



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 06:13 PM BST

PDB ID : 4U3F
Title : Cytochrome bc1 complex from chicken with designed inhibitor bound
Authors : Huang, L.-S.; Zhu, X.-L.; Yang, G.F.; Berry, E.A.
Deposited on : 2014-07-21
Resolution : 3.23 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

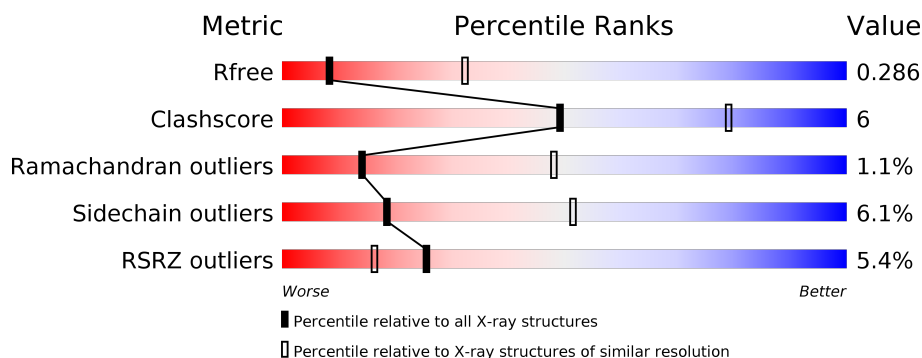
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.23 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1619 (3.28-3.20)
Clashscore	141614	1755 (3.28-3.20)
Ramachandran outliers	138981	1728 (3.28-3.20)
Sidechain outliers	138945	1727 (3.28-3.20)
RSRZ outliers	127900	1567 (3.28-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	446	<div> <div>2%</div> <div>81% 16% ..</div> </div>
1	N	446	<div> <div>2%</div> <div>81% 16% ..</div> </div>
2	B	441	<div> <div>2%</div> <div>72% 21% • 5%</div> </div>
2	O	441	<div> <div>2%</div> <div>73% 20% • •</div> </div>
3	C	380	<div> <div>%</div> <div>84% 15% •</div> </div>
3	P	380	<div> <div>%</div> <div>83% 15% •</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	241	
4	Q	241	
5	E	196	
5	R	196	
6	F	110	
6	S	110	
7	G	81	
7	T	81	
8	H	77	
8	U	77	
9	I	76	
9	V	76	
10	J	61	
10	W	61	

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
11	PEE	P	411	-	-	-	X
3	FME	C	1	-	-	-	X

2 Entry composition

There are 21 unique types of molecules in this entry. The entry contains 32790 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3442	2157	606	658	21			
1	N	442	Total	C	N	O	S	0	0	0
			3437	2154	605	657	21			

- Molecule 2 is a protein called Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	421	Total	C	N	O	S	0	0	0
			3137	1971	544	613	9			
2	O	422	Total	C	N	O	S	0	0	0
			3143	1974	545	614	10			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	380	Total	C	N	O	S	0	0	0
			3021	2025	478	505	13			
3	P	379	Total	C	N	O	S	0	1	0
			3022	2025	480	505	12			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	FME	-	expression tag	UNP P18946
P	1	FME	-	expression tag	UNP P18946

- Molecule 4 is a protein called Mitochondrial cytochrome c1, heme protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1898	1212	327	347	12			
4	Q	241	Total	C	N	O	S	0	0	0
			1898	1212	327	347	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1513	952	263	292	6			
5	R	196	Total	C	N	O	S	0	0	0
			1509	950	263	290	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	101	Total	C	N	O	S	0	0	0
			891	570	159	159	3			
6	S	101	Total	C	N	O	S	0	0	0
			891	570	159	159	3			

- Molecule 7 is a protein called Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	80	Total	C	N	O	0	0	0
			672	437	119	116			
7	T	79	Total	C	N	O	0	0	0
			662	432	117	113			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	68	Total	C	N	O	S	0	0	0
			562	343	104	110	5			
8	U	68	Total	C	N	O	S	0	0	0
			558	341	104	108	5			

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	44	Total	C	N	O	S	0	0	1
			266	157	54	53	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	V	42	Total	C	N	O	S	0	0	1
			265	157	55	51	2			

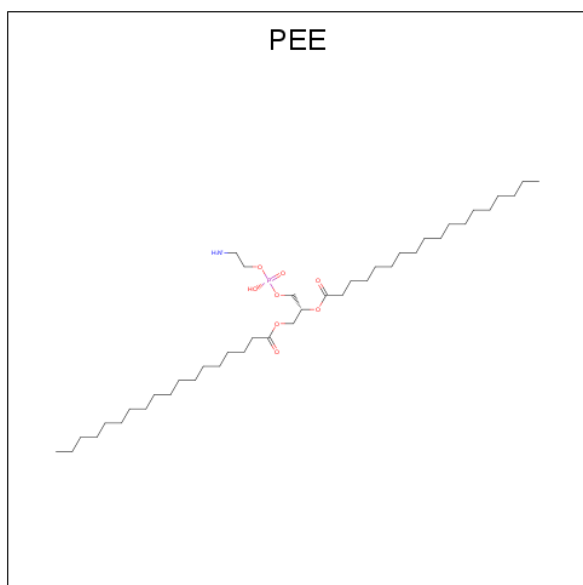
There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	1	AME	-	expression tag	UNP Q5ZLR5
I	29	UNK	LEU	see remark 999	UNP Q5ZLR5
I	30	UNK	ALA	see remark 999	UNP Q5ZLR5
I	31	UNK	PRO	see remark 999	UNP Q5ZLR5
I	32	UNK	ALA	see remark 999	UNP Q5ZLR5
I	33	UNK	ALA	see remark 999	UNP Q5ZLR5
I	37	UNK	LEU	see remark 999	UNP Q5ZLR5
I	38	UNK	ARG	see remark 999	UNP Q5ZLR5
I	39	UNK	ALA	see remark 999	UNP Q5ZLR5
I	40	UNK	GLU	see remark 999	UNP Q5ZLR5
I	41	UNK	LYS	see remark 999	UNP Q5ZLR5
I	42	UNK	VAL	see remark 999	UNP Q5ZLR5
I	43	UNK	VAL	see remark 999	UNP Q5ZLR5
I	44	UNK	LEU	see remark 999	UNP Q5ZLR5
I	45	UNK	ASP	see remark 999	UNP Q5ZLR5
V	-1	AME	-	expression tag	UNP Q5ZLR5
V	27	UNK	LEU	see remark 999	UNP Q5ZLR5
V	28	UNK	ALA	see remark 999	UNP Q5ZLR5
V	29	UNK	PRO	see remark 999	UNP Q5ZLR5
V	30	UNK	ALA	see remark 999	UNP Q5ZLR5
V	31	UNK	ALA	see remark 999	UNP Q5ZLR5
V	32	UNK	LEU	see remark 999	UNP Q5ZLR5
V	33	UNK	ARG	see remark 999	UNP Q5ZLR5
V	37	UNK	ALA	see remark 999	UNP Q5ZLR5
V	38	UNK	GLU	see remark 999	UNP Q5ZLR5
V	39	UNK	LYS	see remark 999	UNP Q5ZLR5
V	40	UNK	VAL	see remark 999	UNP Q5ZLR5
V	41	UNK	VAL	see remark 999	UNP Q5ZLR5
V	42	UNK	LEU	see remark 999	UNP Q5ZLR5
V	43	UNK	ASP	see remark 999	UNP Q5ZLR5

- Molecule 10 is a protein called Mitochondrial ubiquinol-cytochrome c reductase 7.2 kda protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	61	Total	C	N	O	0	0	0
			497	321	87	89			
10	W	60	Total	C	N	O	0	0	1
			479	311	86	82			

- Molecule 11 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: C₄₁H₈₃NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	A	1	Total	C	N	O	P	0	0
			26	16	1	8	1		
11	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
11	C	1	Total	C	N	O	P	0	0
			11	5	1	4	1		
11	C	1	Total	C	N	O	P	0	0
			47	37	1	8	1		
11	C	1	Total	C	O			0	0
			15	13	2				
11	E	1	Total	C	N	O	P	0	0
			48	38	1	8	1		
11	E	1	Total	C				0	0
			15	15					
11	N	1	Total	C	N	O	P	0	0
			8	2	1	4	1		
11	P	1	Total	C	O			0	0
			15	13	2				

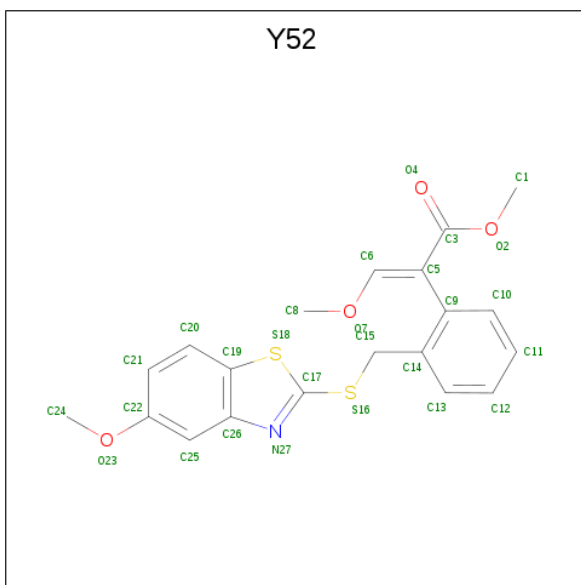
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	P	1	Total 49	C 39	N 1	O 8	P 1	0	0
11	P	1	Total 41	C 31	N 1	O 8	P 1	0	0
11	P	1	Total 12	C 10	O 2			0	0
11	P	1	Total 25	C 15	N 1	O 8	P 1	0	0
11	R	1	Total 49	C 39	N 1	O 8	P 1	0	0

- # HEM

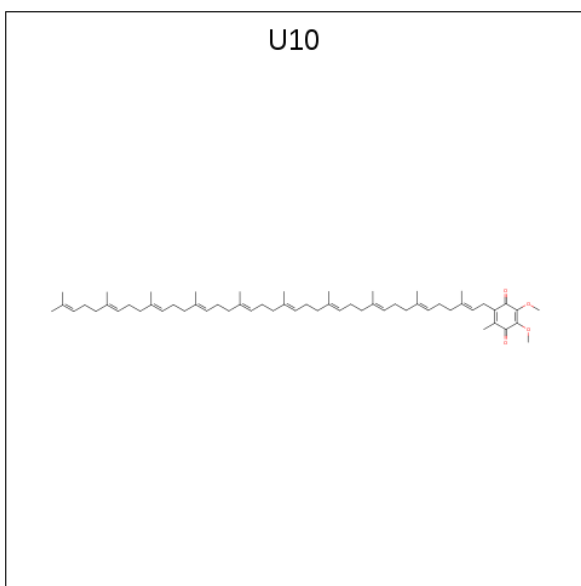
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
12	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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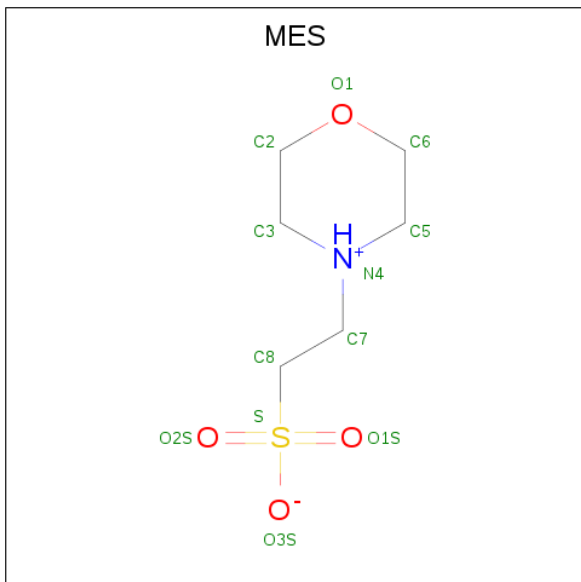
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total 27	C 20	N 1	O 4	S 2	0	0
13	P	1	Total 27	C 20	N 1	O 4	S 2	0	0

- Molecule 14 is UBIQUINONE-10 (three-letter code: U10) (formula: $\text{C}_{59}\text{H}_{90}\text{O}_4$).



