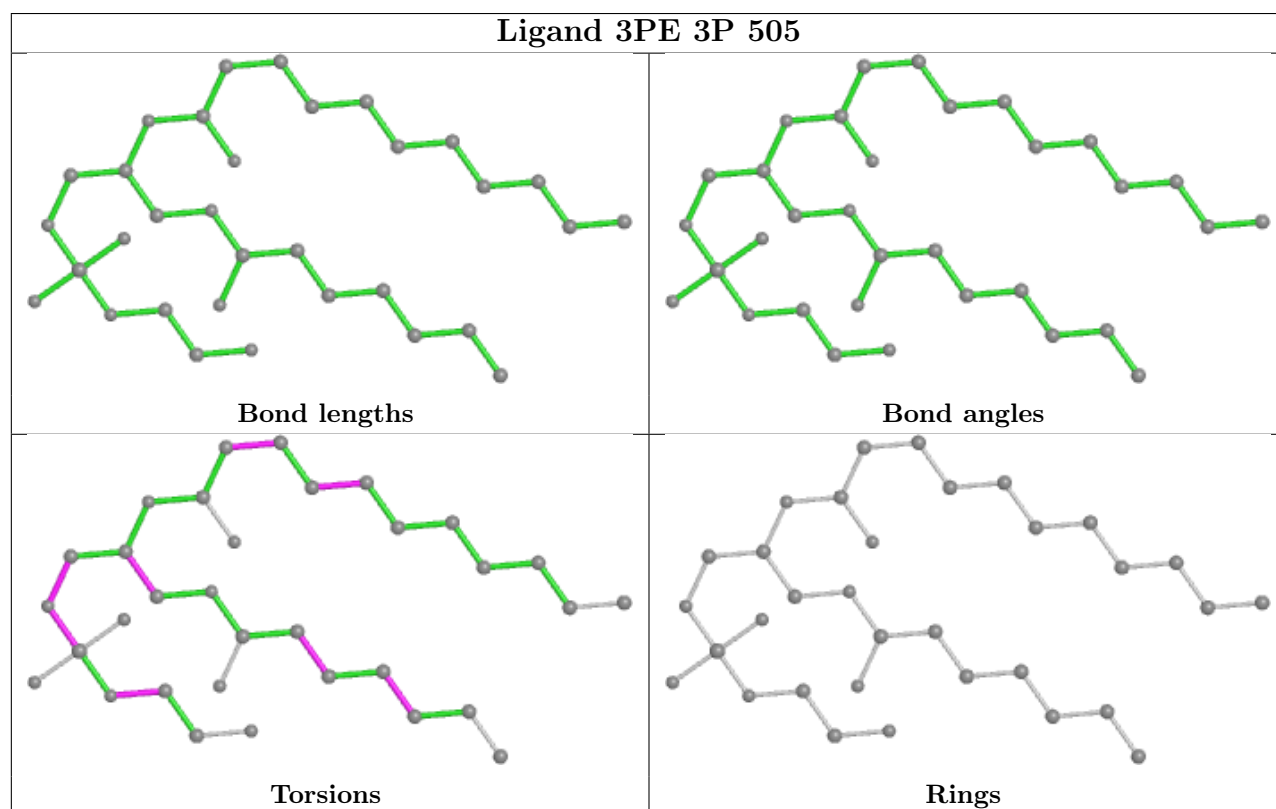
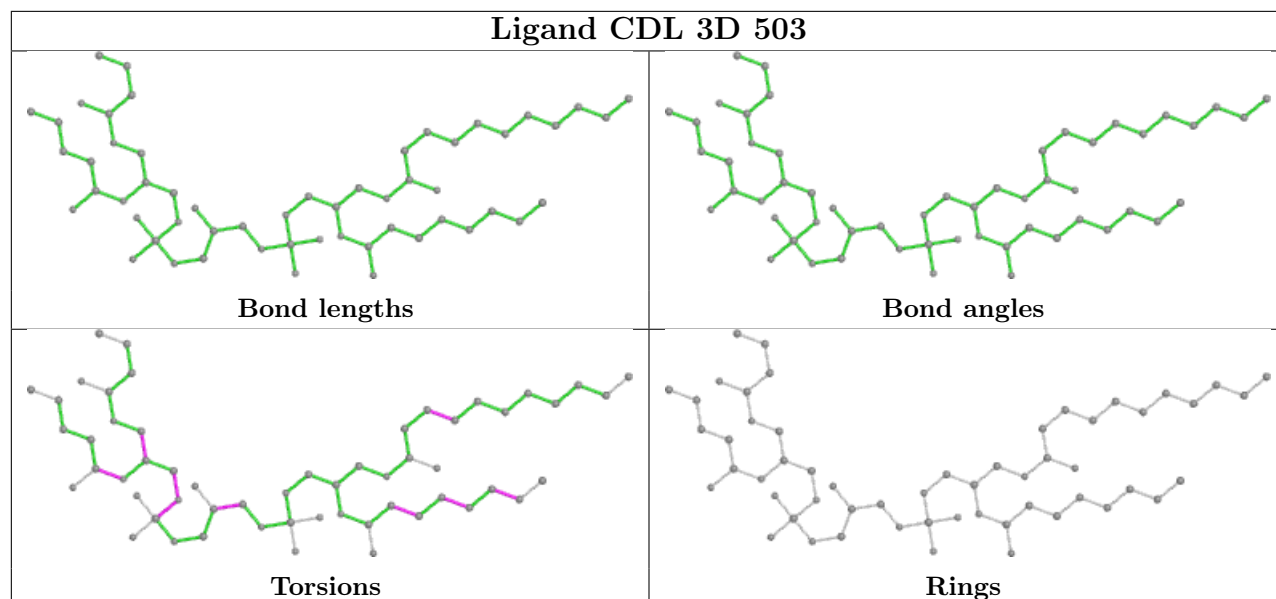
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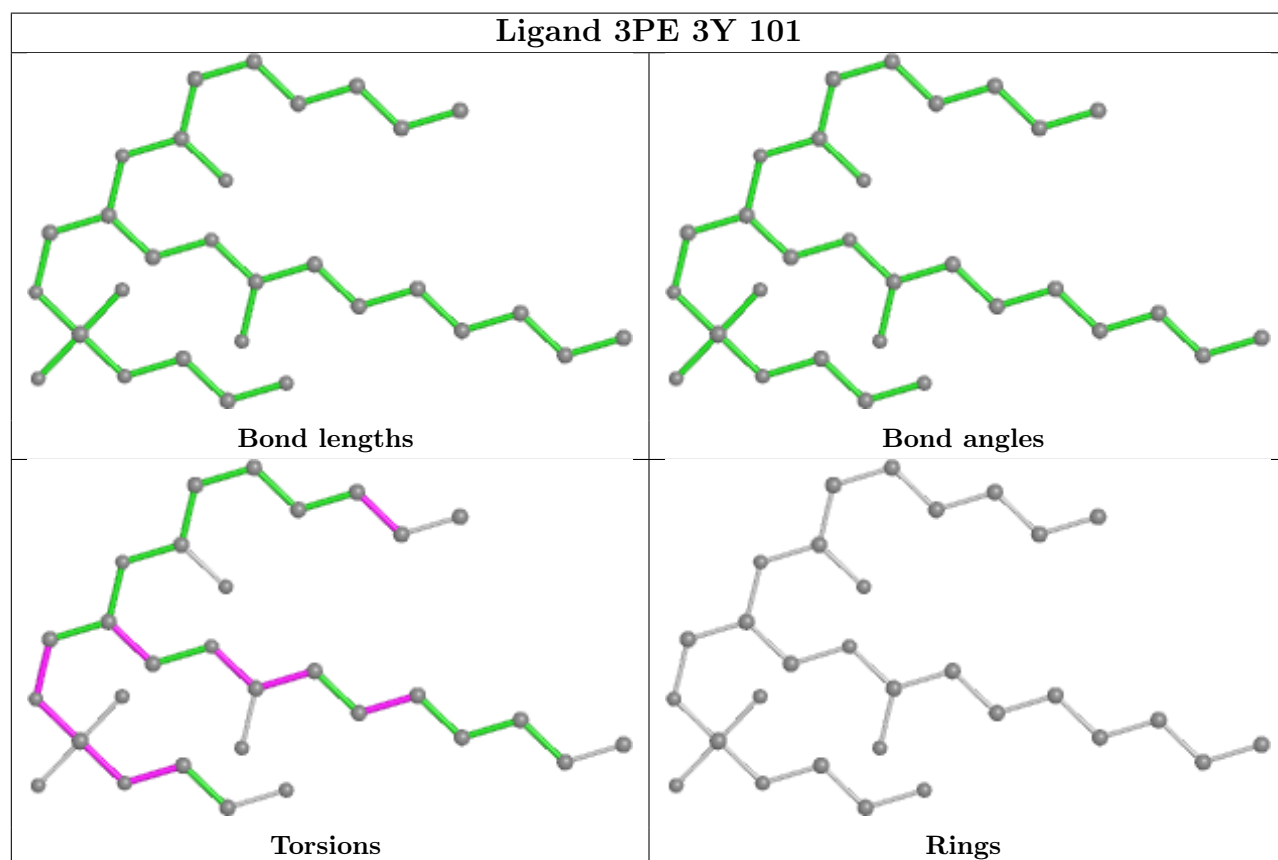
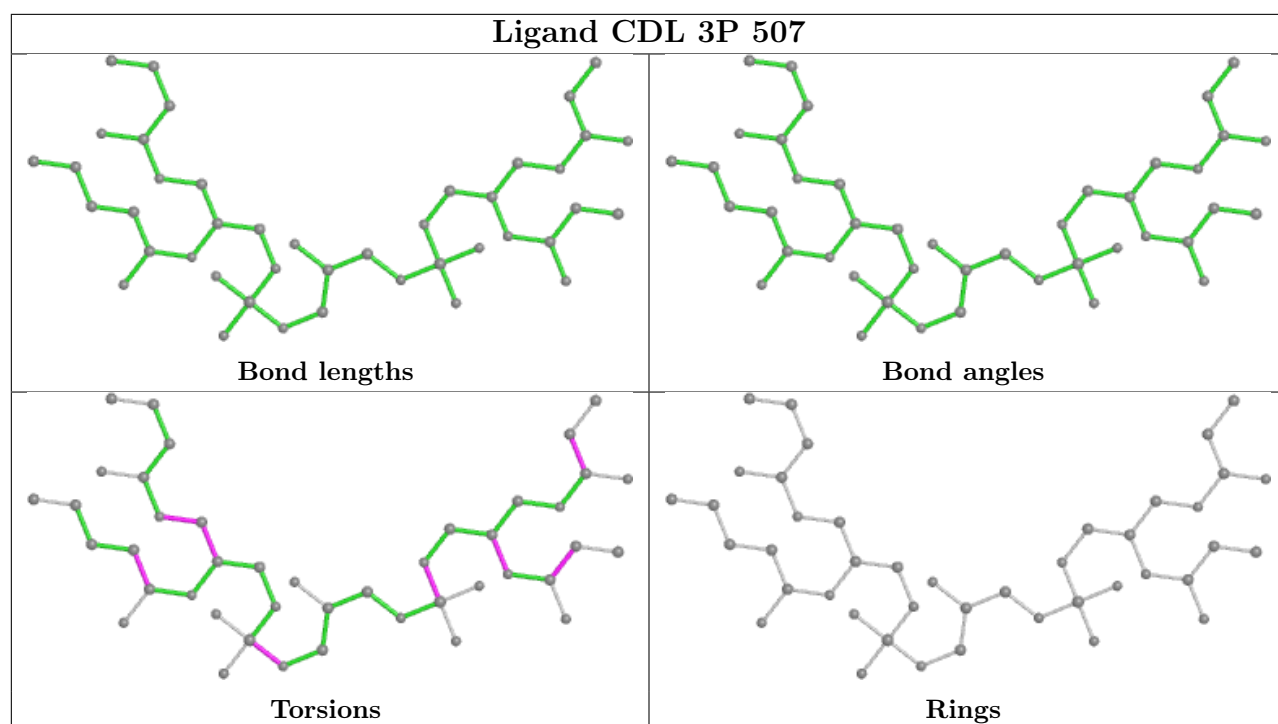
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	3Q	501	HEC	2	0
15	3D	501	HEC	4	0
12	3G	101	3PE	1	0
12	3Q	503	3PE	7	0