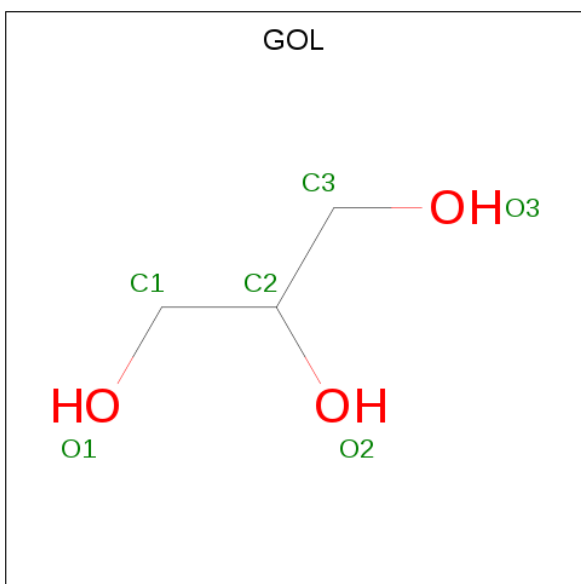
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total 19	C 15	O 4	0	0
14	P	1	Total 19	C 15	O 4	0	0

- Molecule 15 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 16 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



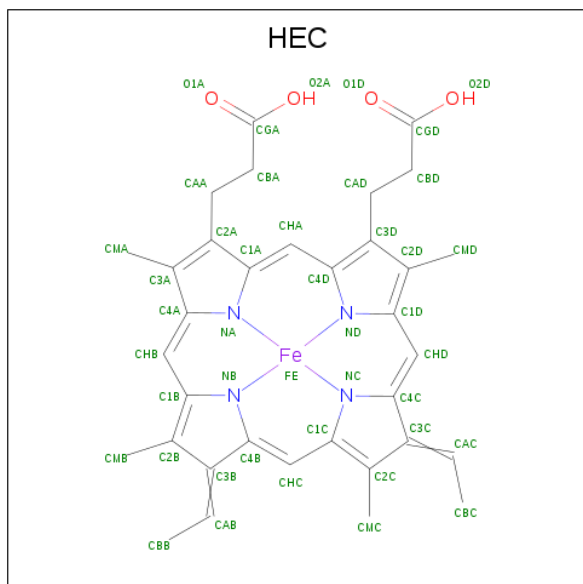
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	C	1	Total	C	O	0	0
			6	3	3		

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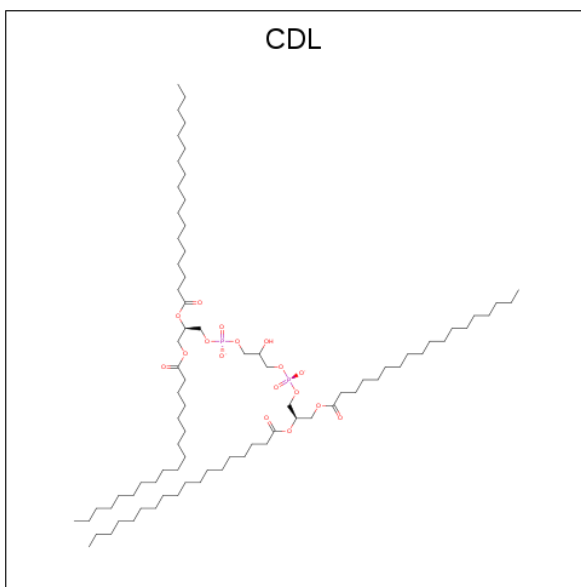
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	P	1	Total	C	O	0	0
			6	3	3		

- Molecule 17 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



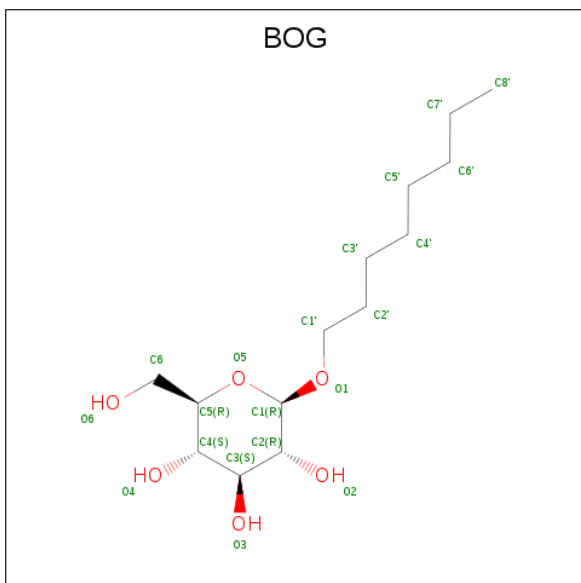
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
17	Q	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 18 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



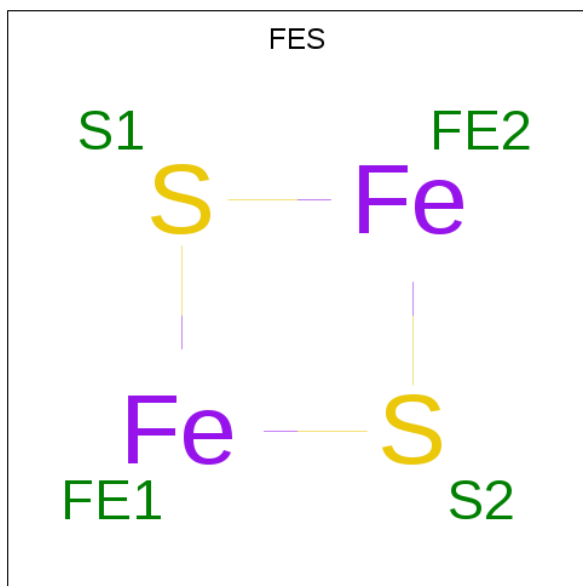
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	D	1	Total	C	O	P	0	0
			42	23	17	2		
18	G	1	Total	C	O	P	0	0
			40	21	17	2		
18	Q	1	Total	C	O	P	0	0
			42	23	17	2		
18	T	1	Total	C	O	P	0	0
			40	21	17	2		

- Molecule 19 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	D	1	Total	C	O	0	0
			20	14	6		
19	P	1	Total	C	O	0	0
			20	14	6		
19	Q	1	Total	C	O	0	0
			20	14	6		

- Molecule 20 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	E	1	Total	Fe	S	0	0
			4	2	2		
20	R	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 21 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	A	2	Total	O	0	0
			2	2		
21	B	1	Total	O	0	0
			1	1		
21	C	2	Total	O	0	0
			2	2		
21	F	1	Total	O	0	0
			1	1		
21	N	1	Total	O	0	0
			1	1		

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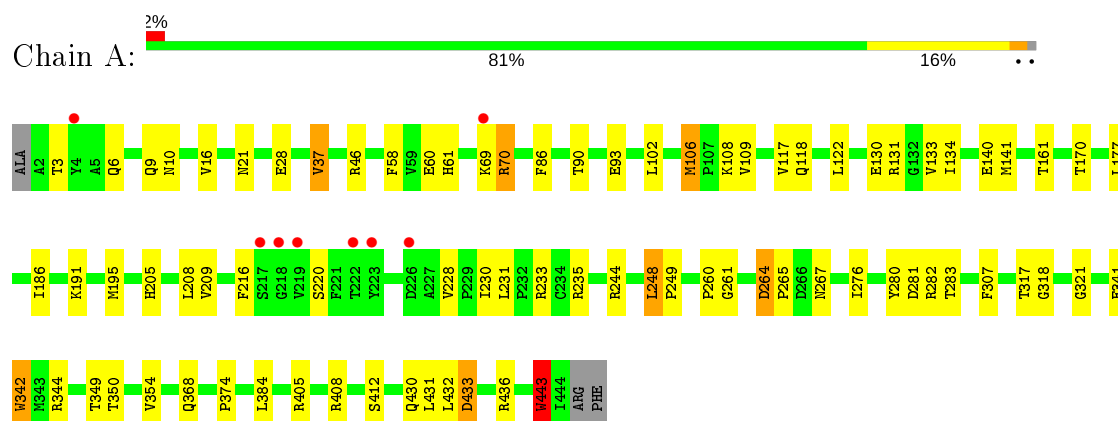
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	O	2	Total	O	0	0
			2	2		
21	P	2	Total	O	0	0
			2	2		

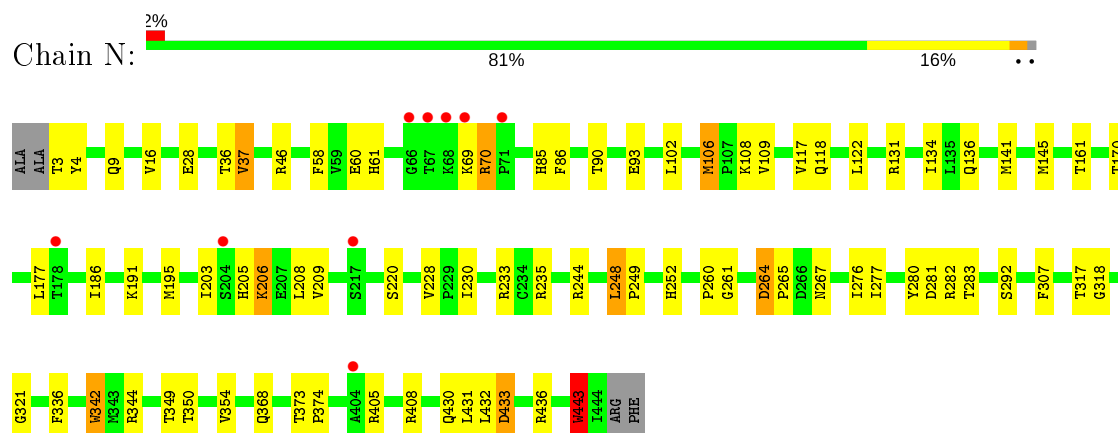
3 Residue-property plots

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

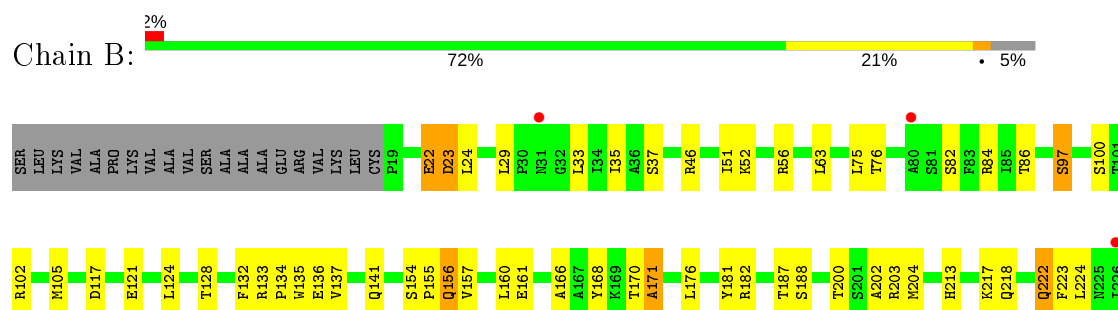
- Molecule 1: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i

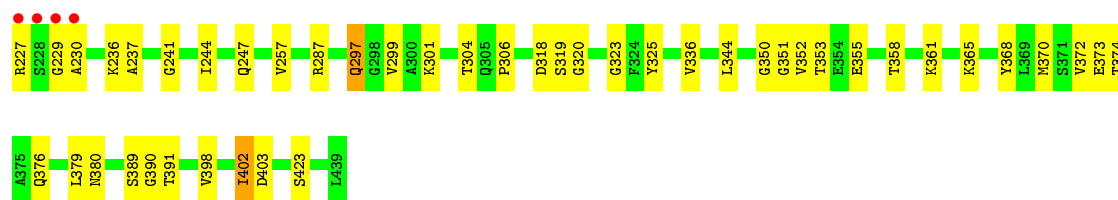


- Molecule 1: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein i

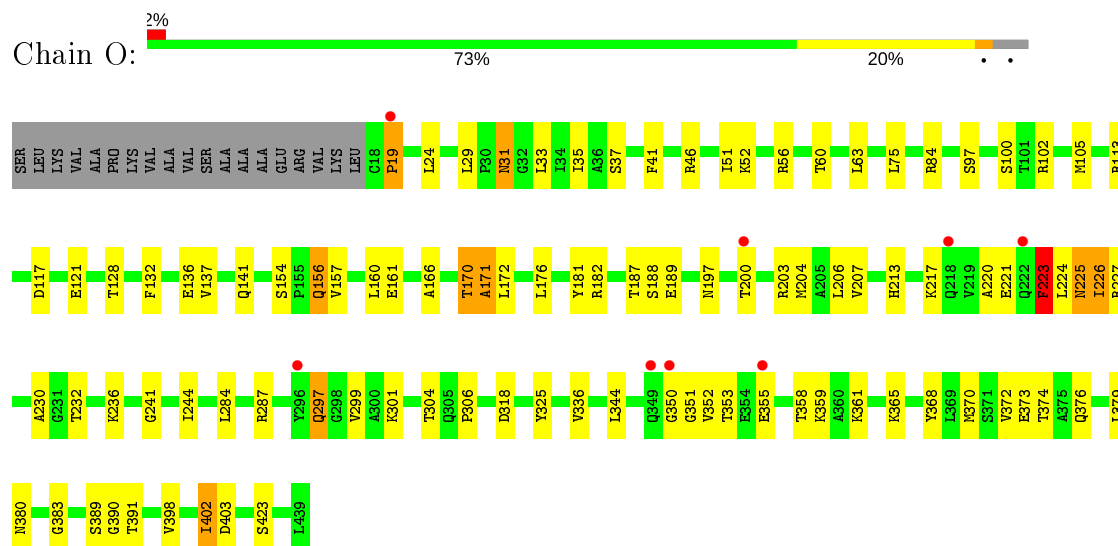


- Molecule 2: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2

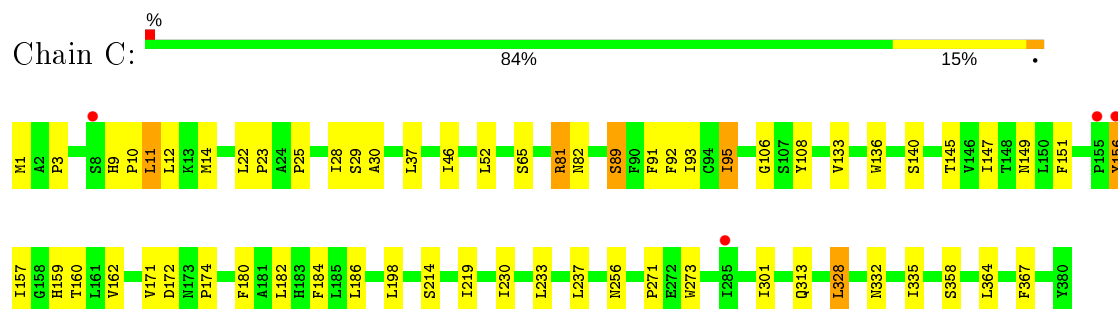




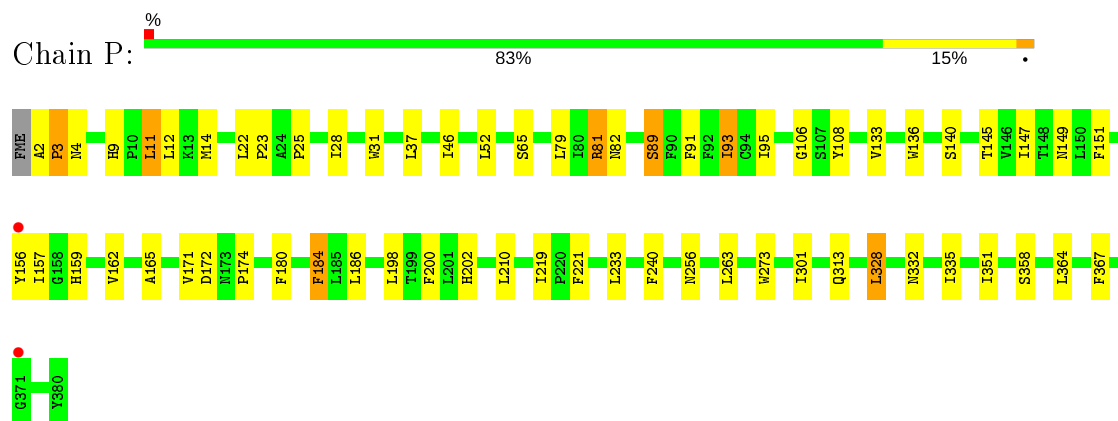
- Molecule 2: Mitochondrial ubiquinol-cytochrome-c reductase complex core protein 2