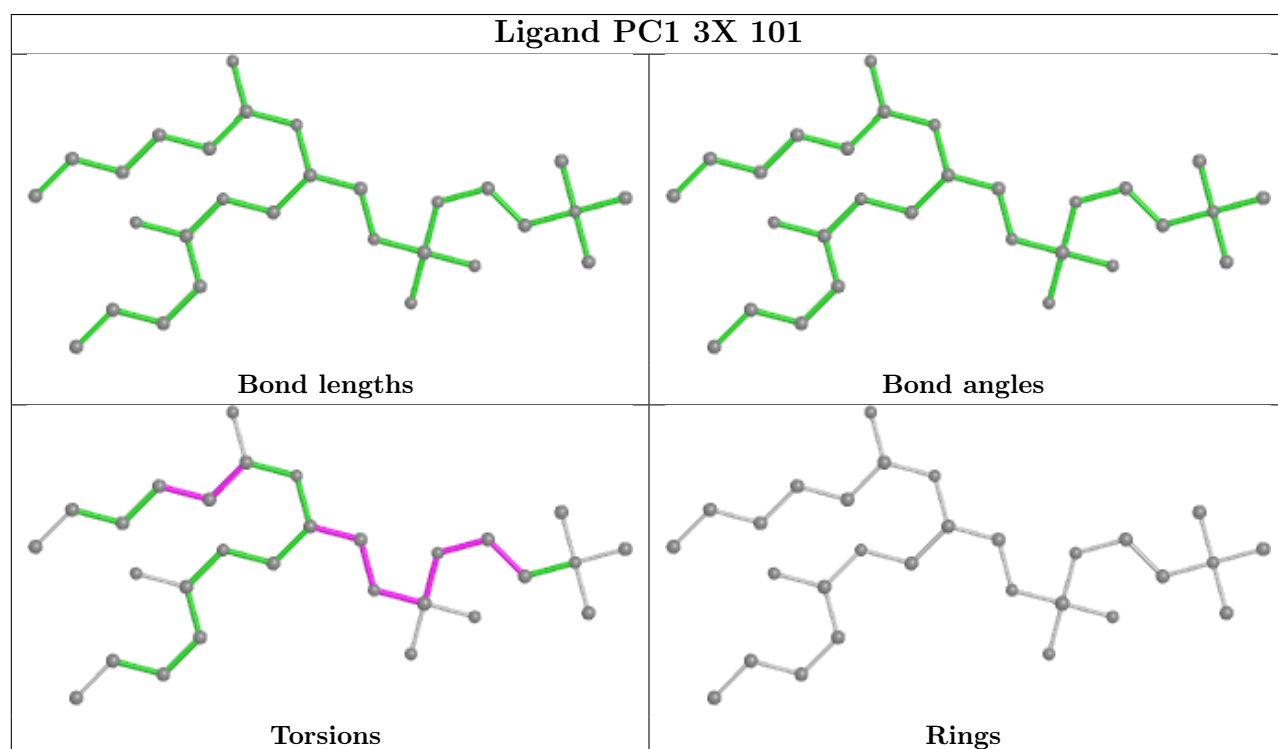
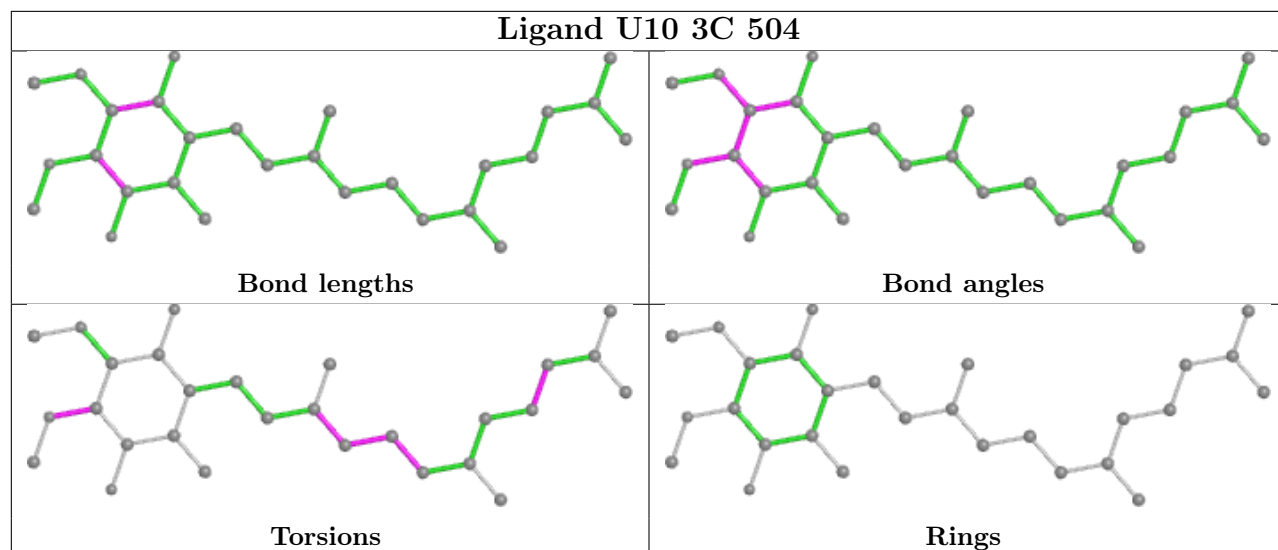
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

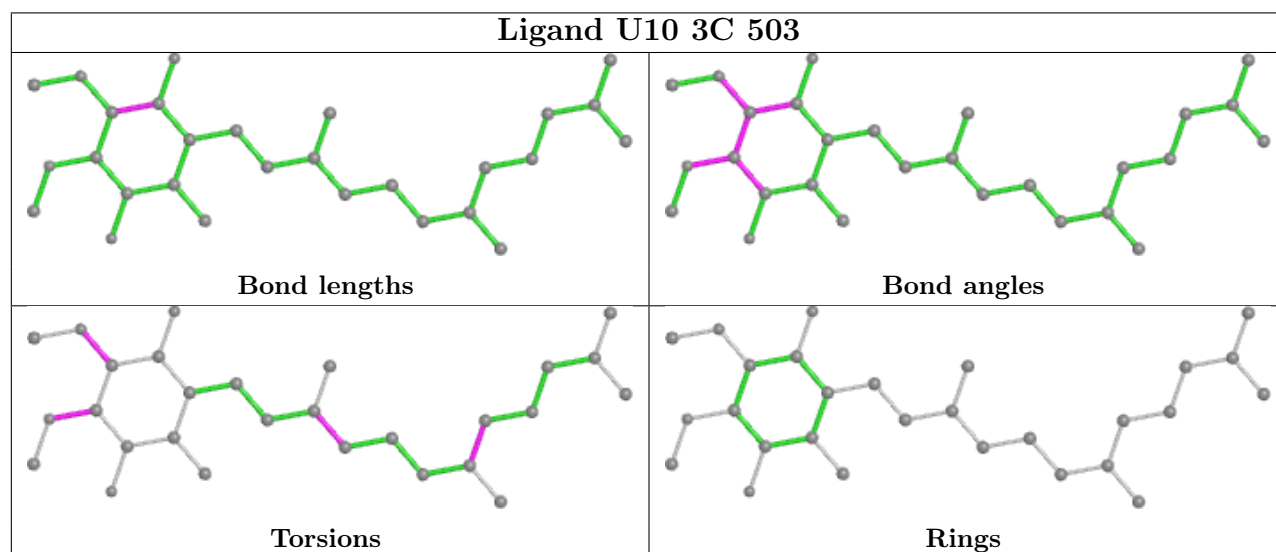
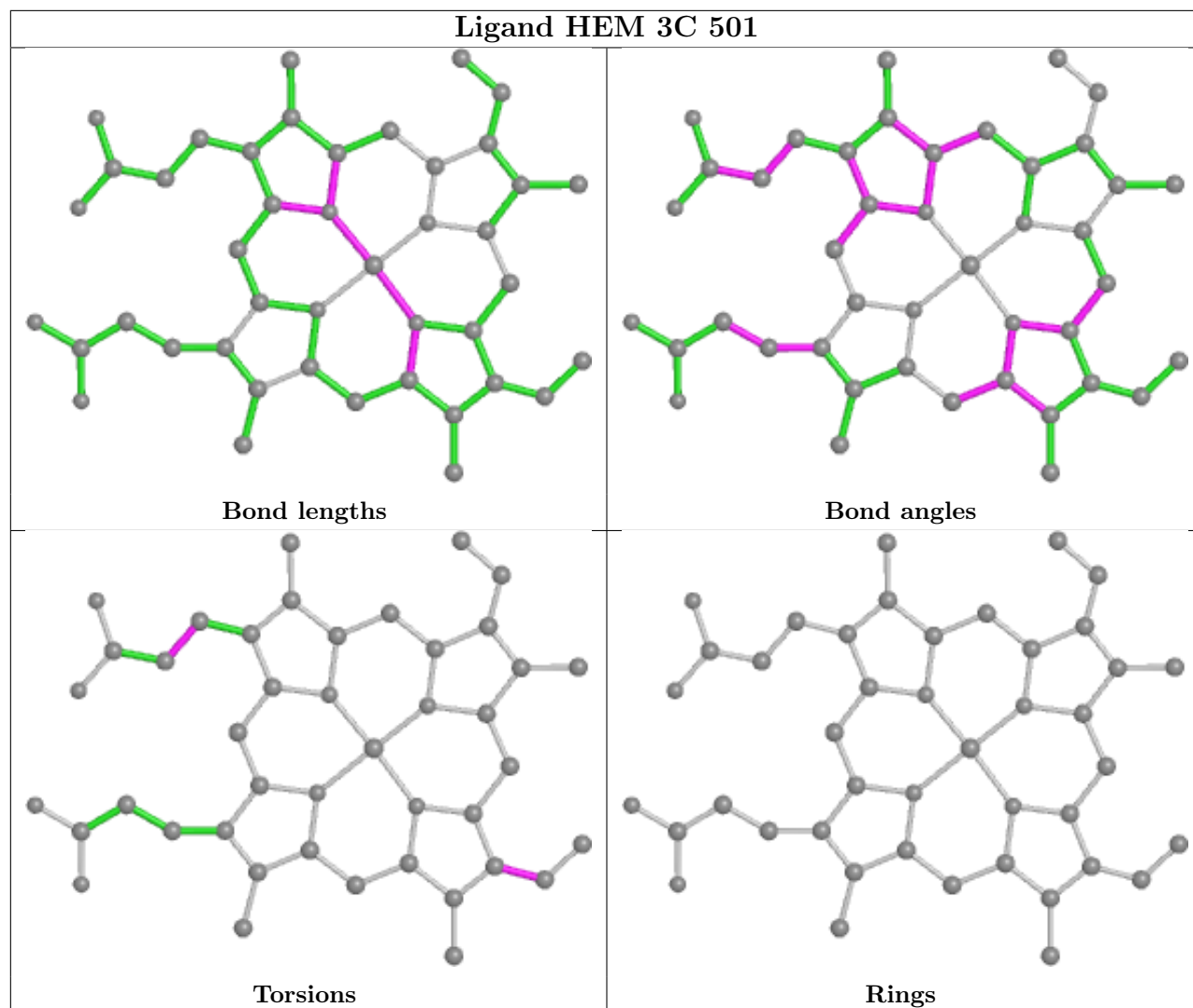


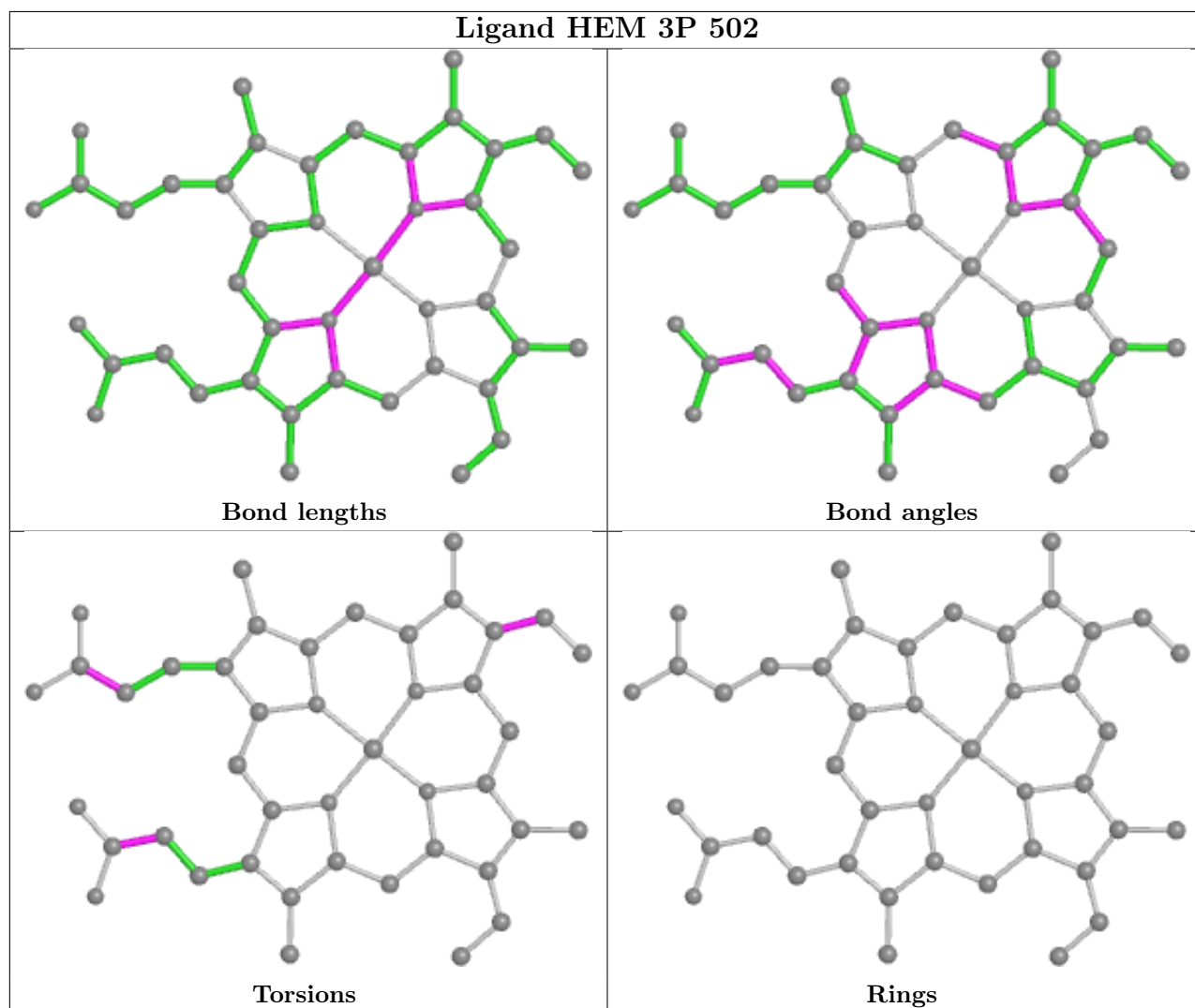
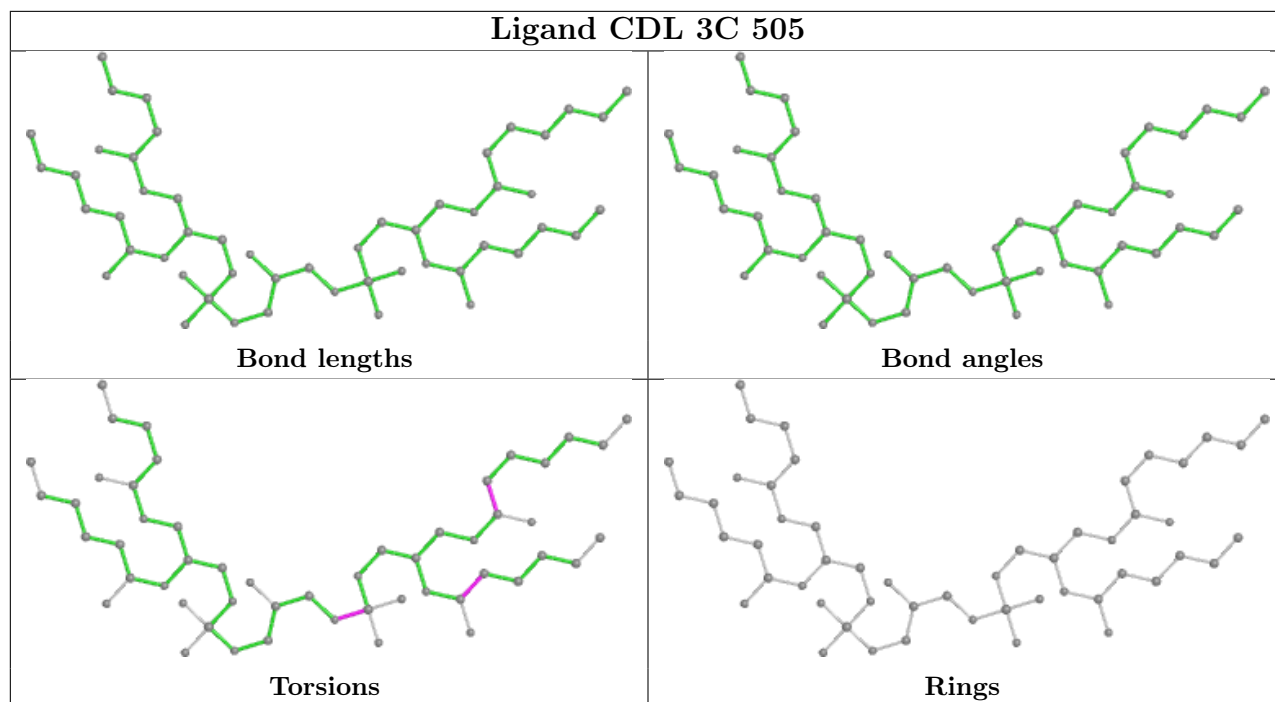




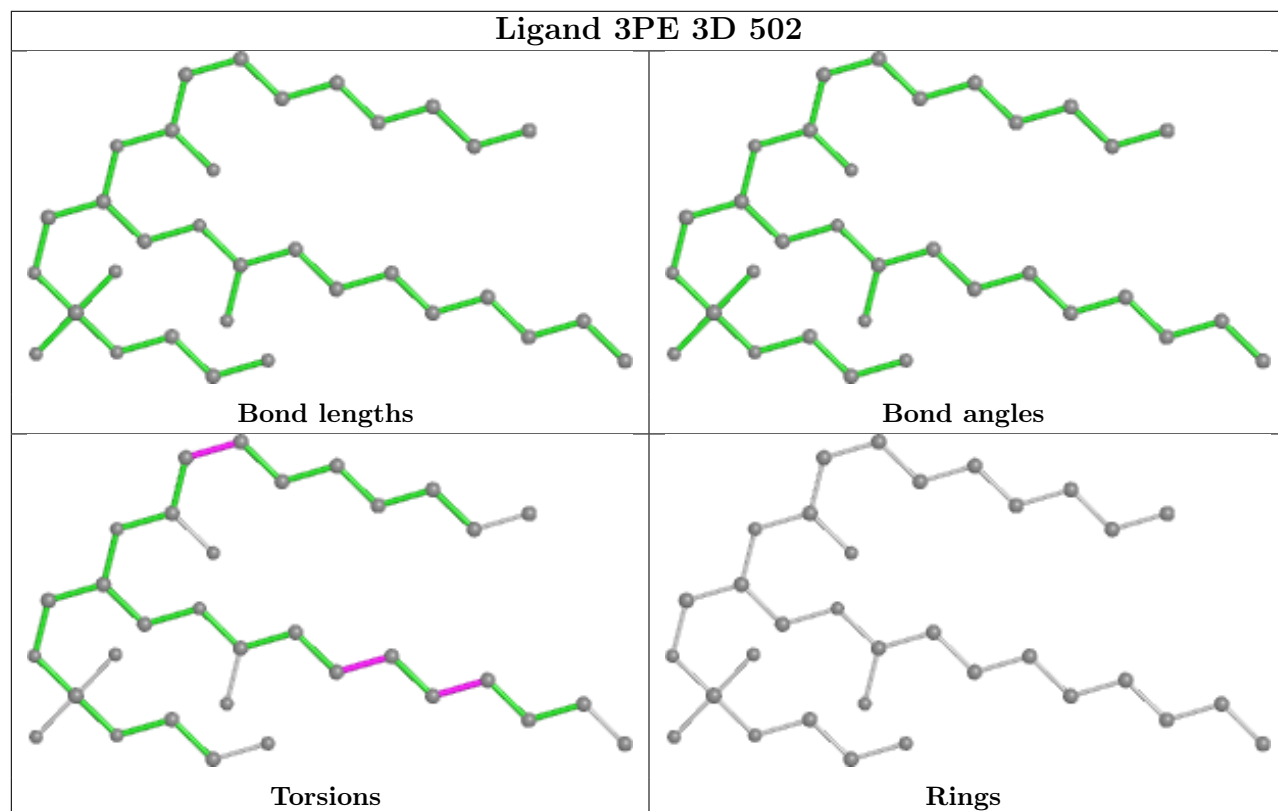
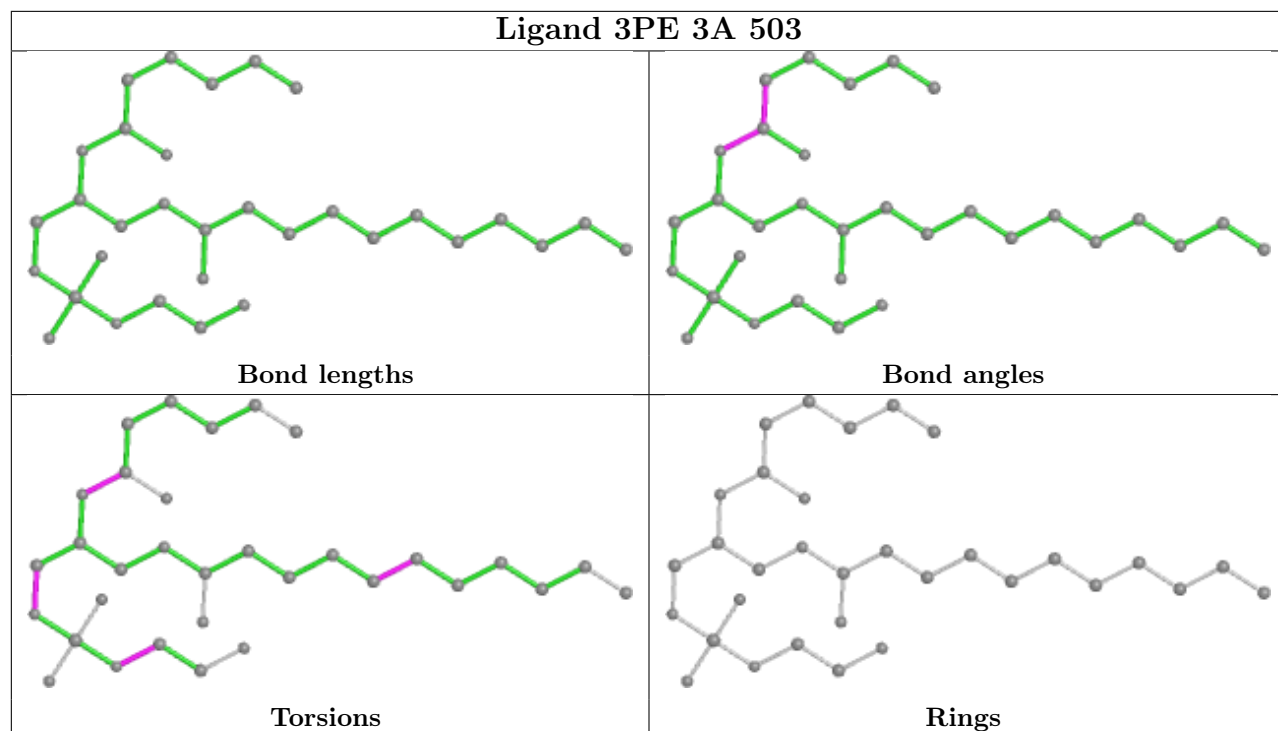