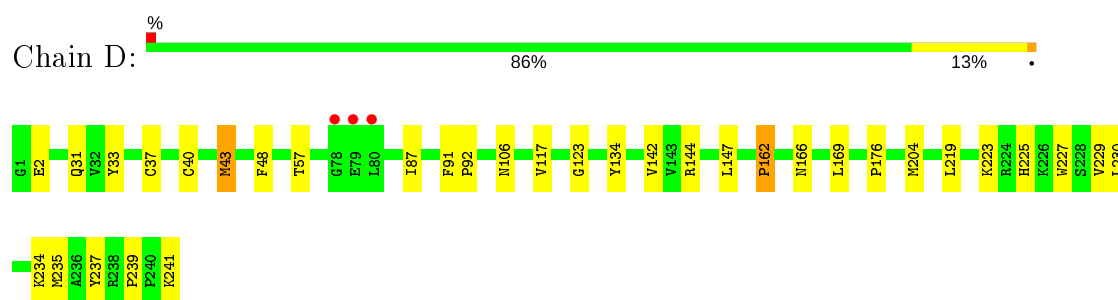
- Molecule 3: Cytochrome b



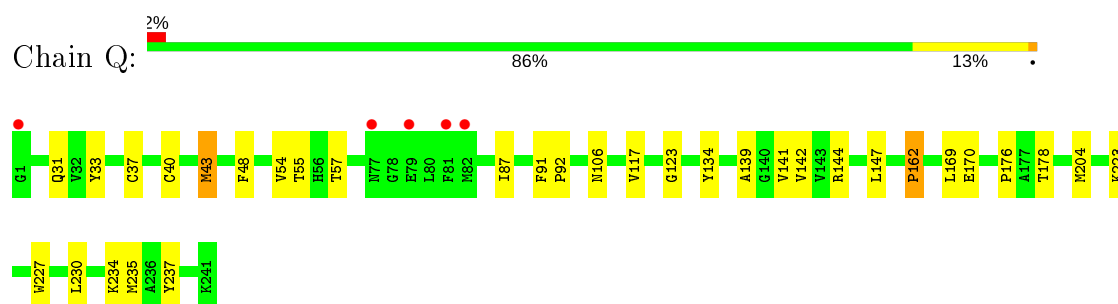
- Molecule 3: Cytochrome b



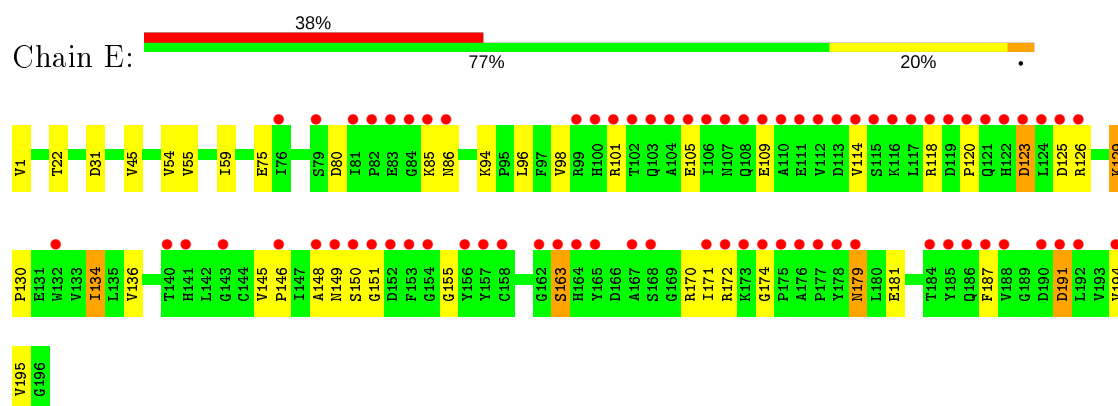
- Molecule 4: Mitochondrial cytochrome c1, heme protein



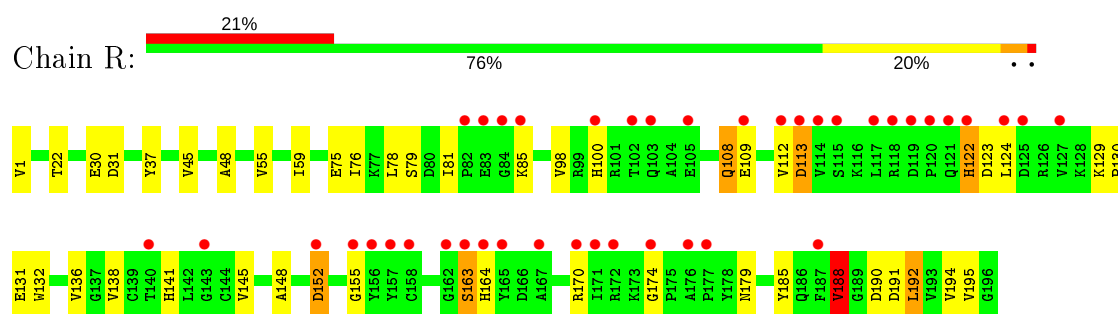
- Molecule 4: Mitochondrial cytochrome c1, heme protein



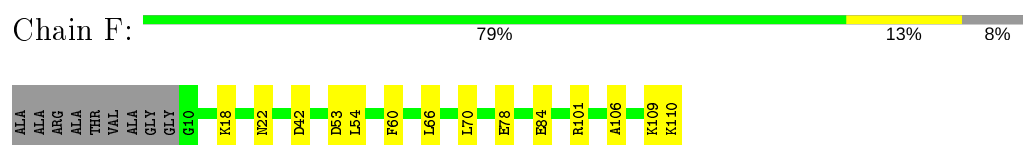
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



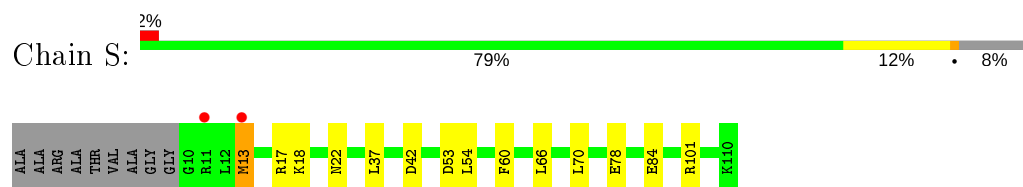
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial



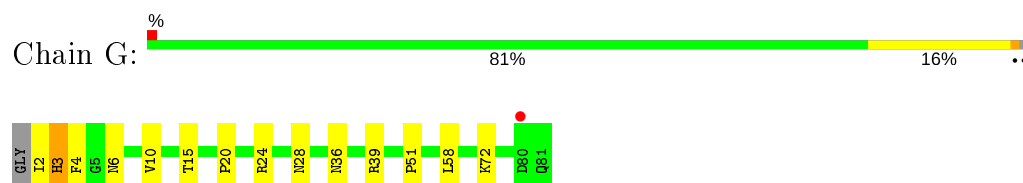
- Molecule 6: Cytochrome b-c1 complex subunit 7



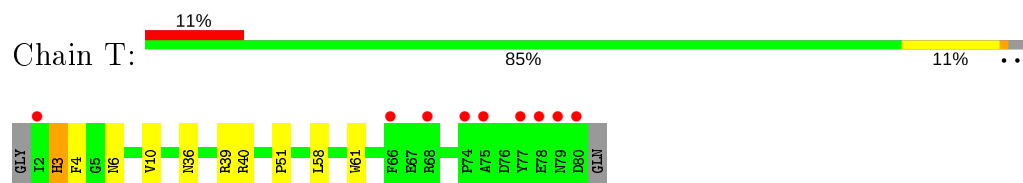
- Molecule 6: Cytochrome b-c1 complex subunit 7



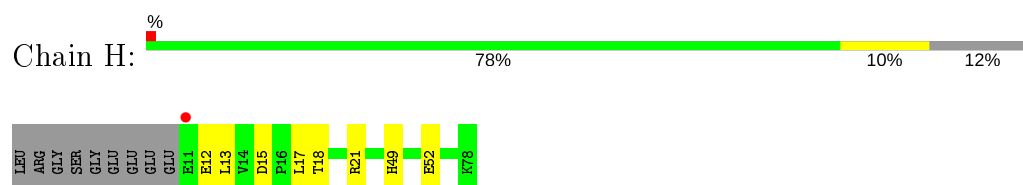
- Molecule 7: Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c



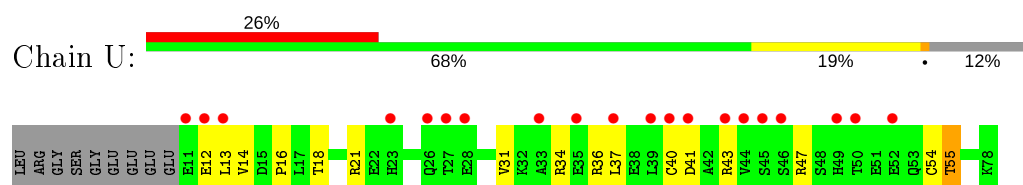
- Molecule 7: Mitochondrial ubiquinol-cytochrome c reductase ubiquinone-binding protein qp-c



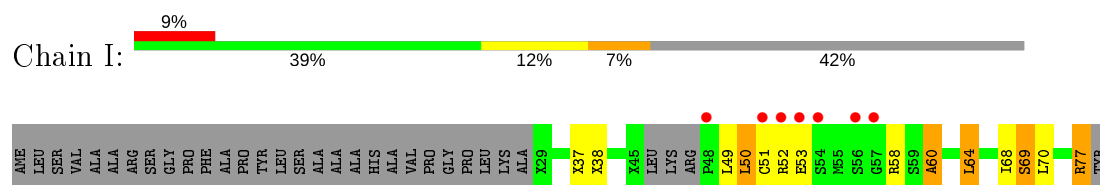
- Molecule 8: Cytochrome b-c1 complex subunit 6



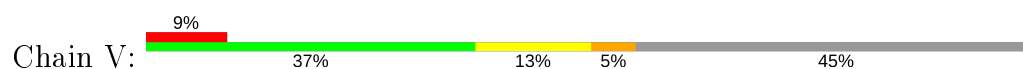
- Molecule 8: Cytochrome b-c1 complex subunit 6

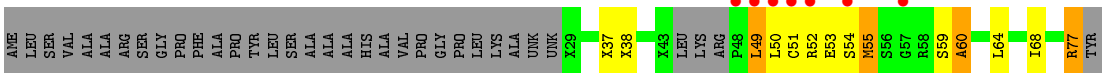


- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

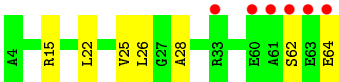
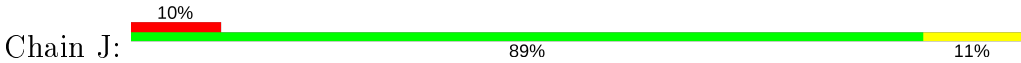


- Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

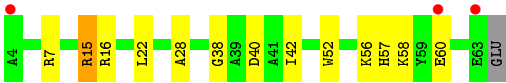
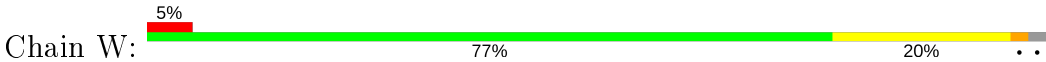




● Molecule 10: Mitochondrial ubiquinol-cytochrome c reductase 7.2 kda protein



● Molecule 10: Mitochondrial ubiquinol-cytochrome c reductase 7.2 kda protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	167.25Å 181.48Å 239.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.23 54.30 – 3.23	Depositor EDS
% Data completeness (in resolution range)	98.3 (15.00-3.23) 82.2 (54.30-3.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.30	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 3.26Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1745)	Depositor
R, R_{free}	0.236 , 0.284 0.243 , 0.286	Depositor DCC
R_{free} test set	2286 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å ²)	49.5	Xtriage
Anisotropy	0.509	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	32790	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: GOL, CDL, Y52, U10, FES, MES, HEC, PEE, FME, HEM, BOG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.21	0/3513	0.40	0/4760
1	N	0.21	0/3508	0.39	0/4753
2	B	0.21	0/3192	0.40	0/4330
2	O	0.22	0/3198	0.40	0/4339
3	C	0.22	0/3114	0.39	0/4263
3	P	0.22	0/3102	0.39	0/4245
4	D	0.20	0/1956	0.37	0/2658
4	Q	0.20	0/1956	0.37	0/2658
5	E	0.20	0/1547	0.38	0/2103
5	R	0.20	0/1543	0.38	0/2098
6	F	0.21	0/911	0.35	0/1219
6	S	0.21	0/911	0.35	0/1219
7	G	0.22	0/694	0.39	0/941
7	T	0.22	0/684	0.39	0/929
8	H	0.21	0/570	0.36	0/763
8	U	0.21	0/566	0.40	0/758
9	I	0.20	0/208	0.48	0/279
9	V	0.21	0/215	0.56	0/288
10	J	0.21	0/508	0.34	0/682
10	W	0.21	0/490	0.35	0/660
All	All	0.21	0/32386	0.39	0/43945

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	216	PHE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3442	0	3354	41	0
1	N	3437	0	3349	40	0
2	B	3137	0	3131	55	0
2	O	3143	0	3135	56	0
3	C	3021	0	3068	35	0
3	P	3022	0	3064	39	0
4	D	1898	0	1846	17	0
4	Q	1898	0	1846	16	0
5	E	1513	0	1480	21	0
5	R	1509	0	1476	22	0
6	F	891	0	893	6	0
6	S	891	0	893	8	0
7	G	672	0	653	11	0
7	T	662	0	645	10	0
8	H	562	0	545	3	0
8	U	558	0	541	8	0
9	I	266	0	223	14	0
9	V	265	0	239	11	0
10	J	497	0	490	3	0
10	W	479	0	478	6	0
11	A	26	0	26	1	0
11	C	122	0	174	2	0
11	E	63	0	99	5	0
11	N	8	0	7	0	0
11	P	142	0	193	7	0
11	R	49	0	75	5	0
12	C	86	0	60	7	0
12	P	86	0	60	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	C	27	0	19	2	0
13	P	27	0	19	1	0
14	C	19	0	17	1	0
14	P	19	0	17	3	0
15	C	12	0	13	0	0
16	C	6	0	8	1	0
16	P	6	0	8	1	0
17	D	43	0	30	0	0
17	Q	43	0	30	0	0
18	D	42	0	28	1	0
18	G	40	0	24	1	0
18	Q	42	0	28	0	0
18	T	40	0	24	3	0
19	D	20	0	28	0	0
19	P	20	0	28	3	0
19	Q	20	0	28	0	0
20	E	4	0	0	0	0
20	R	4	0	0	0	0
21	A	2	0	0	0	0
21	B	1	0	0	1	0
21	C	2	0	0	0	0
21	F	1	0	0	0	0
21	N	1	0	0	0	0
21	O	2	0	0	1	0
21	P	2	0	0	0	0
All	All	32790	0	32392	385	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 6.