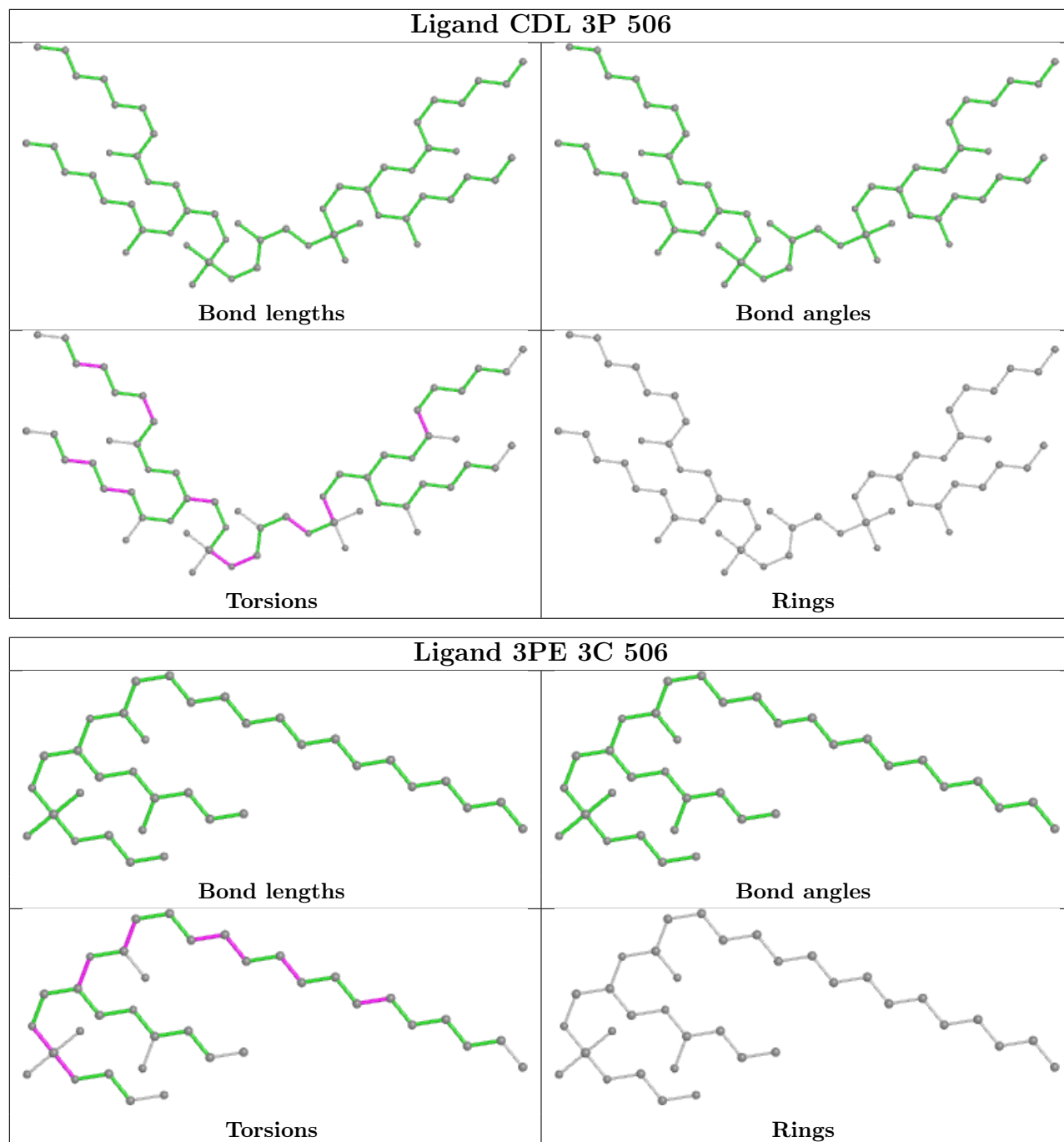


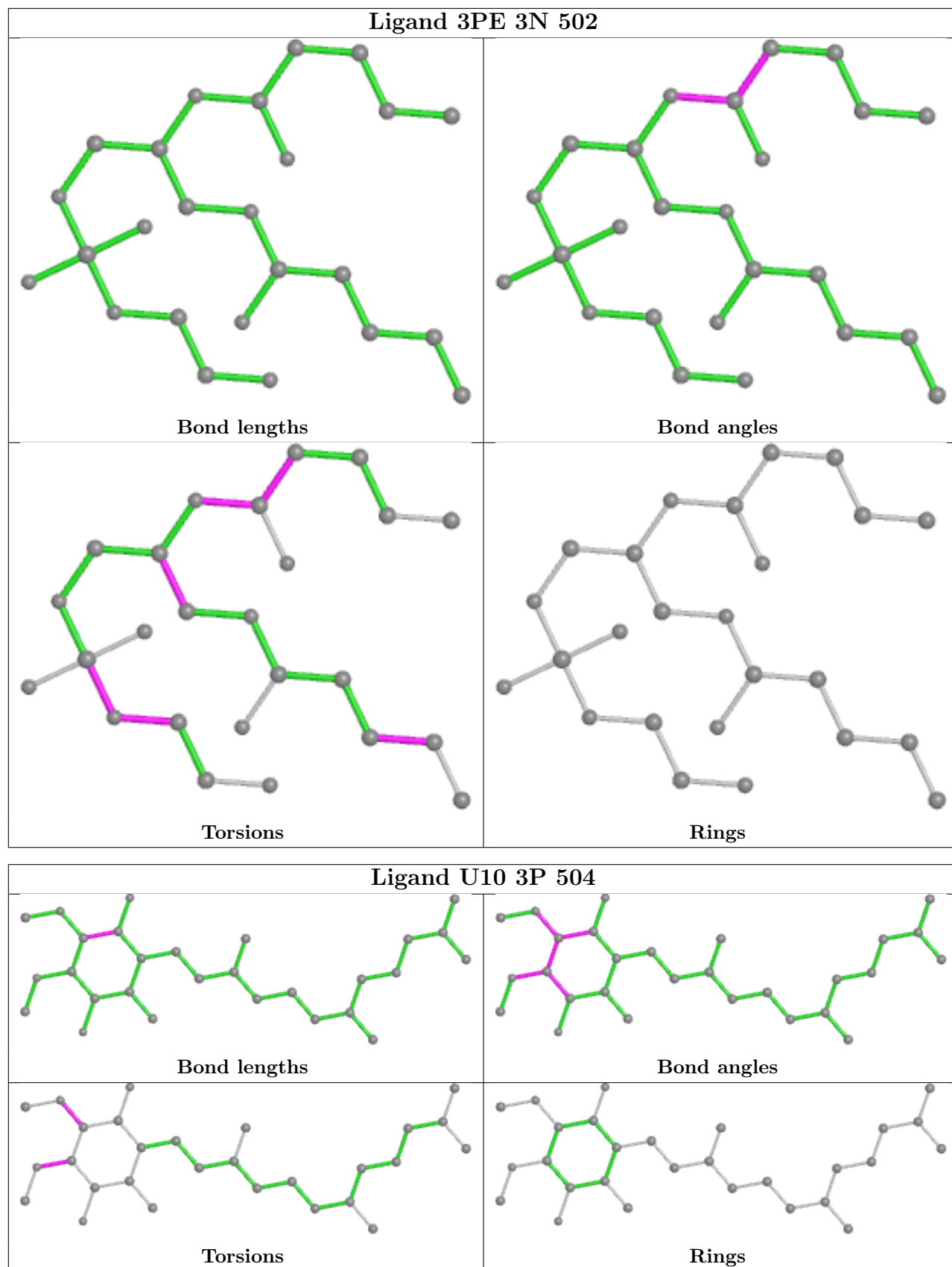


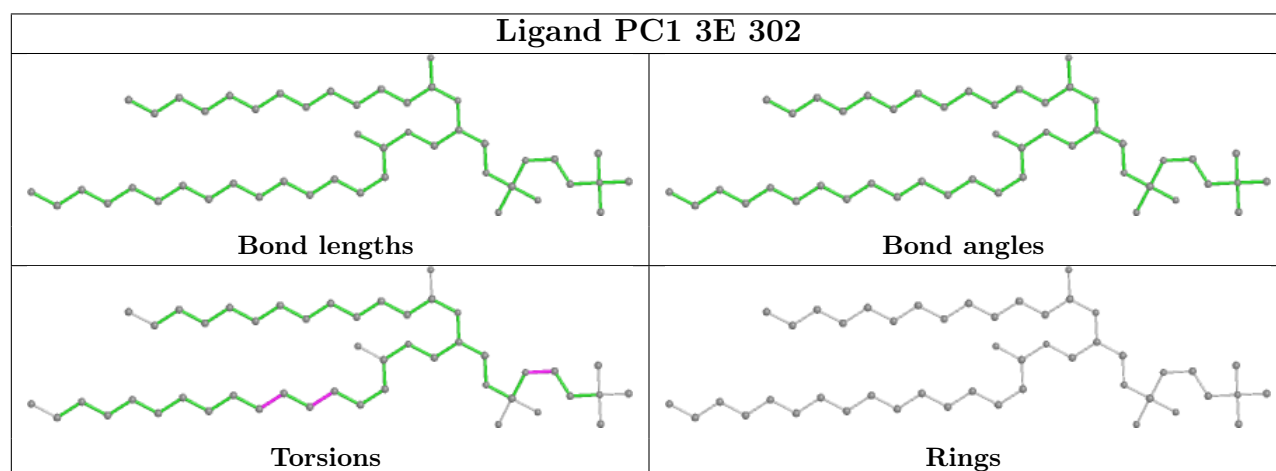
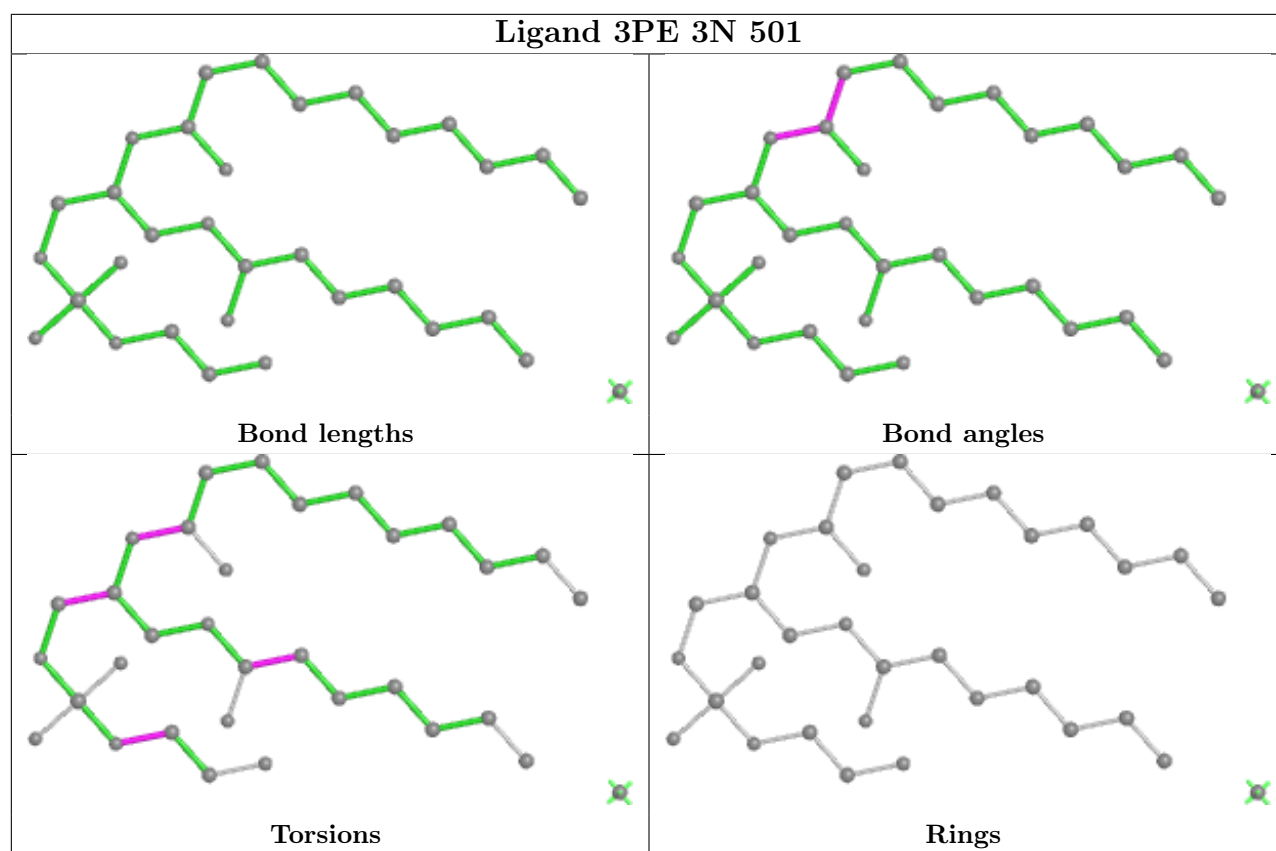


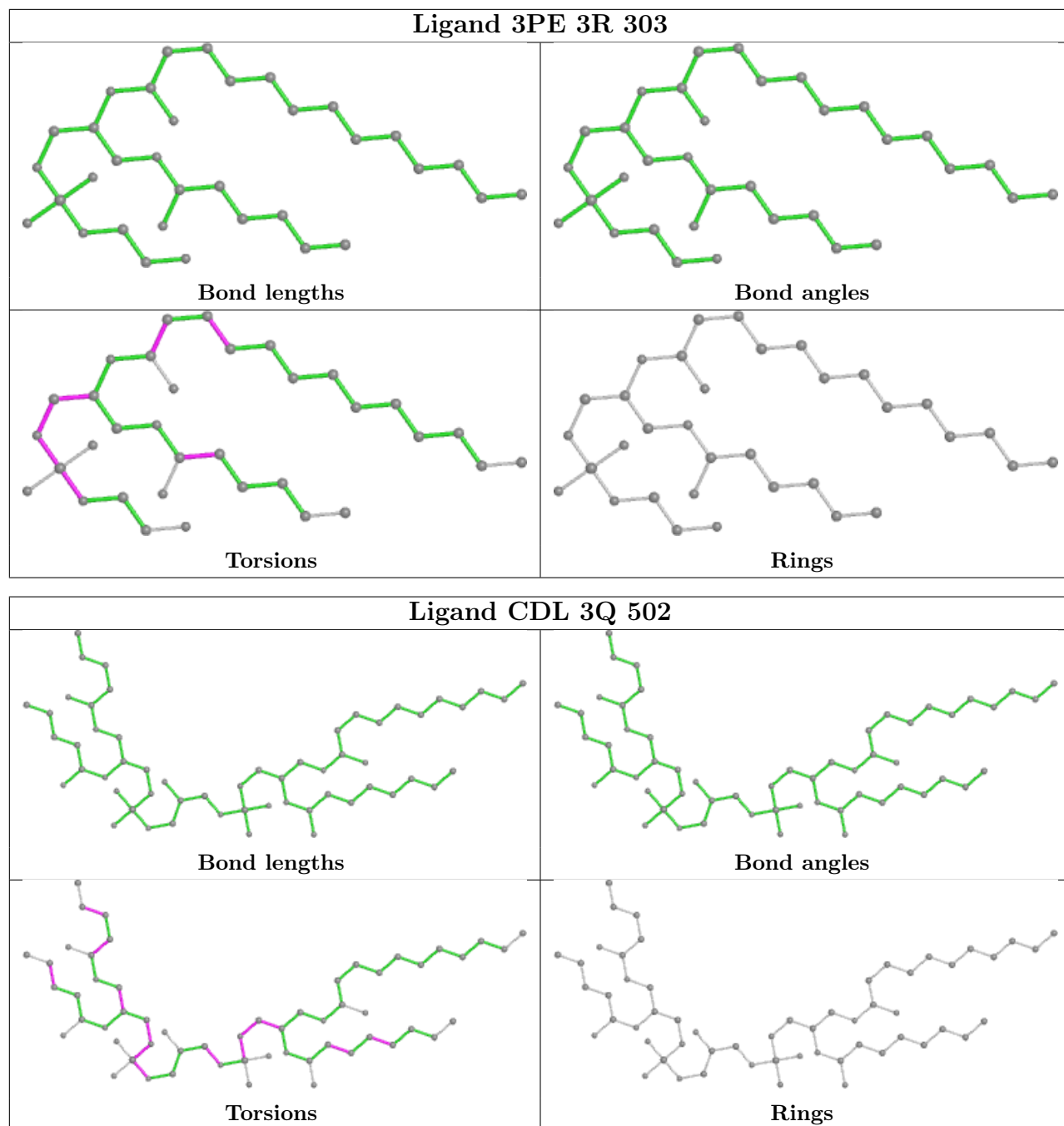


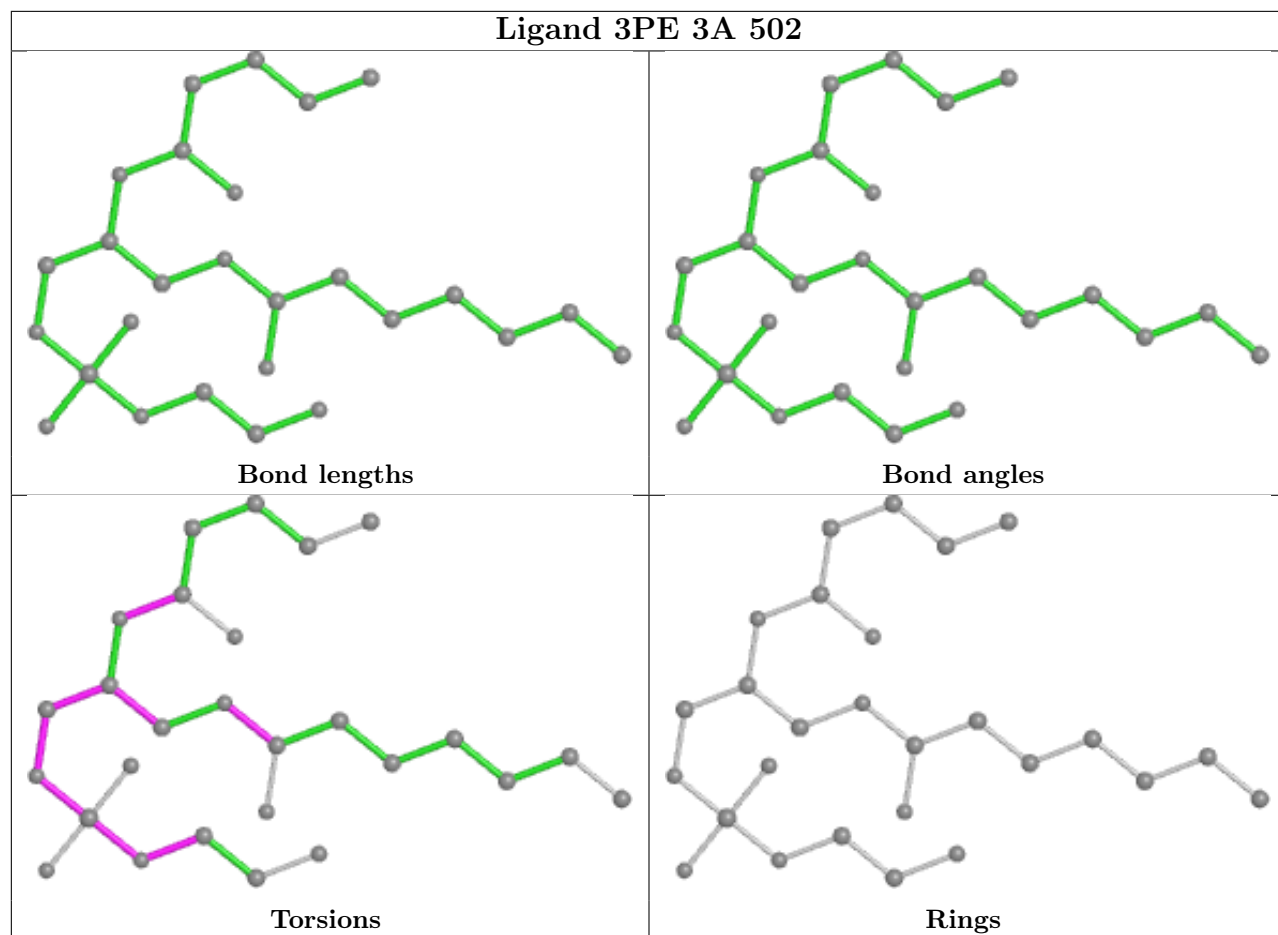


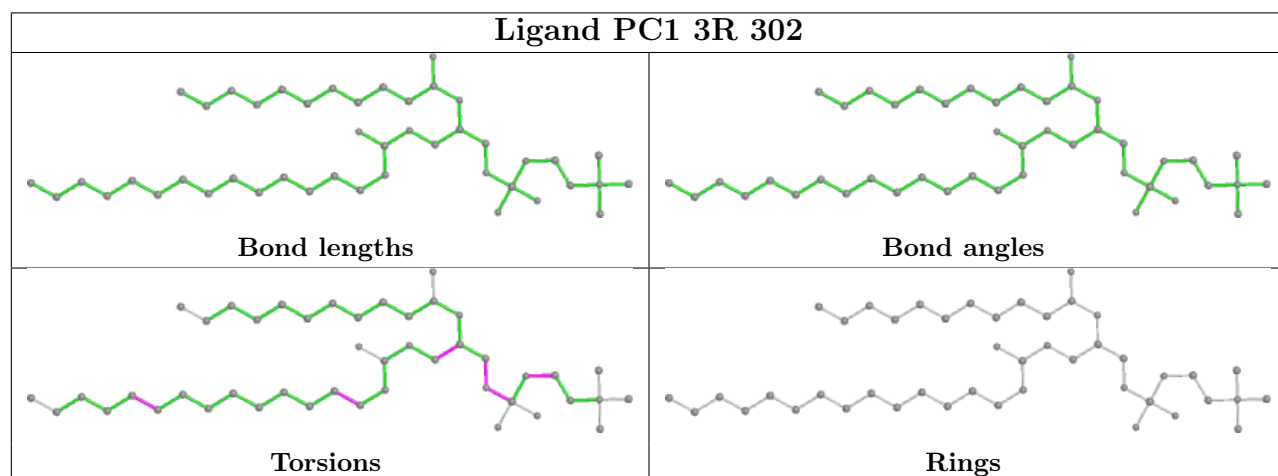
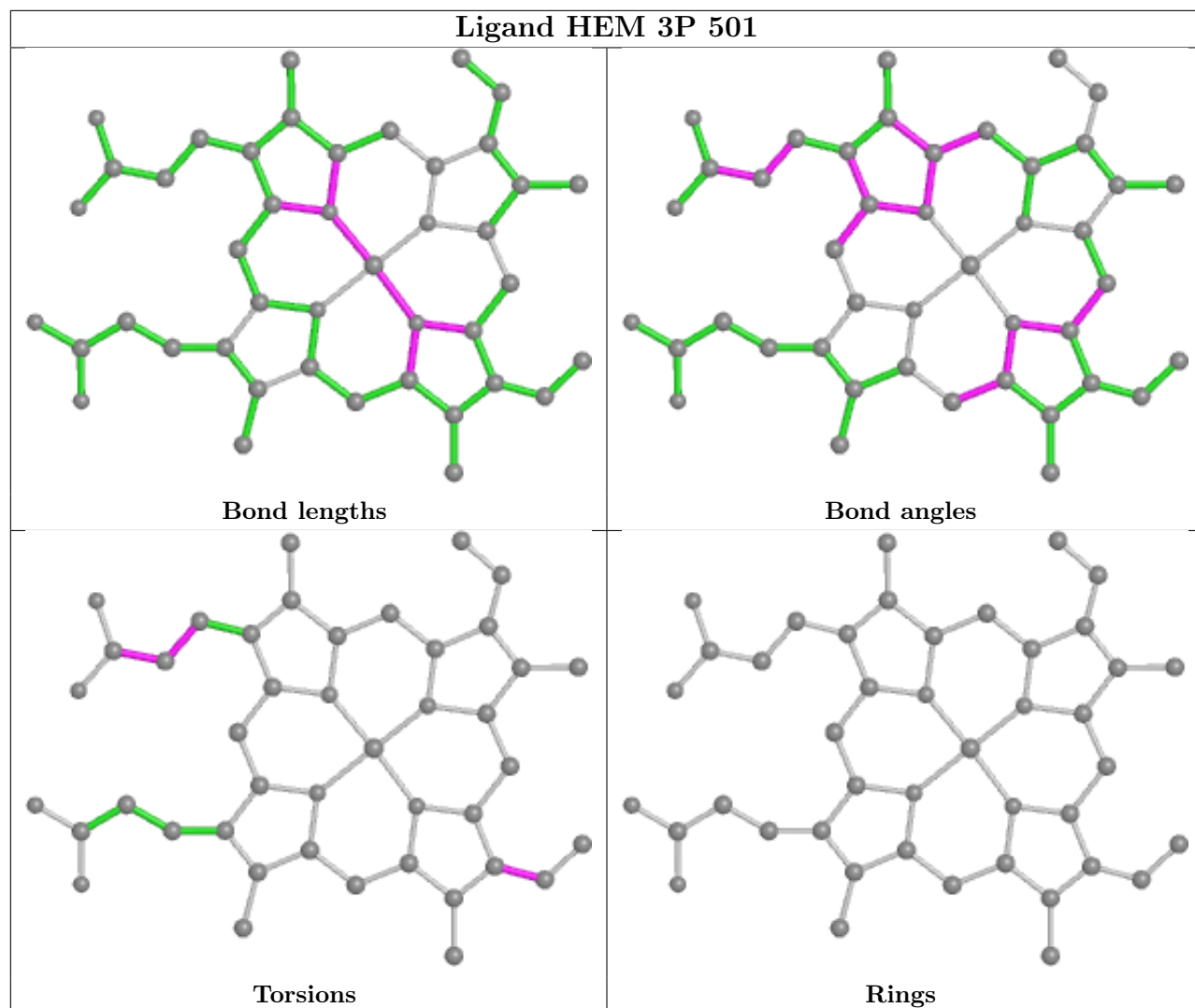


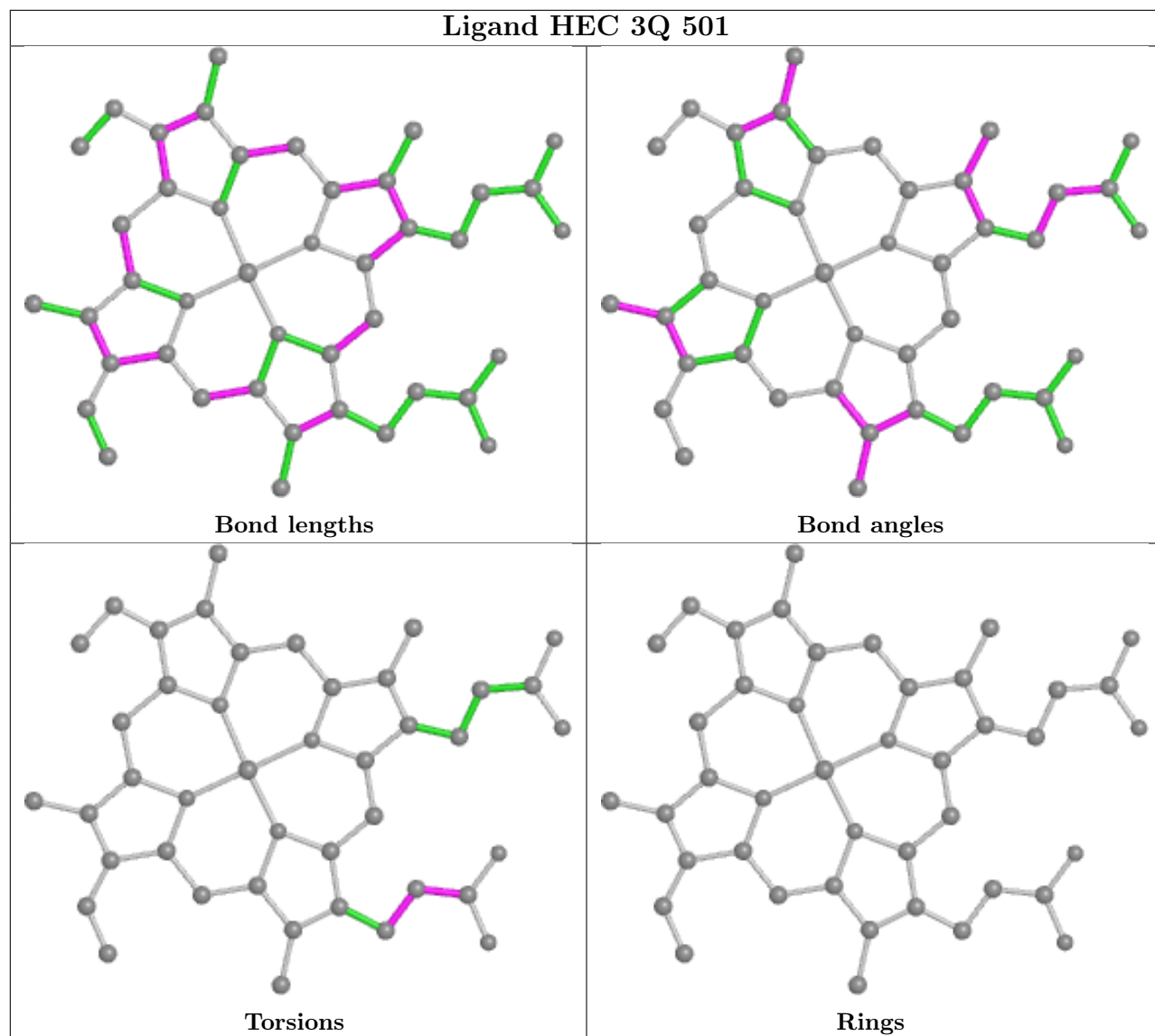




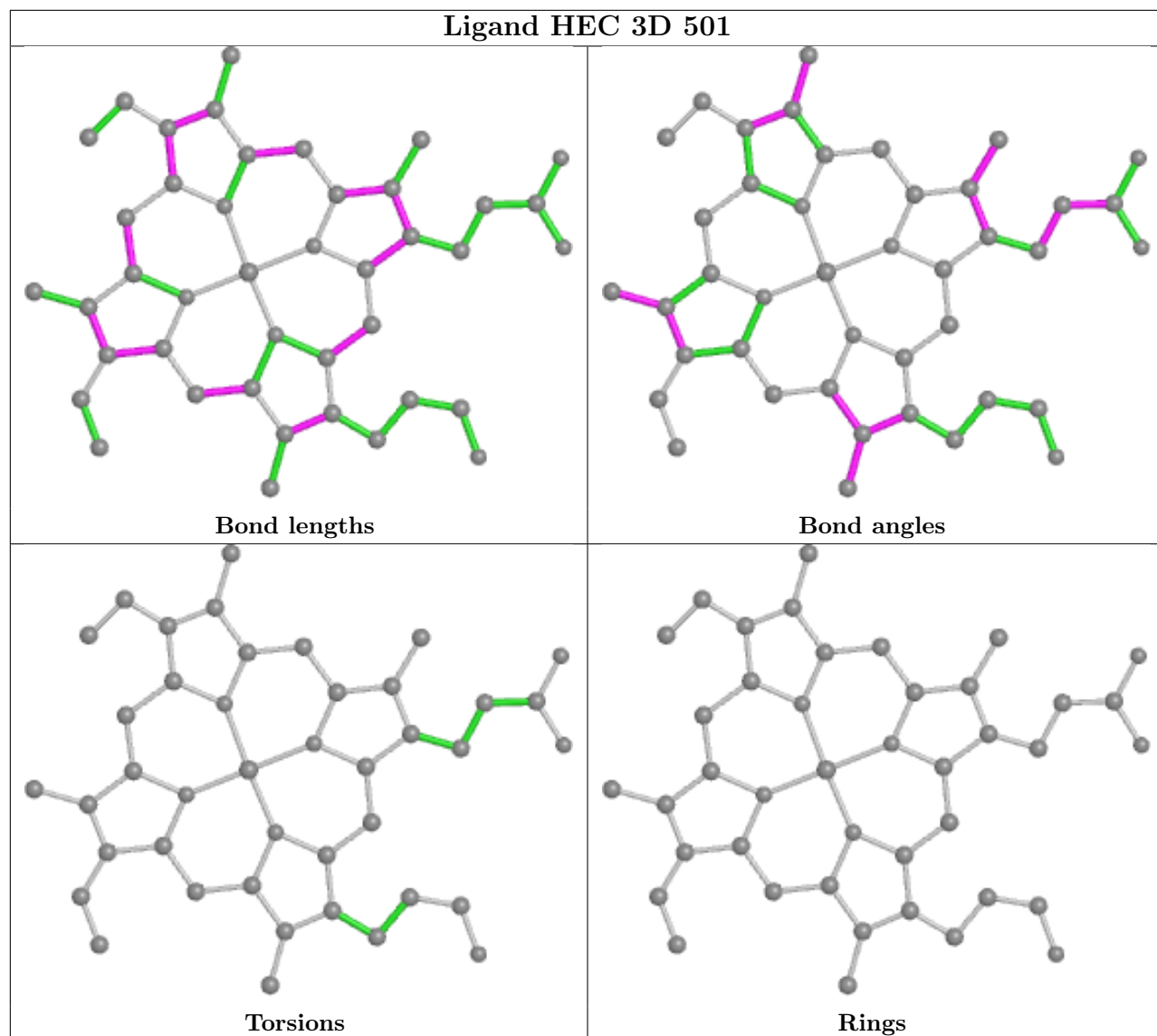


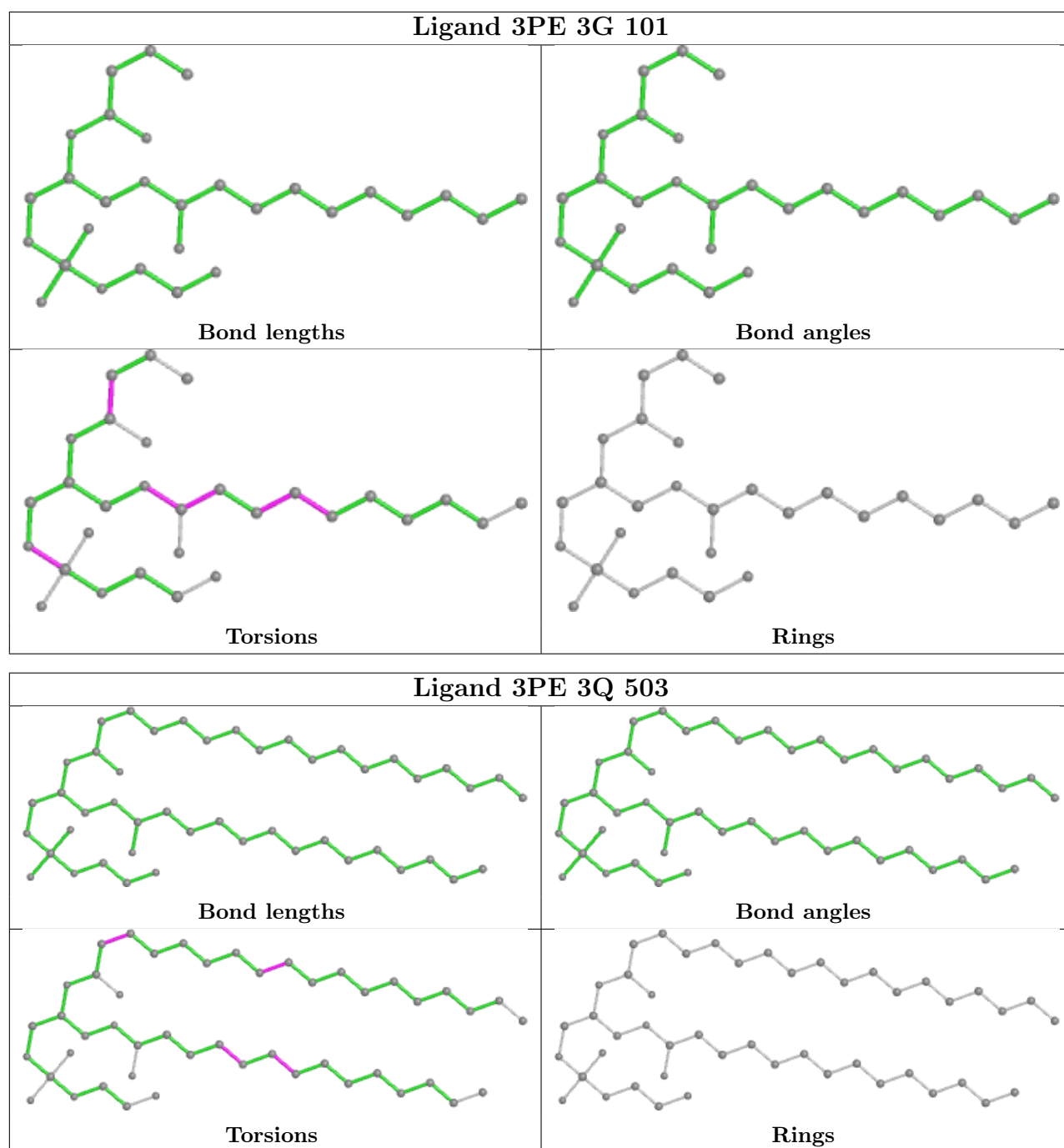












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
7	3G	1
8	3H	1
5	3I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	3G	75:ASN	C	82:PRO	N	4.50
1	3H	77:GLU	C	78:ASP	N	3.04
1	3I	49:PHE	C	50:LEU	N	1.97

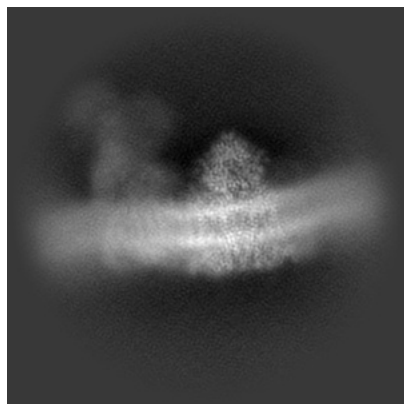
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42221. These allow visual inspection of the internal detail of the map and identification of artifacts.