All (385) 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:V:37:UNK:HG3	9:V:38:UNK:H	1.37	0.90
9:V:49:LEU:HB2	9:V:55:MET:HB3	1.57	0.85
9:I:37:UNK:HG3	9:I:38:UNK:N	1.94	0.81
9:I:37:UNK:HG3	9:I:38:UNK:H	1.47	0.78
2:B:361:LYS:HD2	2:B:403:ASP:HA	1.67	0.76
2:O:361:LYS:HD2	2:O:403:ASP:HA	1.66	0.76
9:V:37:UNK:CG	9:V:38:UNK:H	2.00	0.75
2:O:389:SER:O	2:O:391:THR:N	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:328:LEU:HD12	7:G:51:PRO:HB3	1.71	0.72
2:O:226:ILE:HG22	2:O:227:ARG:H	1.55	0.72
2:B:389:SER:O	2:B:391:THR:N	2.22	0.71
2:B:306:PRO:HB3	9:I:52:ARG:HB2	1.73	0.70
4:D:166:ASN:HD21	8:H:15:ASP:HB2	1.56	0.70
8:U:40:CYS:SG	8:U:43:ARG:NH2	2.64	0.70
1:N:248:LEU:HD13	1:N:249:PRO:HD2	1.73	0.70
2:O:46:ARG:HG2	2:O:379:LEU:HD22	1.73	0.69
1:A:248:LEU:HD13	1:A:249:PRO:HD2	1.73	0.69
2:B:52:LYS:O	2:B:203:ARG:NH2	2.26	0.69
2:B:236:LYS:HE3	2:B:318:ASP:HB2	1.75	0.69
9:V:37:UNK:HG3	9:V:38:UNK:N	2.01	0.68
5:R:188:VAL:HG23	5:R:192:LEU:HB3	1.76	0.68
3:C:89:SER:HG	3:C:273:TRP:HE1	1.42	0.68
9:I:37:UNK:CG	9:I:38:UNK:H	2.07	0.67
2:O:46:ARG:NH2	2:O:376:GLN:OE1	2.28	0.67
2:O:52:LYS:O	2:O:203:ARG:NH2	2.26	0.67
3:C:81:ARG:HH12	16:C:508:GOL:H2	1.60	0.66
1:A:261:GLY:O	1:A:267:ASN:ND2	2.28	0.66
1:A:244:ARG:HE	7:G:10:VAL:HB	1.59	0.66
2:B:46:ARG:HG2	2:B:379:LEU:HD22	1.78	0.66
11:E:502:PEE:H62	10:J:25:VAL:HG22	1.78	0.66
1:N:261:GLY:O	1:N:267:ASN:ND2	2.29	0.66
1:A:106:MET:HE3	1:A:208:LEU:HA	1.80	0.64
3:C:23:PRO:HG2	7:G:3:HIS:HB3	1.78	0.64
3:P:328:LEU:HD12	7:T:51:PRO:HB3	1.79	0.64
2:B:86:THR:HA	9:I:70:LEU:HD11	1.81	0.63
4:D:239:PRO:HG2	4:D:241:LYS:HB2	1.79	0.63
1:A:131:ARG:NH2	1:A:177:LEU:O	2.31	0.63
1:N:131:ARG:NH2	1:N:177:LEU:O	2.32	0.63
9:I:60:ALA:HA	9:I:77:ARG:HH22	1.64	0.62
3:P:89:SER:HG	3:P:273:TRP:HE1	1.44	0.62
2:B:46:ARG:NH2	2:B:376:GLN:OE1	2.33	0.61
6:F:42:ASP:OD1	6:F:101:ARG:NH1	2.34	0.61
12:C:502:HEM:HMC2	12:C:502:HEM:HBC2	1.84	0.60
5:E:101:ARG:NH2	5:E:130:PRO:O	2.34	0.60
6:F:106:ALA:HA	6:F:109:LYS:HE2	1.82	0.60
12:C:501:HEM:HBC2	12:C:501:HEM:HMC1	1.84	0.60
7:T:40:ARG:NH1	18:T:101:CDL:OA4	2.35	0.60
6:S:42:ASP:OD1	6:S:101:ARG:NH1	2.34	0.59
1:A:412:SER:O	10:J:15:ARG:NH2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:P:403:HEM:HBC2	12:P:403:HEM:HMC2	1.84	0.59
19:P:406:BOG:H4	11:R:502:PEE:H24	1.84	0.59
4:Q:178:THR:HG21	8:U:16:PRO:HD3	1.84	0.59
11:E:502:PEE:H42	11:E:503:PEE:H32	1.84	0.58
2:O:225:ASN:HD22	2:O:226:ILE:H	1.50	0.58
12:P:402:HEM:HBC2	12:P:402:HEM:HMC1	1.84	0.58
11:A:501:PEE:H57	11:E:502:PEE:H57	1.86	0.58
4:D:144:ARG:HB3	4:D:147:LEU:HD12	1.85	0.58
4:Q:144:ARG:HB3	4:Q:147:LEU:HD12	1.85	0.58
3:C:151:PHE:HB2	3:C:162:VAL:HG22	1.86	0.58
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.37	0.58
1:N:60:GLU:OE1	2:O:287:ARG:NH2	2.37	0.57
7:T:36:ASN:OD1	7:T:39:ARG:NH1	2.37	0.57
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.70	0.57
5:E:118:ARG:NH1	5:E:172:ARG:O	2.37	0.57
3:P:202:HIS:NE2	14:P:405:U10:O2	2.38	0.57
2:B:56:ARG:HG2	2:B:171:ALA:HB1	1.87	0.57
3:P:23:PRO:HG2	7:T:3:HIS:HB3	1.87	0.57
1:N:106:MET:HE3	1:N:208:LEU:HA	1.87	0.57
3:P:301:ILE:HD11	3:P:364:LEU:HD21	1.86	0.57
3:P:335:ILE:HD13	7:T:58:LEU:HD23	1.87	0.57
1:N:321:GLY:HA2	1:N:342:TRP:HZ2	1.69	0.56
3:C:301:ILE:HD11	3:C:364:LEU:HD21	1.86	0.56
12:P:402:HEM:HMB1	12:P:402:HEM:HBB2	1.88	0.56
12:C:501:HEM:HMB1	12:C:501:HEM:HBB2	1.87	0.56
5:R:113:ASP:OD2	5:R:113:ASP:N	2.34	0.56
12:P:403:HEM:HMB1	12:P:403:HEM:HBB2	1.87	0.56
2:O:287:ARG:HA	9:V:53:GLU:HB3	1.86	0.56
2:B:29:LEU:HD12	2:B:33:LEU:HD23	1.88	0.56
2:B:157:VAL:HG23	9:I:64:LEU:HD21	1.87	0.56
2:B:156:GLN:NE2	21:B:501:HOH:O	2.38	0.55
1:N:244:ARG:HE	7:T:10:VAL:HB	1.70	0.55
14:P:405:U10:H1M1	14:P:405:U10:C8	2.37	0.55
2:O:117:ASP:N	2:O:117:ASP:OD1	2.39	0.55
2:O:56:ARG:HG2	2:O:171:ALA:HB1	1.87	0.55
8:U:18:THR:HA	8:U:21:ARG:HB2	1.88	0.55
5:E:163:SER:HA	5:E:174:GLY:HA3	1.88	0.55
2:O:128:THR:HG21	2:O:224:LEU:HG	1.89	0.55
3:P:151:PHE:HB2	3:P:162:VAL:HG22	1.87	0.55
5:R:76:ILE:HD13	5:R:98:VAL:HG21	1.89	0.55
3:C:198:LEU:HD21	12:C:502:HEM:HMA3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:THR:O	1:A:408:ARG:NH1	2.40	0.54
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.89	0.54
12:C:502:HEM:HBB2	12:C:502:HEM:HMB1	1.88	0.54
1:A:161:THR:HG21	1:A:235:ARG:H	1.71	0.54
3:P:198:LEU:HD21	12:P:403:HEM:HMA3	1.88	0.54
3:P:93:ILE:HD12	3:P:240:PHE:HZ	1.72	0.54
5:E:136:VAL:HB	5:E:181:GLU:HB3	1.89	0.54
2:O:350:GLY:O	2:O:352:VAL:N	2.39	0.54
3:C:335:ILE:HD13	7:G:58:LEU:HD23	1.89	0.54
1:N:349:THR:O	1:N:408:ARG:NH1	2.40	0.54
3:C:180:PHE:HE1	3:P:180:PHE:HE1	1.56	0.53
1:A:6:GLN:HA	1:A:9:GLN:HE21	1.73	0.53
8:U:13:LEU:HB2	8:U:14:VAL:HA	1.90	0.53
2:B:353:THR:HG22	2:B:355:GLU:H	1.73	0.53
3:C:25:PRO:HB2	3:C:28:ILE:HG23	1.91	0.53
2:O:63:LEU:HB2	2:O:182:ARG:HD3	1.90	0.53
3:C:147:ILE:HG13	13:C:503:Y52:H12	1.91	0.52
1:N:4:TYR:HB2	2:O:113:ARG:HB2	1.92	0.52
2:O:353:THR:HG22	2:O:355:GLU:H	1.73	0.52
2:O:75:LEU:HD22	2:O:136:GLU:HB3	1.92	0.52
3:P:25:PRO:HB2	3:P:28:ILE:HG23	1.91	0.52
2:O:306:PRO:HB3	9:V:52:ARG:N	2.25	0.51
2:O:157:VAL:HG23	9:V:64:LEU:HD21	1.91	0.51
1:A:117:VAL:HG23	1:A:118:GLN:HG3	1.93	0.51
3:P:81:ARG:HH12	16:P:408:GOL:H2	1.74	0.51
5:R:79:SER:OG	5:R:191:ASP:OD2	2.29	0.51
2:O:189:GLU:OE2	2:O:189:GLU:N	2.43	0.51
3:P:172:ASP:HB3	3:P:174:PRO:HD2	1.93	0.51
14:P:405:U10:H1M1	14:P:405:U10:H8	1.93	0.51
2:B:299:VAL:HG11	2:B:336:VAL:HG13	1.92	0.51
3:C:182:LEU:HD21	11:C:509:PEE:H3	1.92	0.51
3:P:147:ILE:HG13	13:P:404:Y52:H12	1.91	0.51
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.92	0.51
5:E:45:VAL:HG13	10:J:28:ALA:HA	1.92	0.51
2:O:37:SER:HB3	2:O:213:HIS:ND1	2.26	0.51
1:N:145:MET:HB3	1:N:252:HIS:CE1	2.46	0.51
1:A:244:ARG:NE	7:G:10:VAL:HB	2.26	0.51
2:O:157:VAL:HG23	9:V:64:LEU:HD11	1.93	0.51
1:N:117:VAL:HG23	1:N:118:GLN:HG3	1.93	0.51
2:B:117:ASP:OD1	2:B:117:ASP:N	2.39	0.50
2:B:154:SER:O	2:B:157:VAL:HG12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:299:VAL:HG11	2:O:336:VAL:HG13	1.92	0.50
2:B:350:GLY:O	2:B:352:VAL:N	2.39	0.50
2:O:84:ARG:NH2	2:O:121:GLU:OE2	2.45	0.50
3:P:52:LEU:HD11	3:P:81:ARG:HA	1.93	0.50
2:O:154:SER:O	2:O:157:VAL:HG12	2.11	0.50
4:Q:237:TYR:HB2	6:S:60:PHE:CD1	2.47	0.50
5:E:171:ILE:HG22	5:E:179:ASN:OD1	2.12	0.49
2:B:132:PHE:O	2:B:188:SER:OG	2.27	0.49
2:B:84:ARG:NH2	2:B:121:GLU:OE2	2.45	0.49
3:C:29:SER:HB2	18:G:101:CDL:HB21	1.94	0.49
2:O:31:ASN:N	2:O:31:ASN:OD1	2.43	0.49
5:R:122:HIS:CG	5:R:123:ASP:H	2.31	0.49
3:C:172:ASP:HB3	3:C:174:PRO:HD2	1.94	0.49
1:N:161:THR:HG21	1:N:235:ARG:H	1.77	0.49
1:N:443:TRP:HA	1:N:443:TRP:CE3	2.48	0.49
2:O:161:GLU:OE1	2:O:176:LEU:N	2.45	0.49
2:O:365:LYS:HG3	2:O:402:ILE:HD12	1.95	0.49
1:A:443:TRP:HA	1:A:443:TRP:CE3	2.48	0.49
2:B:128:THR:HG21	2:B:224:LEU:HD22	1.95	0.49
2:O:181:TYR:CZ	2:O:182:ARG:HG3	2.48	0.49
1:A:140:GLU:HG3	9:I:51:CYS:SG	2.52	0.49
2:B:137:VAL:O	2:B:141:GLN:HG2	2.13	0.48
9:I:49:LEU:HD21	9:I:58:ARG:NE	2.28	0.48
19:P:406:BOG:H3'2	11:R:502:PEE:H46	1.95	0.48
3:C:332:ASN:ND2	3:C:358:SER:OG	2.45	0.48
2:B:181:TYR:CZ	2:B:182:ARG:HG3	2.48	0.48
2:B:365:LYS:HG3	2:B:402:ILE:HD12	1.95	0.48
5:E:125:ASP:HB3	5:E:126:ARG:HD2	1.95	0.48
2:B:247:GLN:NE2	2:O:60:THR:OG1	2.46	0.48
2:B:161:GLU:OE1	2:B:176:LEU:N	2.46	0.48
2:B:157:VAL:HG23	9:I:64:LEU:HD11	1.96	0.48
3:C:219:ILE:HG21	4:D:230:LEU:HD11	1.94	0.48
3:C:52:LEU:HD11	3:C:81:ARG:HA	1.93	0.48
2:O:132:PHE:O	2:O:188:SER:OG	2.27	0.48
10:W:57:HIS:CE1	10:W:58:LYS:HG3	2.49	0.48
1:A:191:LYS:O	1:A:195:MET:HG3	2.14	0.48
2:B:35:ILE:HD13	2:B:217:LYS:HA	1.95	0.48
4:D:235:MET:HB3	7:G:15:THR:HG22	1.96	0.48
1:N:102:LEU:H	1:N:102:LEU:HD12	1.79	0.48
2:B:203:ARG:HD2	2:B:230:ALA:O	2.14	0.48
5:E:129:LYS:HD2	5:E:130:PRO:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:191:LYS:O	1:N:195:MET:HG3	2.14	0.48
2:B:37:SER:HB3	2:B:213:HIS:ND1	2.29	0.47
4:D:33:TYR:CD1	4:D:37:CYS:HB2	2.49	0.47
3:P:9:HIS:HB3	3:P:12:LEU:HB2	1.96	0.47
5:R:81:ILE:HG22	5:R:100:HIS:HB2	1.95	0.47
2:O:137:VAL:O	2:O:141:GLN:HG2	2.14	0.47
4:Q:33:TYR:CD1	4:Q:37:CYS:HB2	2.49	0.47
5:E:55:VAL:O	5:E:59:ILE:HG12	2.14	0.47
1:N:368:GLN:O	1:N:374:PRO:HB2	2.14	0.47
2:O:35:ILE:HD13	2:O:217:LYS:HA	1.96	0.47
3:C:52:LEU:HD13	12:C:501:HEM:HBD1	1.96	0.47
5:R:55:VAL:O	5:R:59:ILE:HG12	2.15	0.47
6:F:53:ASP:OD1	6:F:54:LEU:N	2.48	0.47
3:C:145:THR:O	3:C:149:ASN:HB2	2.15	0.47
5:E:75:GLU:HB3	5:E:194:VAL:HG22	1.96	0.47
1:N:205:HIS:HB3	1:N:206:LYS:HE3	1.97	0.47
1:N:46:ARG:NH1	1:N:93:GLU:OE2	2.44	0.47
2:O:217:LYS:O	2:O:221:GLU:HG2	2.14	0.47
2:B:241:GLY:HA2	2:B:423:SER:HB3	1.97	0.46
2:O:203:ARG:HD2	2:O:230:ALA:O	2.15	0.46
2:B:22:GLU:H	2:B:22:GLU:HG3	1.54	0.46
2:B:56:ARG:NH1	2:B:318:ASP:OD2	2.47	0.46
3:C:9:HIS:HB3	3:C:12:LEU:HB2	1.97	0.46
5:E:191:ASP:N	5:E:191:ASP:OD2	2.47	0.46
3:P:52:LEU:HD13	12:P:402:HEM:HBD1	1.96	0.46
3:P:351:ILE:HD11	7:T:61:TRP:HZ3	1.79	0.46
3:P:332:ASN:ND2	3:P:358:SER:OG	2.45	0.46
5:R:30:GLU:OE1	10:W:7:ARG:NH2	2.49	0.46
3:C:10:PRO:HG2	3:P:200:PHE:CE1	2.50	0.46
5:R:152:ASP:HB2	5:R:164:HIS:CG	2.50	0.46
5:R:30:GLU:HB2	10:W:7:ARG:HG2	1.97	0.46
1:A:368:GLN:O	1:A:374:PRO:HB2	2.14	0.46
1:A:102:LEU:H	1:A:102:LEU:HD12	1.79	0.46
3:P:145:THR:O	3:P:149:ASN:HB2	2.15	0.46
5:E:145:VAL:HA	5:E:146:PRO:HD3	1.79	0.46
5:E:94:LYS:HG2	3:P:263:LEU:HD21	1.98	0.46
2:O:56:ARG:NH1	2:O:318:ASP:OD2	2.49	0.46
1:N:37:VAL:HG13	1:N:109:VAL:HG11	1.98	0.46
5:R:136:VAL:HG12	5:R:138:VAL:HG23	1.98	0.45
6:S:53:ASP:OD1	6:S:54:LEU:N	2.48	0.45
5:R:131:GLU:HG2	5:R:132:TRP:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:GLU:OE1	1:A:344:ARG:NH1	2.45	0.45
1:A:46:ARG:NH1	1:A:93:GLU:OE2	2.44	0.45
2:B:23:ASP:N	2:B:23:ASP:OD1	2.34	0.45
7:G:72:LYS:HZ2	8:H:52:GLU:CG	2.30	0.45
5:R:108:GLN:HB3	5:R:108:GLN:HE21	1.55	0.45
1:A:37:VAL:HG13	1:A:109:VAL:HG11	1.98	0.45
3:C:186:LEU:HD21	11:C:509:PEE:H2	1.99	0.45
5:E:150:SER:OG	5:E:151:GLY:N	2.49	0.45
5:R:37:TYR:CE2	11:R:502:PEE:H10	2.52	0.45
3:P:79:LEU:HD22	4:Q:204:MET:HE1	1.97	0.45
3:C:46:ILE:HA	12:C:501:HEM:HMC2	1.98	0.45
1:A:141:MET:HB3	1:A:141:MET:HE2	1.79	0.45
1:A:317:THR:OG1	1:A:318:GLY:N	2.51	0.45
1:N:69:LYS:HE3	1:N:70:ARG:HH21	1.81	0.45
1:A:69:LYS:HE3	1:A:70:ARG:HH21	1.81	0.44
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.52	0.44
1:N:280:TYR:HB3	1:N:307:PHE:CE2	2.52	0.44
1:A:191:LYS:HA	1:A:191:LYS:HE2	2.00	0.44
1:A:281:ASP:O	1:A:283:THR:N	2.50	0.44
3:C:133:VAL:HA	3:C:140:SER:HB3	1.99	0.44
2:O:206:LEU:HD23	2:O:220:ALA:HB2	2.00	0.44
3:P:133:VAL:HA	3:P:140:SER:HB3	2.00	0.44
3:P:89:SER:OG	3:P:273:TRP:NE1	2.30	0.44
4:Q:48:PHE:HB2	4:Q:87:ILE:HA	1.99	0.44
6:S:13:MET:O	6:S:17:ARG:HG2	2.18	0.44
3:P:165:ALA:HB1	11:P:409:PEE:H60	1.99	0.44
4:Q:134:TYR:CG	4:Q:162:PRO:HG3	2.53	0.44
4:Q:237:TYR:HB2	6:S:60:PHE:CG	2.53	0.44
5:R:48:ALA:HB1	11:R:502:PEE:H66	1.99	0.44
2:B:168:TYR:CD2	2:B:237:ALA:HB1	2.53	0.44
4:D:48:PHE:HB2	4:D:87:ILE:HA	2.00	0.44
3:C:89:SER:OG	3:C:273:TRP:NE1	2.31	0.44
1:A:61:HIS:CE1	1:A:134:ILE:HG12	2.53	0.44
1:N:191:LYS:HE2	1:N:191:LYS:HA	2.00	0.44
6:S:18:LYS:O	6:S:22:ASN:ND2	2.50	0.44
1:A:280:TYR:HB3	1:A:307:PHE:CE2	2.52	0.44
2:B:370:MET:HA	2:B:373:GLU:HG3	2.00	0.44
2:B:287:ARG:HG2	9:I:53:GLU:HB3	2.00	0.44
1:N:281:ASP:O	1:N:283:THR:N	2.50	0.44
1:N:433:ASP:OD1	1:N:436:ARG:HG2	2.18	0.44
2:O:370:MET:HA	2:O:373:GLU:HG3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:207:VAL:HG21	2:O:383:GLY:HA2	2.00	0.44
3:P:219:ILE:HG21	4:Q:230:LEU:HD11	2.00	0.44
1:A:433:ASP:OD1	1:A:436:ARG:HG2	2.18	0.43
2:O:197:ASN:HB3	2:O:232:THR:HB	2.00	0.43
5:E:98:VAL:HG22	5:E:134:ILE:HG22	1.99	0.43
5:E:123:ASP:OD1	5:E:170:ARG:NH2	2.51	0.43
5:R:75:GLU:HG2	5:R:194:VAL:HG22	1.99	0.43
2:B:166:ALA:HB2	2:B:244:ILE:HG13	2.00	0.43
5:E:118:ARG:HD3	5:E:171:ILE:HG23	2.00	0.43
1:N:61:HIS:CE1	1:N:134:ILE:HG12	2.53	0.43
11:P:409:PEE:H64	11:P:409:PEE:H10	2.00	0.43
1:N:136:GLN:HE21	9:V:50:LEU:HB2	1.83	0.43
1:A:264:ASP:HA	1:A:265:PRO:HD3	1.90	0.43
4:D:225:HIS:O	7:G:20:PRO:HB3	2.18	0.43
5:R:185:TYR:HB3	5:R:195:VAL:HG13	2.01	0.43
7:T:40:ARG:HD2	18:T:101:CDL:OA4	2.17	0.43
1:A:46:ARG:HD3	1:A:231:LEU:HD13	2.01	0.43
1:A:3:THR:OG1	1:A:6:GLN:OE1	2.23	0.43
14:C:504:U10:C8	14:C:504:U10:H1M1	2.49	0.43
4:D:204:MET:HB3	4:D:204:MET:HE2	1.84	0.43
3:P:210:LEU:HD12	6:S:66:LEU:HD23	2.01	0.43
3:P:31:TRP:NE1	11:P:407:PEE:O4	2.51	0.43
3:P:46:ILE:HA	12:P:402:HEM:HMC2	1.99	0.43
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.53	0.43
6:F:18:LYS:O	6:F:22:ASN:ND2	2.50	0.43
1:N:36:THR:HG21	1:N:373:THR:HA	2.01	0.43
8:U:31:VAL:HA	8:U:34:ARG:HB3	1.99	0.43
1:N:264:ASP:HA	1:N:265:PRO:HD3	1.90	0.43
3:P:106:GLY:HA2	3:P:108:TYR:CE2	2.53	0.43
1:N:317:THR:OG1	1:N:318:GLY:N	2.50	0.43
5:E:86:ASN:HD22	5:E:148:ALA:HB1	1.84	0.42
2:O:29:LEU:HD12	2:O:33:LEU:HD23	2.01	0.42
4:D:223:LYS:HE2	4:D:227:TRP:CD1	2.54	0.42
1:N:122:LEU:HD11	1:N:186:ILE:HD12	2.02	0.42
1:N:244:ARG:NE	7:T:10:VAL:HB	2.34	0.42
2:B:368:TYR:O	2:B:372:VAL:HG23	2.20	0.42
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.53	0.42
2:O:166:ALA:HB2	2:O:244:ILE:HG13	2.01	0.42
2:O:306:PRO:HB3	9:V:52:ARG:H	1.85	0.42
2:O:241:GLY:HA2	2:O:423:SER:HB3	2.01	0.42
4:D:91:PHE:HA	4:D:92:PRO:HD3	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:60:ALA:HA	9:V:77:ARG:HH22	1.85	0.42
3:P:9:HIS:CE1	3:P:11:LEU:HB2	2.55	0.42
2:B:319:SER:OG	2:B:320:GLY:N	2.53	0.42
3:C:136:TRP:HH2	3:C:171:VAL:HG12	1.85	0.42
3:C:230:ILE:HG22	4:D:219:LEU:HD13	2.01	0.42
5:E:96:LEU:HD21	5:E:195:VAL:HG21	2.01	0.42
19:P:406:BOG:H1'1	11:R:502:PEE:H33	2.02	0.42
1:A:60:GLU:OE1	2:B:287:ARG:NH2	2.49	0.42
4:D:33:TYR:CZ	4:D:43:MET:HG3	2.55	0.42
1:N:60:GLU:OE2	1:N:90:THR:HG22	2.20	0.42
3:P:221:PHE:HE2	11:P:401:PEE:H26	1.84	0.42
4:Q:139:ALA:HB3	8:U:54:CYS:SG	2.60	0.42
4:Q:223:LYS:HE2	4:Q:227:TRP:CD1	2.54	0.42
3:C:37:LEU:HD21	3:C:233:LEU:HA	2.02	0.42
1:N:321:GLY:HA2	1:N:342:TRP:CZ2	2.52	0.42
1:A:205:HIS:O	1:A:209:VAL:HG13	2.20	0.41
1:A:21:ASN:OD1	1:A:21:ASN:N	2.50	0.41
1:A:60:GLU:OE2	1:A:90:THR:HG22	2.20	0.41
3:C:9:HIS:CE1	3:C:11:LEU:HB2	2.55	0.41
1:A:140:GLU:CD	9:I:50:LEU:H	2.20	0.41
1:A:122:LEU:HD11	1:A:186:ILE:HD12	2.02	0.41
3:P:186:LEU:HD21	11:P:409:PEE:H1	2.02	0.41
5:R:163:SER:HA	5:R:174:GLY:HA3	2.01	0.41
3:C:271:PRO:HB3	13:C:503:Y52:C14	2.51	0.41
1:N:336:PHE:CE2	3:P:4:ASN:HB3	2.55	0.41
5:R:78:LEU:HB3	5:R:132:TRP:CZ2	2.54	0.41
3:C:92:PHE:HA	3:C:95:ILE:HG22	2.02	0.41
3:C:30:ALA:HB2	18:D:502:CDL:HA31	2.03	0.41
2:O:156:GLN:NE2	21:O:502:HOH:O	2.46	0.41
4:Q:91:PHE:HA	4:Q:92:PRO:HD3	1.74	0.41
7:T:40:ARG:HB3	18:T:101:CDL:HA31	2.02	0.41
2:B:257:VAL:O	2:B:323:GLY:HA3	2.21	0.41
1:N:277:ILE:O	1:N:292:SER:OG	2.28	0.41
2:O:368:TYR:O	2:O:372:VAL:HG23	2.20	0.41
5:R:170:ARG:HA	5:R:179:ASN:HB3	2.02	0.41
2:B:124:LEU:HD21	2:B:223:PHE:HB3	2.02	0.41
1:N:141:MET:HB3	1:N:141:MET:HE2	1.77	0.41
1:N:205:HIS:O	1:N:209:VAL:HG13	2.20	0.41
1:N:276:ILE:HD11	1:N:354:VAL:HG12	2.02	0.41
11:P:411:PEE:H13	11:P:411:PEE:H50	2.03	0.41
4:D:117:VAL:O	4:D:123:GLY:HA2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:223:PHE:HA	2:O:223:PHE:HD2	1.77	0.41
2:O:297:GLN:O	2:O:301:LYS:HG3	2.20	0.41
3:P:136:TRP:HH2	3:P:171:VAL:HG12	1.85	0.41
3:P:37:LEU:HD21	3:P:233:LEU:HA	2.03	0.41
4:Q:54:VAL:HG12	4:Q:55:THR:HG23	2.03	0.41
4:Q:141:VAL:HG21	8:U:55:THR:HG23	2.03	0.41
2:B:202:ALA:HB3	2:B:229:GLY:O	2.21	0.41
2:B:76:THR:HG22	2:B:82:SER:H	1.86	0.41
3:C:237:LEU:HD21	11:E:503:PEE:H29	2.02	0.41
1:N:106:MET:HG3	1:N:203:ILE:HD13	2.03	0.41
2:O:51:ILE:HG12	2:O:204:MET:HG2	2.03	0.41
11:P:407:PEE:H25	11:P:407:PEE:H32	1.92	0.41
4:Q:117:VAL:O	4:Q:123:GLY:HA2	2.20	0.41
5:R:45:VAL:HG13	10:W:28:ALA:HA	2.03	0.41
2:B:133:ARG:HA	2:B:134:PRO:HD3	1.87	0.41
2:B:218:GLN:O	2:B:222:GLN:HB2	2.20	0.41
3:C:214:SER:HA	6:F:66:LEU:HD11	2.03	0.41
8:H:17:LEU:HD21	8:H:21:ARG:HH21	1.86	0.41
2:O:200:THR:O	2:O:204:MET:HG3	2.20	0.41
3:P:2:ALA:HA	3:P:3:PRO:HD2	1.72	0.41
4:Q:33:TYR:CZ	4:Q:43:MET:HG3	2.55	0.41
1:A:276:ILE:HD11	1:A:354:VAL:HG12	2.03	0.41
4:D:237:TYR:HB2	6:F:60:PHE:CD1	2.56	0.41
5:E:54:VAL:HG11	11:E:502:PEE:H43	2.03	0.41
4:D:229:VAL:HG23	7:G:20:PRO:HG3	2.02	0.41
7:G:24:ARG:NH2	7:G:28:ASN:H	2.18	0.41
9:I:51:CYS:HB3	9:I:52:ARG:H	1.70	0.41
5:R:129:LYS:HA	5:R:130:PRO:HD3	1.85	0.41
2:B:100:SER:HB2	2:B:105:MET:HG2	2.02	0.41
2:B:154:SER:HA	2:B:155:PRO:HD3	1.94	0.41
2:O:100:SER:HB2	2:O:105:MET:HG2	2.03	0.41
3:P:184:PHE:CZ	12:P:402:HEM:HBC1	2.56	0.41
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.57	0.40
2:O:19:PRO:HB3	2:O:41:PHE:CD1	2.56	0.40
1:N:85:HIS:CD2	2:O:284:LEU:HD22	2.55	0.40
10:W:38:GLY:O	10:W:42:ILE:HG13	2.21	0.40
2:B:200:THR:O	2:B:204:MET:HG3	2.21	0.40
2:B:51:ILE:HG12	2:B:204:MET:HG2	2.03	0.40
2:O:170:THR:O	2:O:172:LEU:N	2.54	0.40
2:O:359:LYS:HB2	2:O:359:LYS:HE3	1.91	0.40
10:W:52:TRP:O	10:W:56:LYS:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:LEU:HD12	1:A:384:LEU:HA	1.95	0.40
2:B:297:GLN:O	2:B:301:LYS:HG3	2.20	0.40
2:B:97:SER:HA	9:I:69:SER:HA	2.03	0.40
2:O:56:ARG:NH2	2:O:236:LYS:HA	2.37	0.40
8:U:37:LEU:O	8:U:41:ASP:N	2.49	0.40
5:E:105:GLU:O	5:E:109:GLU:HB2	2.21	0.40
1:A:130:GLU:HA	1:A:133:VAL:HB	2.04	0.40
6:S:37:LEU:HA	6:S:37:LEU:HD23	1.93	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	441/446 (99%)	421 (96%)	16 (4%)	4 (1%)	17	52
1	N	440/446 (99%)	419 (95%)	17 (4%)	4 (1%)	17	52
2	B	419/441 (95%)	397 (95%)	18 (4%)	4 (1%)	15	50
2	O	420/441 (95%)	397 (94%)	17 (4%)	6 (1%)	11	43
3	C	378/380 (100%)	365 (97%)	11 (3%)	2 (0%)	29	64
3	P	378/380 (100%)	364 (96%)	12 (3%)	2 (0%)	29	64
4	D	239/241 (99%)	226 (95%)	11 (5%)	2 (1%)	19	55
4	Q	239/241 (99%)	225 (94%)	12 (5%)	2 (1%)	19	55
5	E	194/196 (99%)	168 (87%)	20 (10%)	6 (3%)	4	24
5	R	194/196 (99%)	175 (90%)	14 (7%)	5 (3%)	5	28
6	F	99/110 (90%)	97 (98%)	2 (2%)	0	100	100
6	S	99/110 (90%)	98 (99%)	1 (1%)	0	100	100
7	G	78/81 (96%)	74 (95%)	4 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	T	77/81 (95%)	72 (94%)	5 (6%)	0	100	100
8	H	66/77 (86%)	64 (97%)	2 (3%)	0	100	100
8	U	66/77 (86%)	56 (85%)	9 (14%)	1 (2%)	10	41
9	I	28/76 (37%)	17 (61%)	9 (32%)	2 (7%)	1	7
9	V	28/76 (37%)	19 (68%)	7 (25%)	2 (7%)	1	7
10	J	59/61 (97%)	55 (93%)	3 (5%)	1 (2%)	9	39
10	W	58/61 (95%)	54 (93%)	3 (5%)	1 (2%)	9	39
All	All	4000/4218 (95%)	3763 (94%)	193 (5%)	44 (1%)	14	48