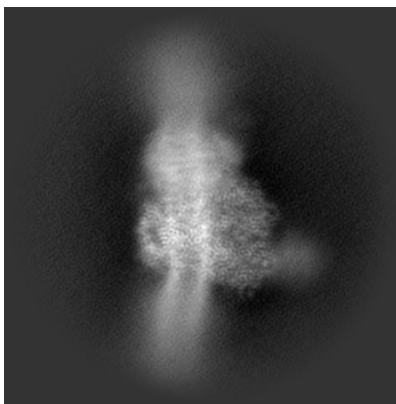
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

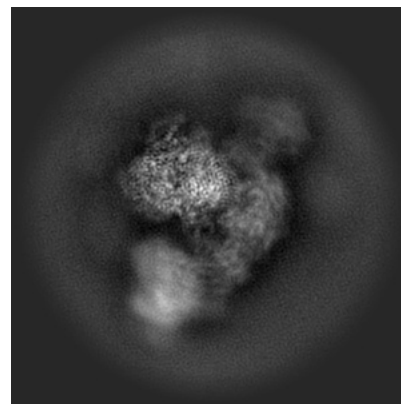
#### 6.1.1 Primary map



X

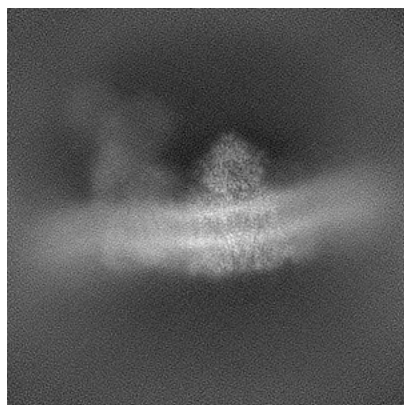


Y

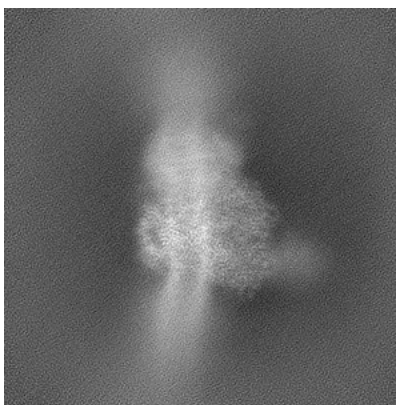


Z

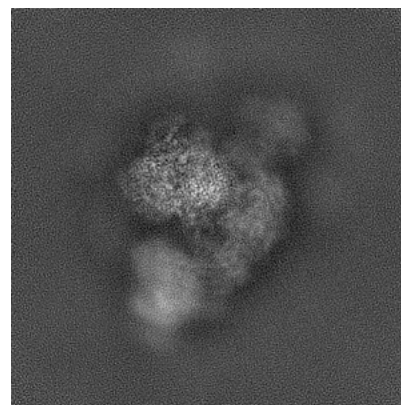
#### 6.1.2 Raw map



X



Y

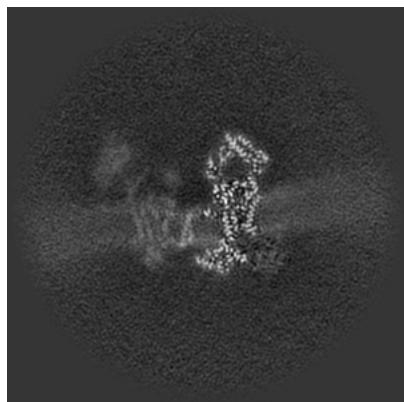


Z

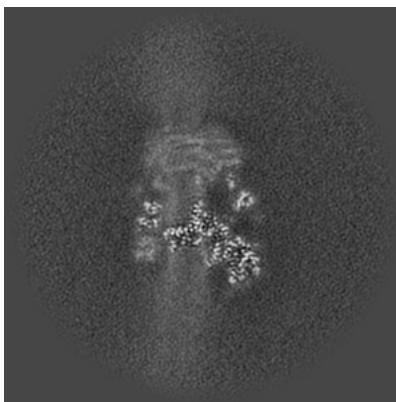
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

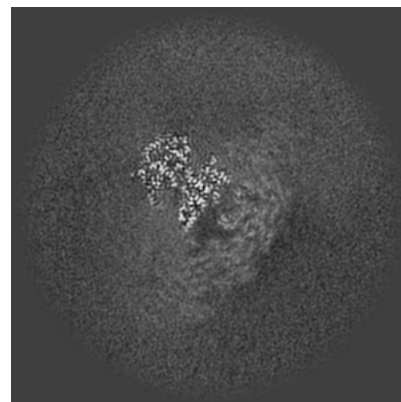
### 6.2.1 Primary map



X Index: 160

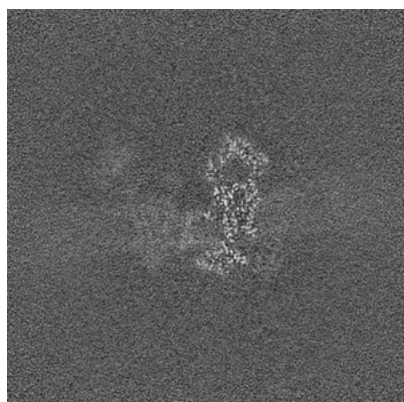


Y Index: 160

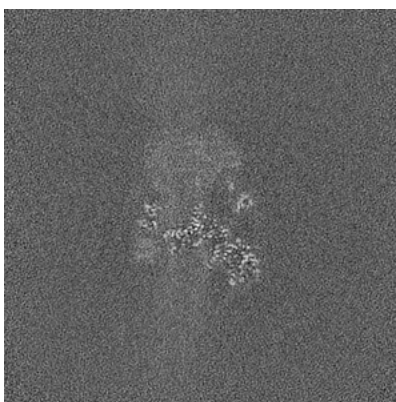


Z Index: 160

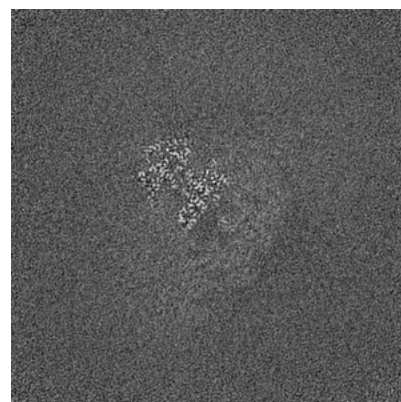
### 6.2.2 Raw map



X Index: 160



Y Index: 160



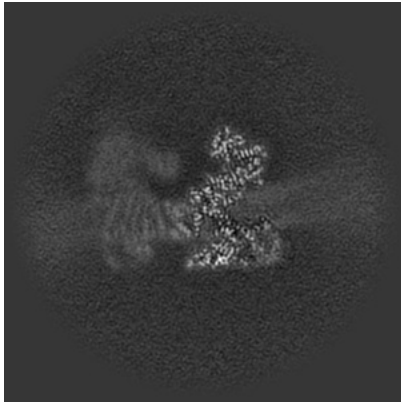
Z Index: 160

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

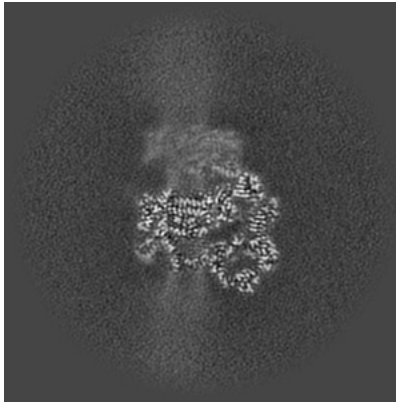


## 6.3 Largest variance slices [i](#)

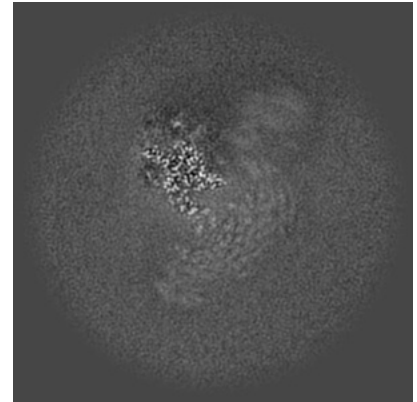
### 6.3.1 Primary map



X Index: 147

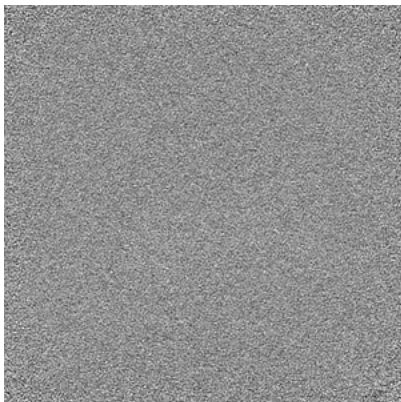


Y Index: 175

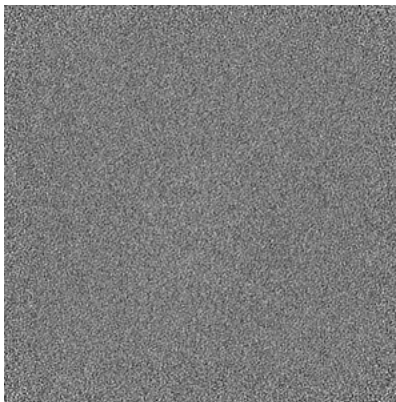


Z Index: 133

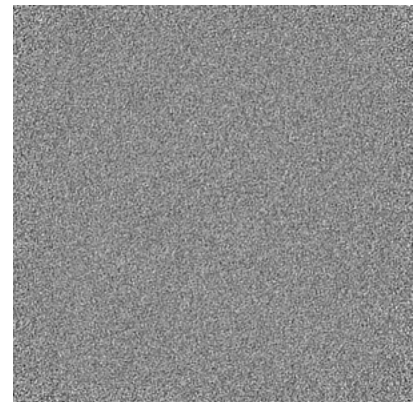
### 6.3.2 Raw map



X Index: 0



Y Index: 0

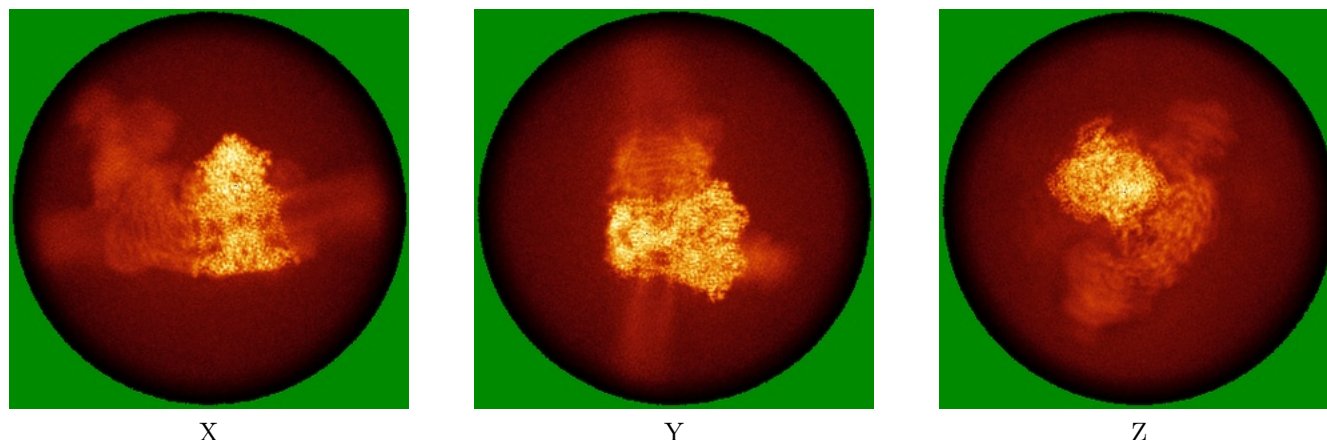


Z Index: 0

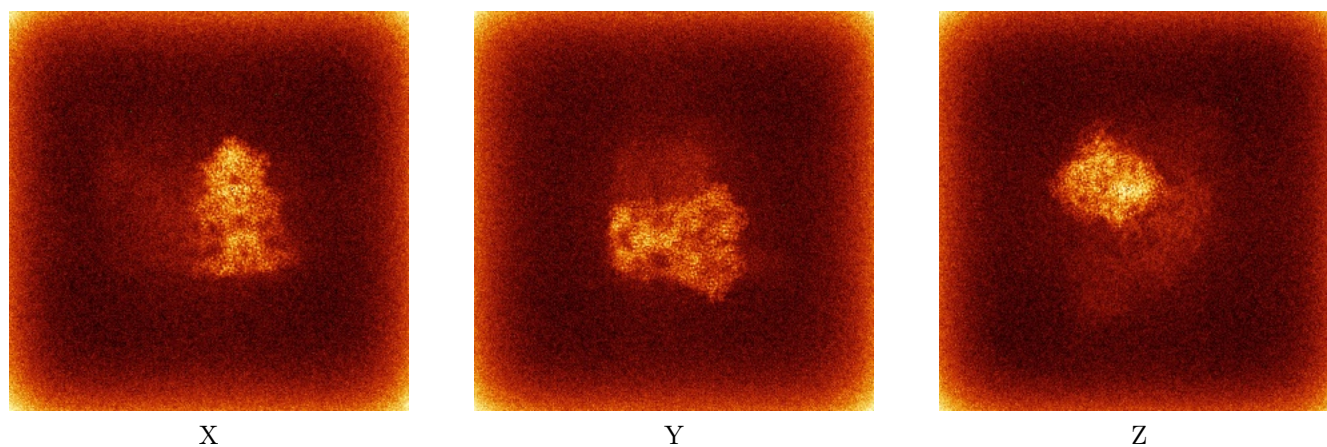
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