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	390	GLY
2	O	19	PRO
2	O	226	ILE
2	O	390	GLY
9	V	59	SER
2	B	171	ALA
2	B	351	GLY
5	E	149	ASN
2	O	171	ALA
2	O	351	GLY
5	R	148	ALA
5	R	188	VAL
1	A	282	ARG
1	A	433	ASP
3	C	3	PRO
3	C	156	TYR
4	D	176	PRO
10	J	62	SER
1	N	282	ARG
1	N	433	ASP
2	O	223	PHE
3	P	3	PRO
4	Q	176	PRO
1	A	443	TRP
5	E	114	VAL
5	E	179	ASN
9	I	60	ALA
1	N	443	TRP

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Mol	Chain	Res	Type
8	U	12	GLU
2	B	227	ARG
5	E	120	PRO
5	E	155	GLY
5	E	163	SER
9	I	64	LEU
3	P	156	TYR
5	R	155	GLY
5	R	163	SER
9	V	60	ALA
10	W	15	ARG
5	R	141	HIS
4	D	162	PRO
4	Q	162	PRO
1	A	260	PRO
1	N	260	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	365/368 (99%)	342 (94%)	23 (6%)	18	50
1	N	365/368 (99%)	339 (93%)	26 (7%)	14	45
2	B	331/347 (95%)	312 (94%)	19 (6%)	20	54
2	O	332/347 (96%)	313 (94%)	19 (6%)	20	54
3	C	328/328 (100%)	309 (94%)	19 (6%)	20	53
3	P	327/328 (100%)	310 (95%)	17 (5%)	23	56
4	D	200/200 (100%)	191 (96%)	9 (4%)	27	61
4	Q	200/200 (100%)	190 (95%)	10 (5%)	24	58
5	E	166/166 (100%)	156 (94%)	10 (6%)	19	52
5	R	165/166 (99%)	150 (91%)	15 (9%)	9	32
6	F	93/96 (97%)	89 (96%)	4 (4%)	29	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	S	93/96 (97%)	89 (96%)	4 (4%)	29	62
7	G	71/71 (100%)	67 (94%)	4 (6%)	21	55
7	T	70/71 (99%)	67 (96%)	3 (4%)	29	62
8	H	64/71 (90%)	60 (94%)	4 (6%)	18	50
8	U	63/71 (89%)	60 (95%)	3 (5%)	25	59
9	I	22/45 (49%)	18 (82%)	4 (18%)	1	7
9	V	23/45 (51%)	17 (74%)	6 (26%)	0	1
10	J	49/49 (100%)	46 (94%)	3 (6%)	18	51
10	W	47/49 (96%)	42 (89%)	5 (11%)	6	26
All	All	3374/3482 (97%)	3167 (94%)	207 (6%)	18	51

All (207) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	16	VAL
1	A	28	GLU
1	A	37	VAL
1	A	58	PHE
1	A	70	ARG
1	A	86	PHE
1	A	106	MET
1	A	108	LYS
1	A	170	THR
1	A	220	SER
1	A	228	VAL
1	A	230	ILE
1	A	233	ARG
1	A	248	LEU
1	A	264	ASP
1	A	342	TRP
1	A	350	THR
1	A	405	ARG
1	A	430	GLN
1	A	431	LEU
1	A	432	LEU
1	A	443	TRP
2	B	22	GLU
2	B	23	ASP

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Mol	Chain	Res	Type
2	B	24	LEU
2	B	97	SER
2	B	102	ARG
2	B	156	GLN
2	B	160	LEU
2	B	170	THR
2	B	187	THR
2	B	222	GLN
2	B	297	GLN
2	B	304	THR
2	B	325	TYR
2	B	344	LEU
2	B	358	THR
2	B	374	THR
2	B	380	ASN
2	B	398	VAL
2	B	402	ILE
3	C	11	LEU
3	C	14	MET
3	C	22	LEU
3	C	65	SER
3	C	81	ARG
3	C	82	ASN
3	C	89	SER
3	C	91	PHE
3	C	93	ILE
3	C	95	ILE
3	C	156	TYR
3	C	157	ILE
3	C	159	HIS
3	C	160	THR
3	C	184	PHE
3	C	256	ASN
3	C	313	GLN
3	C	328	LEU
3	C	367	PHE
4	D	2	GLU
4	D	31	GLN
4	D	40	CYS
4	D	43	MET
4	D	57	THR
4	D	106	ASN

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Mol	Chain	Res	Type
4	D	142	VAL
4	D	169	LEU
4	D	234	LYS
5	E	1	VAL
5	E	22	THR
5	E	31	ASP
5	E	80	ASP
5	E	85	LYS
5	E	123	ASP
5	E	129	LYS
5	E	134	ILE
5	E	187	PHE
5	E	191	ASP
6	F	70	LEU
6	F	78	GLU
6	F	84	GLU
6	F	110	LYS
7	G	2	ILE
7	G	3	HIS
7	G	4	PHE
7	G	6	ASN
8	H	12	GLU
8	H	13	LEU
8	H	18	THR
8	H	49	HIS
9	I	50	LEU
9	I	68	ILE
9	I	69	SER
9	I	77	ARG
10	J	22	LEU
10	J	26	LEU
10	J	64	GLU
1	N	3	THR
1	N	9	GLN
1	N	16	VAL
1	N	28	GLU
1	N	37	VAL
1	N	58	PHE
1	N	70	ARG
1	N	86	PHE
1	N	106	MET
1	N	108	LYS

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Mol	Chain	Res	Type
1	N	170	THR
1	N	206	LYS
1	N	220	SER
1	N	228	VAL
1	N	230	ILE
1	N	233	ARG
1	N	248	LEU
1	N	264	ASP
1	N	342	TRP
1	N	344	ARG
1	N	350	THR
1	N	405	ARG
1	N	430	GLN
1	N	431	LEU
1	N	432	LEU
1	N	443	TRP
2	O	24	LEU
2	O	31	ASN
2	O	97	SER
2	O	102	ARG
2	O	156	GLN
2	O	160	LEU
2	O	170	THR
2	O	187	THR
2	O	223	PHE
2	O	225	ASN
2	O	297	GLN
2	O	304	THR
2	O	325	TYR
2	O	344	LEU
2	O	358	THR
2	O	374	THR
2	O	380	ASN
2	O	398	VAL
2	O	402	ILE
3	P	11	LEU
3	P	14	MET
3	P	22	LEU
3	P	65	SER
3	P	81	ARG
3	P	82	ASN
3	P	89	SER

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Mol	Chain	Res	Type
3	P	91	PHE
3	P	93	ILE
3	P	95	ILE
3	P	157	ILE
3	P	159	HIS
3	P	184	PHE
3	P	256	ASN
3	P	313	GLN
3	P	328	LEU
3	P	367	PHE
4	Q	31	GLN
4	Q	40	CYS
4	Q	43	MET
4	Q	57	THR
4	Q	106	ASN
4	Q	142	VAL
4	Q	169	LEU
4	Q	170	GLU
4	Q	234	LYS
4	Q	235	MET
5	R	1	VAL
5	R	22	THR
5	R	31	ASP
5	R	85	LYS
5	R	108	GLN
5	R	109	GLU
5	R	112	VAL
5	R	113	ASP
5	R	122	HIS
5	R	124	LEU
5	R	145	VAL
5	R	152	ASP
5	R	188	VAL
5	R	190	ASP
5	R	192	LEU
6	S	13	MET
6	S	70	LEU
6	S	78	GLU
6	S	84	GLU
7	T	3	HIS
7	T	4	PHE
7	T	6	ASN

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Mol	Chain	Res	Type
8	U	36	ARG
8	U	47	ARG
8	U	55	THR
9	V	49	LEU
9	V	51	CYS
9	V	54	SER
9	V	55	MET
9	V	68	ILE
9	V	77	ARG
10	W	15	ARG
10	W	16	ARG
10	W	22	LEU
10	W	40	ASP
10	W	60	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	118	GLN
1	A	173	ASN
1	A	271	HIS
2	B	392	HIS
3	C	313	GLN
3	C	332	ASN
4	D	105	ASN
4	D	166	ASN
5	E	122	HIS
7	G	23	GLN
1	N	118	GLN
1	N	136	GLN
1	N	173	ASN
1	N	271	HIS
2	O	225	ASN
2	O	363	GLN
3	P	313	GLN
3	P	332	ASN
4	Q	105	ASN
5	R	86	ASN
5	R	108	GLN
7	T	23	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	FME	C	1	3	7,8,10	1.95	1 (14%)	5,8,11	1.39	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FME	C	1	3	-	0/5/8/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	FME	CN-N	-5.04	1.33	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	FME	CN-N-CA	2.65	121.87	113.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

36 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	PEE	N	501	-	7,7,50	1.40	1 (14%)	9,9,55	1.25	1 (11%)
11	PEE	E	503	-	14,14,50	0.23	0	13,13,55	0.68	0
19	BOG	D	503	-	20,20,20	0.55	1 (5%)	25,25,25	0.64	0
17	HEC	Q	501	4	26,50,50	2.05	3 (11%)	18,82,82	1.53	3 (16%)
15	MES	C	506	-	12,12,12	2.26	1 (8%)	14,16,16	1.23	3 (21%)
11	PEE	C	509	-	46,46,50	1.02	2 (4%)	49,51,55	1.10	4 (8%)
14	U10	P	405	-	19,19,63	2.18	2 (10%)	23,26,79	1.60	4 (17%)
11	PEE	A	501	-	25,25,50	1.35	2 (8%)	28,30,55	1.56	5 (17%)
11	PEE	P	401	-	11,14,50	0.23	0	10,14,55	0.61	0
11	PEE	R	502	-	48,48,50	0.98	2 (4%)	51,53,55	1.09	6 (11%)
17	HEC	D	501	4	26,50,50	2.03	3 (11%)	18,82,82	1.52	3 (16%)
11	PEE	C	507	-	10,10,50	0.51	0	11,12,55	0.55	0
11	PEE	P	407	-	48,48,50	0.97	2 (4%)	51,53,55	1.00	2 (3%)
18	CDL	D	502	-	41,41,99	1.31	4 (9%)	47,53,111	1.31	5 (10%)
20	FES	R	501	5	0,4,4	0.00	-	-	-	-
12	HEM	C	502	3	27,50,50	1.82	5 (18%)	17,82,82	1.53	2 (11%)
11	PEE	C	505	-	48,48,50	0.94	2 (4%)	51,53,55	1.14	4 (7%)
12	HEM	C	501	3	27,50,50	1.84	5 (18%)	17,82,82	1.52	4 (23%)
16	GOL	P	408	-	5,5,5	0.37	0	5,5,5	0.29	0
19	BOG	P	406	-	20,20,20	0.52	0	25,25,25	0.62	0
18	CDL	T	101	-	39,39,99	1.35	4 (10%)	45,51,111	1.38	5 (11%)
13	Y52	C	503	-	27,29,29	0.68	0	30,39,39	1.10	3 (10%)
11	PEE	P	409	-	40,40,50	1.03	2 (5%)	43,45,55	1.14	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CDL	G	101	-	39,39,99	1.34	4 (10%)	45,51,111	1.36	4 (8%)
16	GOL	C	508	-	5,5,5	0.36	0	5,5,5	0.34	0
18	CDL	Q	502	-	41,41,99	1.30	4 (9%)	47,53,111	1.29	6 (12%)
13	Y52	P	404	-	27,29,29	0.67	0	30,39,39	1.07	2 (6%)
14	U10	C	504	-	19,19,63	2.12	2 (10%)	23,26,79	1.48	2 (8%)
19	BOG	Q	503	-	20,20,20	0.55	1 (5%)	25,25,25	0.61	0
11	PEE	C	510	-	11,14,50	0.25	0	10,14,55	0.59	0
11	PEE	P	411	-	24,24,50	1.30	2 (8%)	27,29,55	1.40	4 (14%)
12	HEM	P	402	3	27,50,50	1.84	5 (18%)	17,82,82	1.51	4 (23%)
11	PEE	P	410	-	8,11,50	0.22	0	7,11,55	0.80	0
12	HEM	P	403	3	27,50,50	1.82	5 (18%)	17,82,82	1.51	3 (17%)
20	FES	E	501	5	0,4,4	0.00	-	-	-	-
11	PEE	E	502	-	47,47,50	0.98	2 (4%)	50,52,55	1.06	4 (8%)

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	PEE	N	501	-	-	0/5/5/54	-
11	PEE	E	503	-	-	1/12/12/54	-
19	BOG	D	503	-	-	0/11/31/31	0/1/1/1
17	HEC	Q	501	4	-	0/6/54/54	-
15	MES	C	506	-	-	3/6/14/14	0/1/1/1
11	PEE	C	509	-	-	13/50/50/54	-
14	U10	P	405	-	-	4/11/35/87	0/1/1/1
11	PEE	A	501	-	-	11/29/29/54	-
11	PEE	P	401	-	-	3/10/12/54	-
11	PEE	R	502	-	-	21/52/52/54	-
17	HEC	D	501	4	-	0/6/54/54	-
11	PEE	C	507	-	-	5/10/10/54	-
11	PEE	P	407	-	-	15/52/52/54	-
18	CDL	D	502	-	-	16/51/51/110	-
20	FES	R	501	5	-	-	0/1/1/1
12	HEM	C	502	3	-	0/6/54/54	-
11	PEE	C	505	-	-	21/52/52/54	-
12	HEM	C	501	3	-	3/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	GOL	P	408	-	-	4/4/4/4	-
19	BOG	P	406	-	-	3/11/31/31	0/1/1/1
18	CDL	T	101	-	-	17/49/49/110	-
13	Y52	C	503	-	-	0/18/20/20	0/3/3/3
11	PEE	P	409	-	-	19/44/44/54	-
18	CDL	G	101	-	-	14/49/49/110	-
16	GOL	C	508	-	-	4/4/4/4	-
18	CDL	Q	502	-	-	14/51/51/110	-
13	Y52	P	404	-	-	0/18/20/20	0/3/3/3
14	U10	C	504	-	-	4/11/35/87	0/1/1/1
19	BOG	Q	503	-	-	2/11/31/31	0/1/1/1
11	PEE	C	510	-	-	5/10/12/54	-
11	PEE	P	411	-	-	9/28/28/54	-
12	HEM	P	402	3	-	3/6/54/54	-
11	PEE	P	410	-	-	4/7/9/54	-
12	HEM	P	403	3	-	0/6/54/54	-
20	FES	E	501	5	-	-	0/1/1/1
11	PEE	E	502	-	-	19/51/51/54	-

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	P	405	U10	C6-C1	8.65	1.51	1.35
14	C	504	U10	C6-C1	8.36	1.50	1.35
15	C	506	MES	C8-S	-7.58	1.66	1.77
17	Q	501	HEC	C3B-C2B	-6.01	1.34	1.40
17	D	501	HEC	C3B-C2B	-5.97	1.34	1.40
17	Q	501	HEC	C3C-C2C	-5.84	1.34	1.40
17	D	501	HEC	C3C-C2C	-5.80	1.34	1.40
11	A	501	PEE	O3-C30	4.66	1.46	1.33
11	C	509	PEE	O2-C10	4.64	1.47	1.34
11	R	502	PEE	O2-C10	4.54	1.47	1.34
11	C	509	PEE	O3-C30	4.44	1.46	1.33
11	E	502	PEE	O2-C10	4.39	1.46	1.34
18	T	101	CDL	OB8-CB7	4.34	1.46	1.33
11	R	502	PEE	O3-C30	4.31	1.45	1.33
18	G	101	CDL	OB8-CB7	4.28	1.45	1.33
11	P	409	PEE	O3-C30	4.28	1.45	1.33
11	P	407	PEE	O2-C10	4.28	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D	502	CDL	OB8-CB7	4.27	1.45	1.33
11	E	502	PEE	O3-C30	4.24	1.45	1.33
11	P	409	PEE	O2-C10	4.22	1.46	1.34
11	P	411	PEE	O3-C30	4.21	1.45	1.33
11	P	407	PEE	O3-C30	4.20	1.45	1.33
18	Q	502	CDL	OB8-CB7	4.20	1.45	1.33
11	C	505	PEE	O3-C30	4.15	1.45	1.33
11	P	411	PEE	O2-C10	4.15	1.46	1.34
11	C	505	PEE	O2-C10	4.15	1.46	1.34
18	D	502	CDL	OA6-CA5	4.14	1.46	1.34
18	T	101	CDL	OA6-CA5	4.13	1.46	1.34
11	A	501	PEE	O2-C10	4.13	1.46	1.34
18	D	502	CDL	OB6-CB5	4.08	1.45	1.34
18	Q	502	CDL	OA6-CA5	4.08	1.45	1.34
18	G	101	CDL	OB6-CB5	4.07	1.45	1.34
18	Q	502	CDL	OB6-CB5	4.07	1.45	1.34
18	T	101	CDL	OB6-CB5	4.05	1.45	1.34
18	G	101	CDL	OA6-CA5	4.02	1.45	1.34
12	C	502	HEM	C3C-CAC	3.94	1.55	1.47
12	P	403	HEM	C3C-CAC	3.94	1.55	1.47
12	P	403	HEM	C3B-CAB	3.88	1.55	1.47
12	C	501	HEM	C3B-CAB	3.88	1.55	1.47
12	C	502	HEM	C3B-CAB	3.86	1.55	1.47
12	C	501	HEM	C3C-CAC	3.85	1.55	1.47
12	P	402	HEM	C3B-CAB	3.85	1.55	1.47
12	P	402	HEM	C3C-CAC	3.83	1.55	1.47
12	P	402	HEM	C3C-C2C	-3.77	1.35	1.40
12	C	501	HEM	C3C-C2C	-3.70	1.35	1.40
12	C	501	HEM	C3B-C2B	-3.64	1.35	1.40
12	P	403	HEM	C3B-C2B	-3.62	1.35	1.40
12	P	402	HEM	C3B-C2B	-3.61	1.35	1.40
12	C	502	HEM	C3C-C2C	-3.57	1.35	1.40
12	P	403	HEM	C3C-C2C	-3.54	1.35	1.40
12	C	502	HEM	C3B-C2B	-3.52	1.35	1.40
11	N	501	PEE	P-O1P	3.36	1.61	1.50
14	C	504	U10	C4-C3	3.13	1.49	1.36
14	P	405	U10	C4-C3	3.06	1.48	1.36
18	Q	502	CDL	OA8-CA7	2.51	1.45	1.33
18	G	101	CDL	OA8-CA7	2.50	1.45	1.33
18	T	101	CDL	OA8-CA7	2.49	1.45	1.33
18	D	502	CDL	OA8-CA7	2.43	1.45	1.33
17	Q	501	HEC	CAD-C3D	2.16	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	P	402	HEM	CAA-C2A	2.16	1.55	1.52
12	C	501	HEM	CAA-C2A	2.11	1.55	1.52
17	D	501	HEC	CAD-C3D	2.10	1.55	1.52
12	P	403	HEM	CAA-C2A	2.06	1.55	1.52
12	C	502	HEM	CAA-C2A	2.03	1.55	1.52
19	Q	503	BOG	O1-C1	2.02	1.43	1.40
19	D	503	BOG	O1-C1	2.01	1.43	1.40