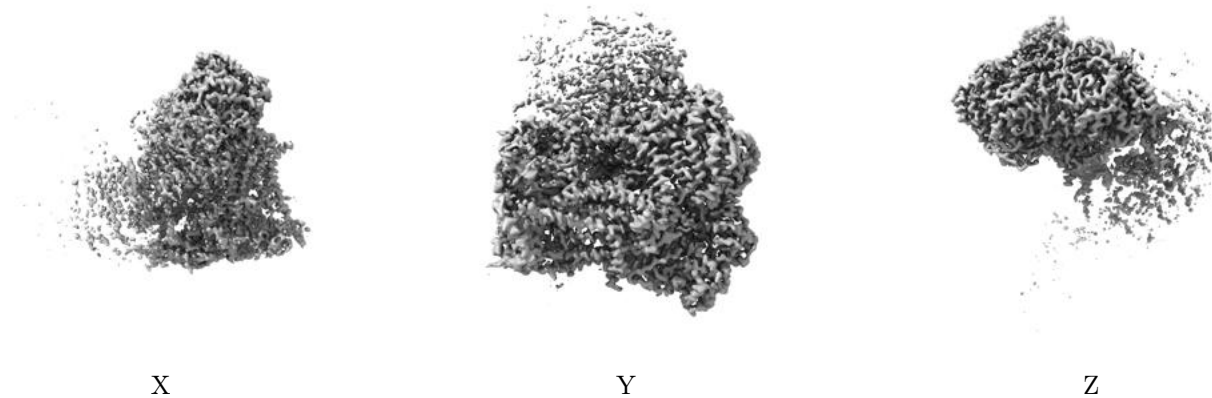
### 6.4.2 Raw map



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

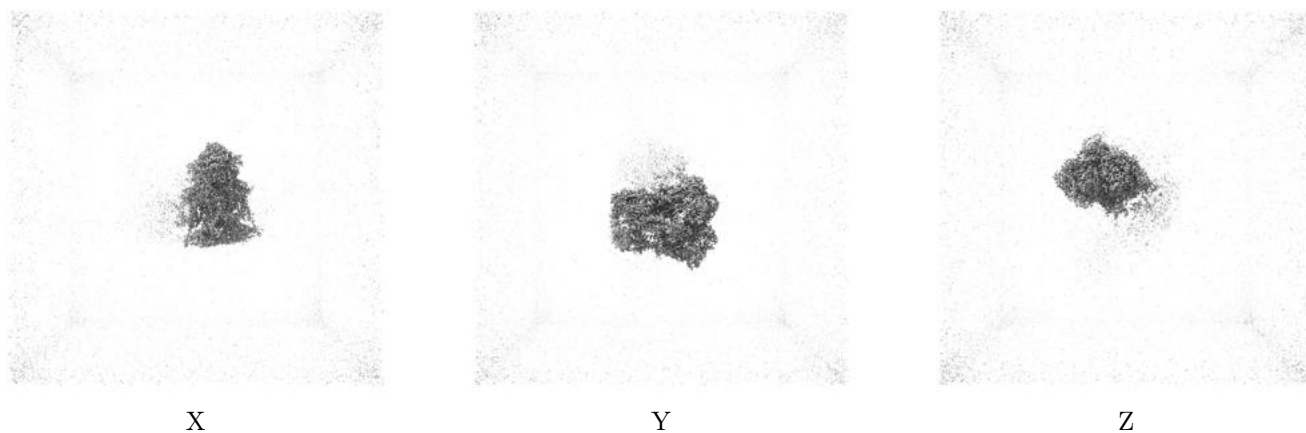
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

## 6.6 Mask visualisation [i](#)

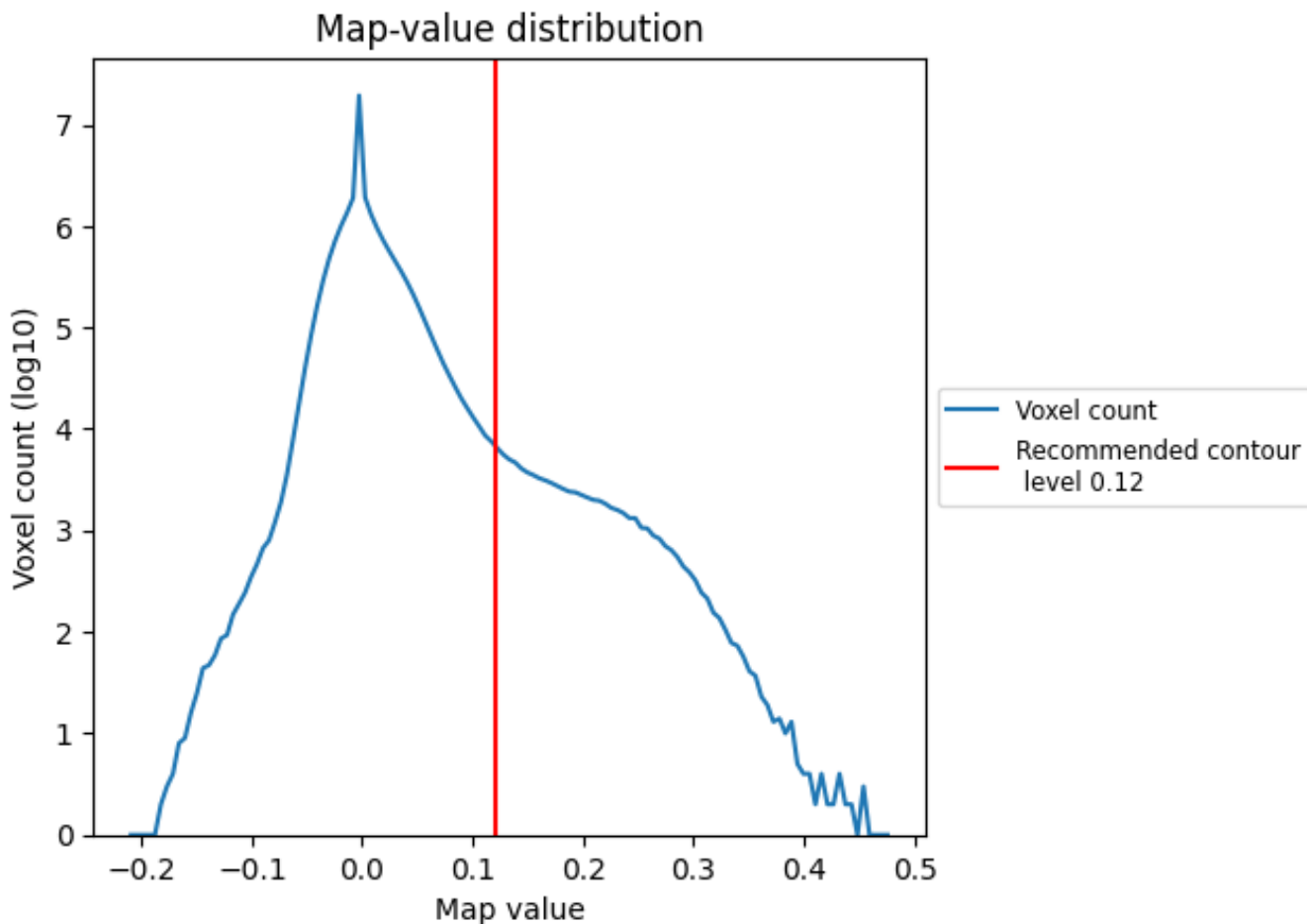
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

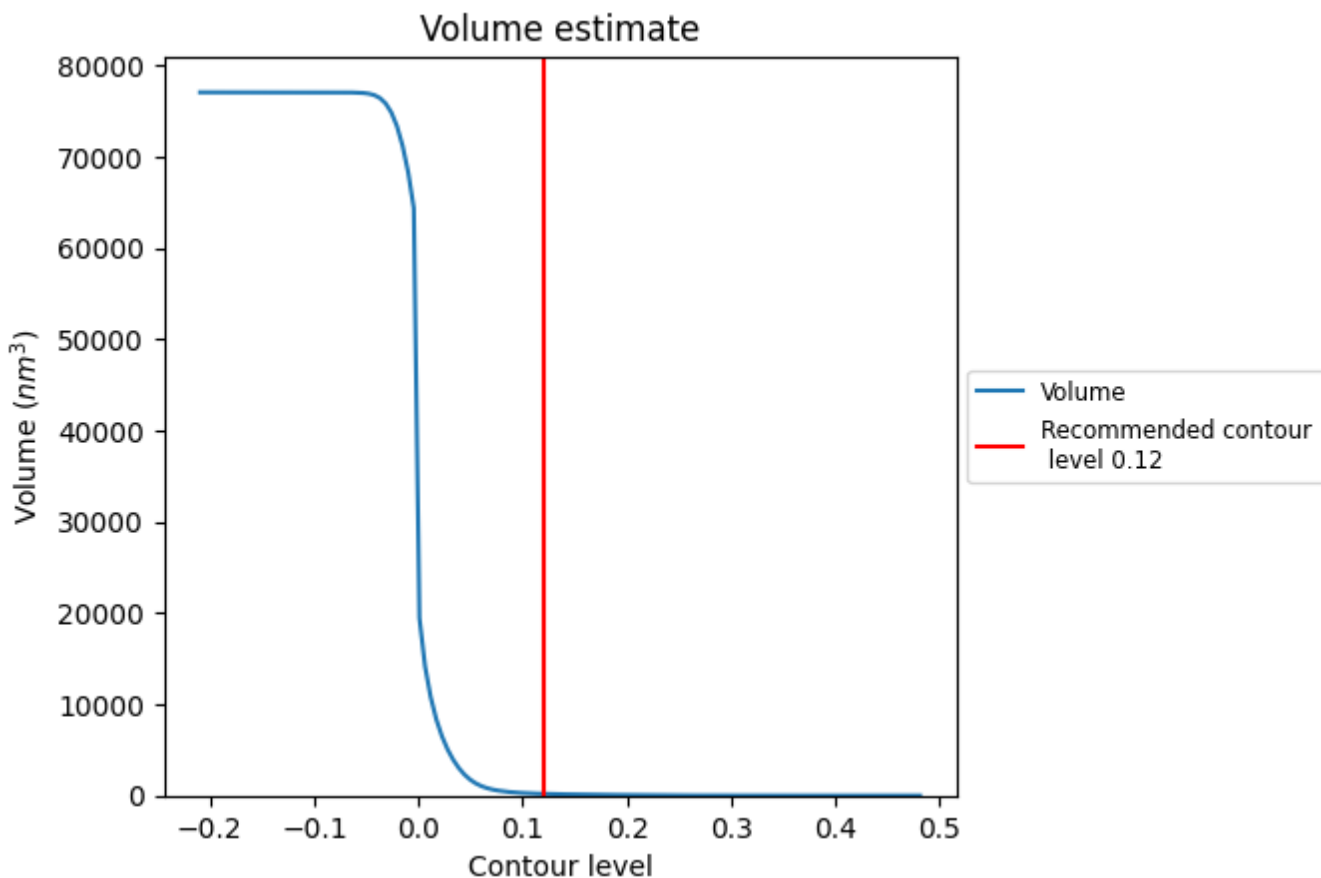
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

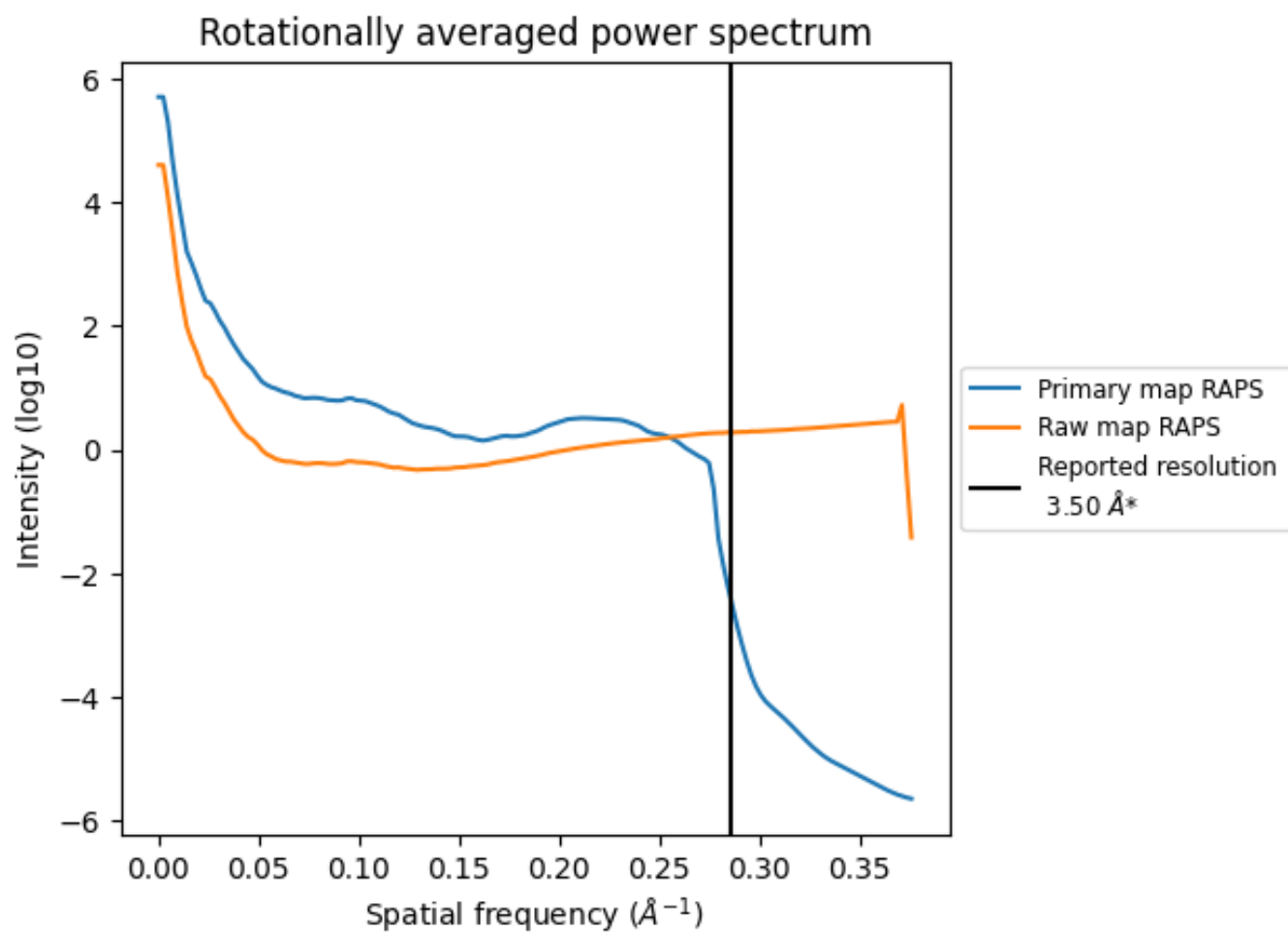
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 191 nm<sup>3</sup>; this corresponds to an approximate mass of 172 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

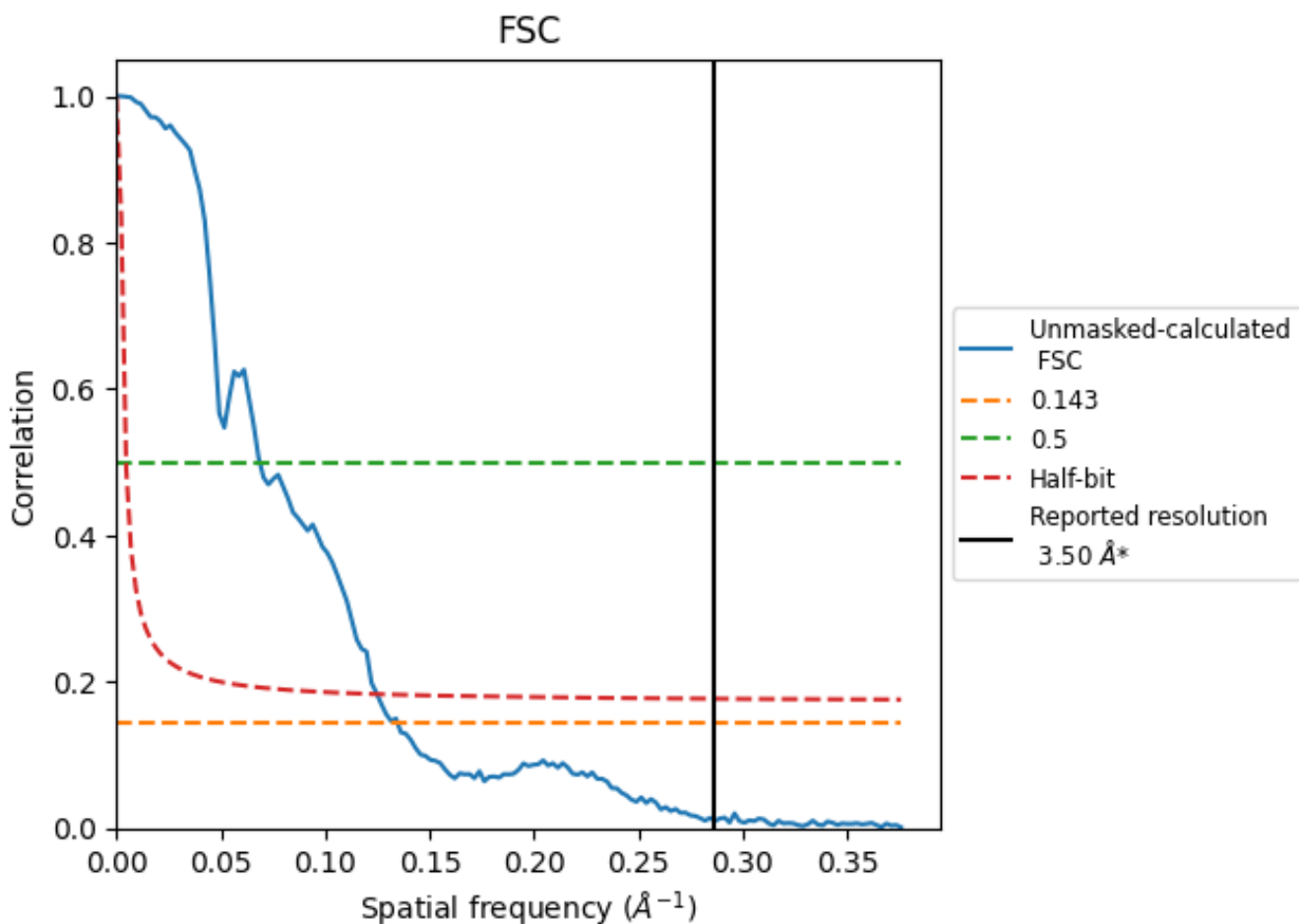


\*Reported resolution corresponds to spatial frequency of  $0.286 \text{ \AA}^{-1}$

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.286 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

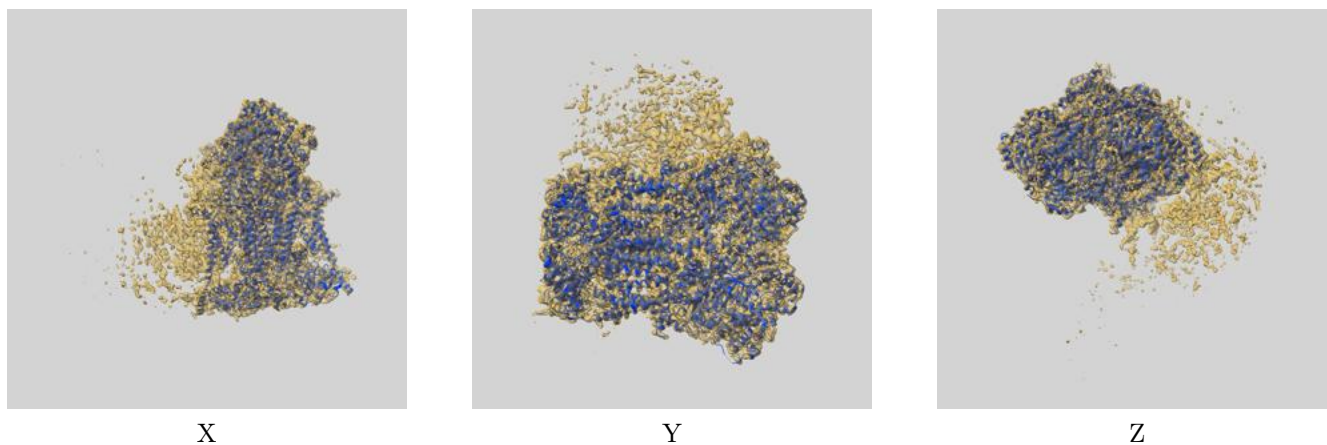
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.42	14.58	8.01

\*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 7.42 differs from the reported value 3.5 by more than 10 %

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

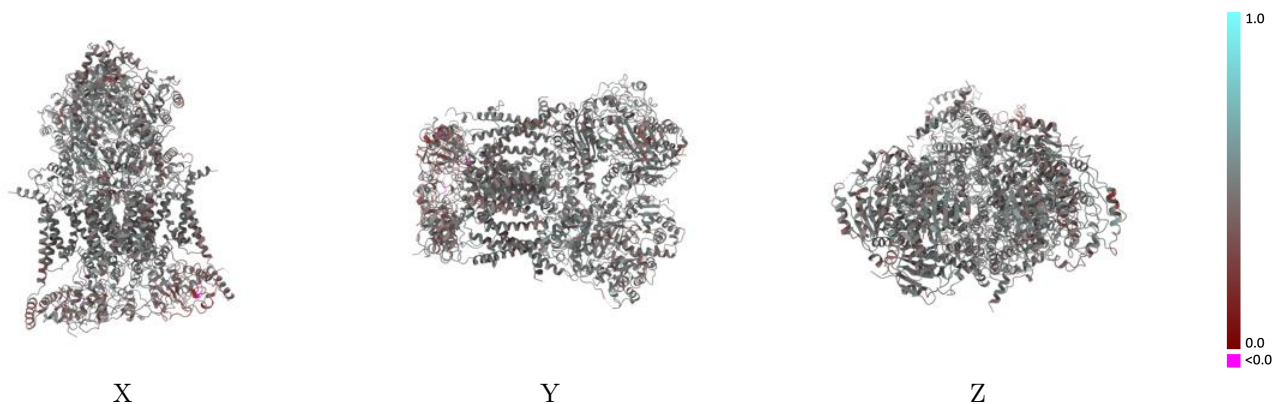
This section contains information regarding the fit between EMDB map EMD-42221 and PDB model 8UGD. Per-residue inclusion information can be found in section [3](#) on page [12](#).

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



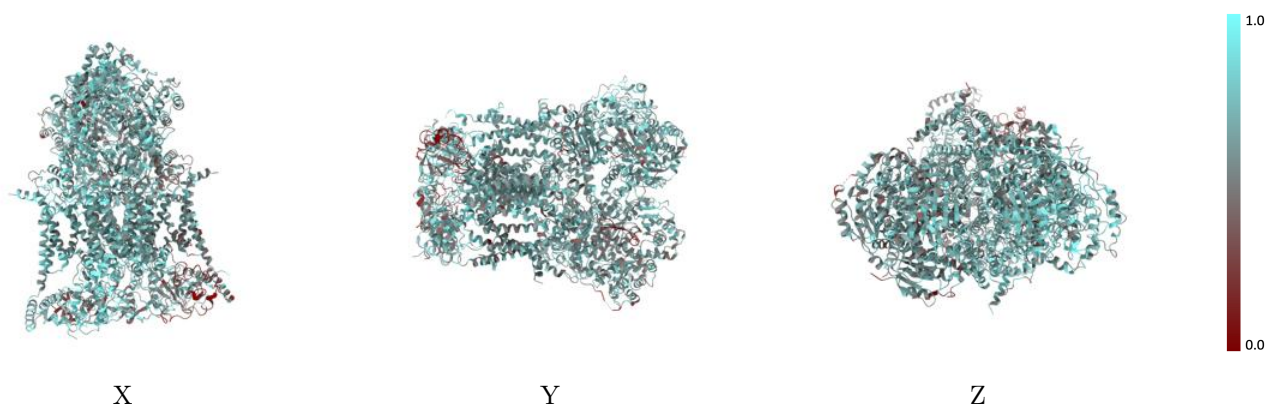
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



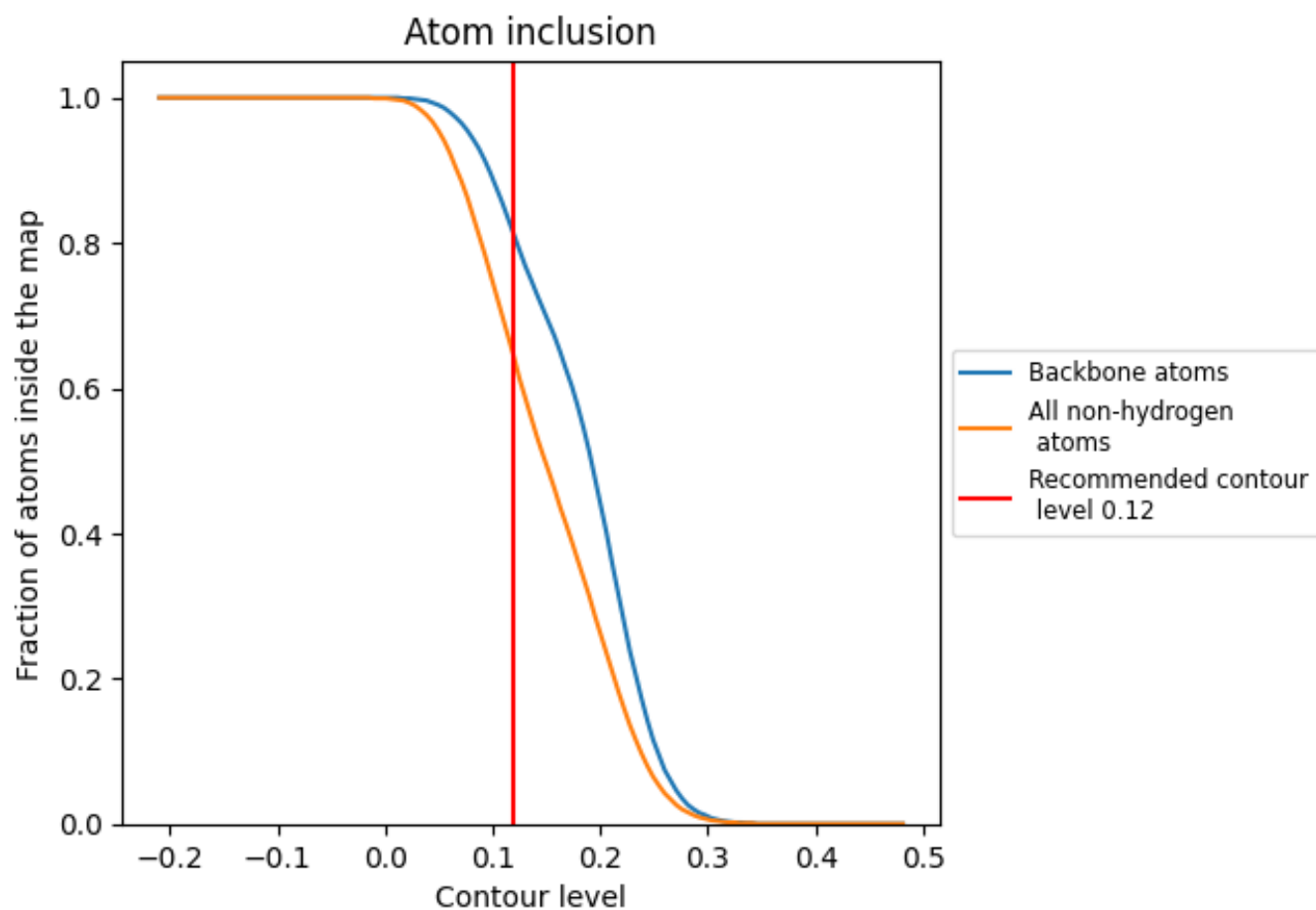
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

## 9.4 Atom inclusion [i](#)

















































At the recommended contour level, 81% of all backbone atoms, 64% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6420	 0.4610
3A	 0.6210	 0.4750
3B	 0.6400	 0.4760
3C	 0.6520	 0.4730
3D	 0.6630	 0.4750
3E	 0.4090	 0.3670
3F	 0.6360	 0.4710
3G	 0.6250	 0.4760
3H	 0.5890	 0.4250
3I	 0.1890	 0.3920
3J	 0.6150	 0.4660
3N	 0.7140	 0.4740
3O	 0.6820	 0.4720
3P	 0.7180	 0.4750
3Q	 0.7360	 0.4710
3R	 0.4340	 0.3710
3S	 0.7230	 0.4890
3T	 0.7490	 0.4740
3U	 0.6810	 0.4280
3V	 0.4090	 0.4510
3W	 0.7610	 0.4820
3X	 0.5850	 0.4600
3Y	 0.5230	 0.4530