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	T	101	CDL	OB6-CB5-C51	4.49	121.18	111.50
11	C	505	PEE	O2-C10-C11	4.48	121.17	111.50
14	C	504	U10	C7-C8-C9	-4.45	119.38	126.79
18	Q	502	CDL	OB6-CB5-C51	4.40	120.98	111.50
11	P	411	PEE	O2-C10-C11	4.40	120.97	111.50
18	G	101	CDL	OB6-CB5-C51	4.36	120.90	111.50
11	A	501	PEE	O2-C10-C11	4.26	120.68	111.50
18	D	502	CDL	OB6-CB5-C51	4.17	120.49	111.50
11	E	502	PEE	O2-C10-C11	4.04	120.21	111.50
14	P	405	U10	C7-C8-C9	-3.97	120.19	126.79
11	R	502	PEE	O2-C10-C11	3.84	119.78	111.50
11	P	409	PEE	O3-C30-C31	3.69	123.50	111.91
14	C	504	U10	C10-C9-C11	3.69	120.21	115.98
11	C	509	PEE	O2-C10-C11	3.68	119.43	111.50
11	P	409	PEE	O2-C10-C11	3.59	119.25	111.50
18	T	101	CDL	OB8-CB7-C71	3.53	120.64	111.38
18	D	502	CDL	OA6-CA5-C11	3.53	120.63	110.80
11	A	501	PEE	O3-C30-C31	3.51	122.93	111.91
11	P	407	PEE	O2-C10-C11	3.41	118.84	111.50
14	P	405	U10	C10-C9-C11	3.40	119.87	115.98
18	T	101	CDL	CB4-OB6-CB5	-3.38	109.48	117.79
11	N	501	PEE	O3P-P-O2P	3.27	120.12	107.64
11	A	501	PEE	O3-C3-C2	3.23	117.83	108.43
18	Q	502	CDL	OA6-CA5-C11	3.23	119.81	110.80
11	C	505	PEE	O3-C30-C31	3.17	121.86	111.91
18	G	101	CDL	CB4-OB6-CB5	-3.15	110.05	117.79
18	G	101	CDL	OB8-CB7-C71	3.14	119.61	111.38
12	C	502	HEM	CBD-CAD-C3D	-3.05	106.86	112.48
12	P	403	HEM	CBD-CAD-C3D	-3.03	106.89	112.48
11	E	502	PEE	O3-C30-C31	3.02	121.38	111.91
13	P	404	Y52	C19-C26-N27	2.99	115.00	108.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	503	Y52	C19-C26-N27	2.95	114.91	108.04
18	T	101	CDL	OA6-CA5-C11	2.94	119.01	110.80
11	A	501	PEE	O2-C10-O4	-2.83	116.85	123.70
14	P	405	U10	C7-C6-C5	-2.79	115.12	118.48
18	G	101	CDL	OA6-CA5-C11	2.78	118.56	110.80
11	C	509	PEE	O3-C30-C31	2.74	120.52	111.91
18	D	502	CDL	OB8-CB7-C71	2.74	120.51	111.91
17	Q	501	HEC	CMB-C2B-C1B	-2.73	124.27	128.46
17	D	501	HEC	CMB-C2B-C1B	-2.69	124.33	128.46
18	D	502	CDL	CB4-OB6-CB5	-2.66	111.24	117.79
11	P	407	PEE	O3-C30-C31	2.61	120.11	111.91
11	C	509	PEE	O2-C2-C1	2.60	117.83	108.40
13	C	503	Y52	C15-S16-C17	-2.60	98.97	101.20
18	Q	502	CDL	CB4-OB6-CB5	-2.58	111.44	117.79
11	C	505	PEE	O2-C10-O4	-2.57	117.50	123.70
11	R	502	PEE	O2-C2-C1	2.55	117.63	108.40
14	P	405	U10	C8-C7-C6	2.50	118.78	112.05
11	P	411	PEE	O3-C30-C31	2.49	119.73	111.91
11	C	509	PEE	C2-O2-C10	2.48	123.89	117.79
11	P	411	PEE	O2-C10-O4	-2.43	117.82	123.70
11	R	502	PEE	O3-C30-C31	2.38	119.39	111.91
11	R	502	PEE	C2-O2-C10	2.36	123.60	117.79
18	Q	502	CDL	OB8-CB7-C71	2.33	119.23	111.91
12	C	501	HEM	CMB-C2B-C3B	2.27	128.93	124.68
11	C	505	PEE	O3-C30-O5	-2.27	117.86	123.59
15	C	506	MES	O3S-S-C8	2.27	109.44	105.77
17	D	501	HEC	CMC-C2C-C1C	-2.25	125.01	128.46
11	A	501	PEE	O3-C30-O5	-2.24	117.95	123.59
11	E	502	PEE	O3-C30-O5	-2.22	118.00	123.59
12	P	402	HEM	CMB-C2B-C3B	2.21	128.82	124.68
13	C	503	Y52	C25-C26-N27	-2.21	124.51	130.83
12	C	501	HEM	C4A-C3A-C2A	2.19	108.52	107.00
12	P	402	HEM	CBD-CAD-C3D	-2.18	108.46	112.48
12	C	501	HEM	CBD-CAD-C3D	-2.17	108.47	112.48
18	Q	502	CDL	OB6-CB5-OB7	-2.17	118.45	123.70
15	C	506	MES	O2S-S-C8	2.17	109.52	106.92
17	Q	501	HEC	CMC-C2C-C1C	-2.17	125.14	128.46
17	Q	501	HEC	C1D-C2D-C3D	2.15	108.49	107.00
13	P	404	Y52	C25-C26-N27	-2.15	124.69	130.83
12	P	402	HEM	CMC-C2C-C3C	2.14	128.69	124.68
18	Q	502	CDL	CA4-OA6-CA5	-2.12	112.58	117.79
12	P	403	HEM	CMC-C2C-C3C	2.10	128.61	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	P	402	HEM	C4A-C3A-C2A	2.10	108.46	107.00
12	C	501	HEM	CMC-C2C-C3C	2.10	128.60	124.68
15	C	506	MES	O1S-S-C8	2.08	109.42	106.92
18	T	101	CDL	OB6-CB5-OB7	-2.07	118.69	123.70
17	D	501	HEC	C1D-C2D-C3D	2.06	108.43	107.00
11	E	502	PEE	C3-C2-C1	-2.06	106.93	111.79
12	C	502	HEM	CMC-C2C-C3C	2.05	128.51	124.68
11	R	502	PEE	O3-C3-C2	2.04	114.38	108.43
11	P	411	PEE	O3-C30-O5	-2.04	118.44	123.59
11	R	502	PEE	O3-C30-O5	-2.04	118.44	123.59
11	P	409	PEE	O3-C30-O5	-2.03	118.47	123.59
12	P	403	HEM	CMB-C2B-C3B	2.01	128.43	124.68
18	D	502	CDL	CA4-OA6-CA5	-2.00	112.87	117.79

There are no chirality outliers.

All (237) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	P	410	PEE	C10-C11-C12-C13
11	C	509	PEE	C1-O3P-P-O1P
11	C	509	PEE	C1-O3P-P-O2P
11	C	509	PEE	C1-O3P-P-O4P
14	P	405	U10	C1-C6-C7-C8
14	P	405	U10	C5-C6-C7-C8
14	P	405	U10	C12-C11-C9-C8
14	P	405	U10	C12-C11-C9-C10
11	A	501	PEE	C1-O3P-P-O1P
11	A	501	PEE	C1-O3P-P-O4P
11	A	501	PEE	C4-O4P-P-O1P
11	P	401	PEE	C10-C11-C12-C13
11	R	502	PEE	C1-O3P-P-O4P
11	C	507	PEE	C4-O4P-P-O1P
11	P	407	PEE	C1-O3P-P-O1P
11	P	407	PEE	C1-O3P-P-O4P
11	P	407	PEE	C4-O4P-P-O3P
11	C	505	PEE	C1-C2-O2-C10
11	C	505	PEE	C11-C10-O2-C2
11	C	505	PEE	C4-O4P-P-O1P
12	C	501	HEM	C1A-C2A-CAA-CBA
12	C	501	HEM	C3D-CAD-CBD-CGD
16	P	408	GOL	O1-C1-C2-O2
16	P	408	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
18	T	101	CDL	CA3-OA5-PA1-OA4
18	T	101	CDL	CB2-OB2-PB2-OB3
18	T	101	CDL	CB2-OB2-PB2-OB4
18	T	101	CDL	CB2-OB2-PB2-OB5
18	T	101	CDL	CB3-OB5-PB2-OB4
18	T	101	CDL	C51-CB5-OB6-CB4
11	P	409	PEE	C11-C10-O2-C2
11	P	409	PEE	C4-O4P-P-O3P
18	G	101	CDL	CB2-C1-CA2-OA2
18	G	101	CDL	CB2-OB2-PB2-OB4
16	C	508	GOL	O1-C1-C2-O2
16	C	508	GOL	C1-C2-C3-O3
18	Q	502	CDL	CA2-OA2-PA1-OA3
18	Q	502	CDL	CA2-OA2-PA1-OA5
18	Q	502	CDL	CB2-OB2-PB2-OB4
18	Q	502	CDL	CB3-OB5-PB2-OB4
14	C	504	U10	C12-C11-C9-C10
11	C	510	PEE	C10-C11-C12-C13
11	P	411	PEE	C11-C10-O2-C2
11	P	411	PEE	C1-O3P-P-O2P
12	P	402	HEM	C1A-C2A-CAA-CBA
12	P	402	HEM	C3D-CAD-CBD-CGD
11	E	502	PEE	C1-O3P-P-O1P
11	E	502	PEE	C1-O3P-P-O2P
11	E	502	PEE	C1-O3P-P-O4P
11	E	502	PEE	C4-O4P-P-O1P
11	A	501	PEE	O4-C10-O2-C2
11	C	505	PEE	O4-C10-O2-C2
18	T	101	CDL	OB7-CB5-OB6-CB4
11	P	411	PEE	O4-C10-O2-C2
11	P	409	PEE	O4-C10-O2-C2
18	D	502	CDL	O1-C1-CA2-OA2
18	D	502	CDL	O1-C1-CB2-OB2
18	Q	502	CDL	O1-C1-CA2-OA2
11	A	501	PEE	C11-C10-O2-C2
18	G	101	CDL	C51-CB5-OB6-CB4
18	Q	502	CDL	C51-CB5-OB6-CB4
19	P	406	BOG	O5-C5-C6-O6
18	T	101	CDL	C71-CB7-OB8-CB6
11	P	407	PEE	O2-C2-C3-O3
11	C	505	PEE	O2-C2-C3-O3
16	P	408	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
18	T	101	CDL	OB9-CB7-OB8-CB6
11	E	502	PEE	C30-C31-C32-C33
18	G	101	CDL	O1-C1-CA2-OA2
18	G	101	CDL	OB7-CB5-OB6-CB4
18	Q	502	CDL	OB7-CB5-OB6-CB4
11	C	509	PEE	C4-O4P-P-O3P
11	C	507	PEE	C1-O3P-P-O4P
18	D	502	CDL	CA3-OA5-PA1-OA2
11	C	505	PEE	C1-O3P-P-O4P
18	T	101	CDL	CA2-OA2-PA1-OA5
18	T	101	CDL	CA3-OA5-PA1-OA2
18	T	101	CDL	CB3-OB5-PB2-OB2
18	G	101	CDL	CA2-OA2-PA1-OA5
18	G	101	CDL	CB2-OB2-PB2-OB5
18	G	101	CDL	CB3-OB5-PB2-OB2
18	Q	502	CDL	CA3-OA5-PA1-OA2
18	Q	502	CDL	CB2-OB2-PB2-OB5
18	Q	502	CDL	CB3-OB5-PB2-OB2
11	P	411	PEE	C1-O3P-P-O4P
11	R	502	PEE	C31-C32-C33-C34
11	C	509	PEE	C31-C30-O3-C3
19	Q	503	BOG	O1-C1'-C2'-C3'
18	Q	502	CDL	C11-CA5-OA6-CA4
11	C	509	PEE	C1-C2-O2-C10
11	P	411	PEE	C1-C2-O2-C10
18	Q	502	CDL	OA7-CA5-OA6-CA4
11	P	410	PEE	C15-C16-C17-C18
11	C	510	PEE	C11-C12-C13-C14
11	C	510	PEE	C15-C16-C17-C18
11	R	502	PEE	C18-C19-C20-C21
11	C	505	PEE	C32-C33-C34-C35
11	E	503	PEE	C18-C19-C20-C21
11	E	502	PEE	C13-C14-C15-C16
11	C	509	PEE	C32-C33-C34-C35
16	P	408	GOL	O1-C1-C2-C3
16	C	508	GOL	O1-C1-C2-C3
11	R	502	PEE	O4-C10-O2-C2
11	E	502	PEE	C31-C32-C33-C34
11	C	509	PEE	O5-C30-O3-C3
11	E	502	PEE	C39-C40-C41-C42
19	Q	503	BOG	C1'-C2'-C3'-C4'
11	R	502	PEE	C11-C10-O2-C2

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Mol	Chain	Res	Type	Atoms
11	R	502	PEE	C23-C24-C25-C26
16	C	508	GOL	O2-C2-C3-O3
11	C	510	PEE	C16-C17-C18-C19
11	E	502	PEE	C12-C13-C14-C15
11	C	505	PEE	C36-C37-C38-C39
11	P	409	PEE	C32-C33-C34-C35
11	P	409	PEE	C33-C34-C35-C36
18	D	502	CDL	C11-CA5-OA6-CA4
11	R	502	PEE	C10-C11-C12-C13
11	C	509	PEE	C11-C10-O2-C2
11	C	509	PEE	O4-C10-O2-C2
18	D	502	CDL	OB6-CB4-CB6-OB8
11	R	502	PEE	C11-C12-C13-C14
11	P	407	PEE	C11-C12-C13-C14
18	D	502	CDL	OA7-CA5-OA6-CA4
18	Q	502	CDL	CB2-C1-CA2-OA2
11	C	505	PEE	C1-C2-C3-O3
14	C	504	U10	C1-C6-C7-C8
11	R	502	PEE	C16-C17-C18-C19
19	P	406	BOG	C4-C5-C6-O6
14	C	504	U10	C5-C6-C7-C8
11	P	401	PEE	C13-C14-C15-C16
11	A	501	PEE	C3-C2-O2-C10
11	R	502	PEE	C1-C2-O2-C10
11	R	502	PEE	C31-C30-O3-C3
18	G	101	CDL	OA5-CA3-CA4-OA6
11	P	411	PEE	O2-C2-C3-O3
11	C	505	PEE	O3P-C1-C2-C3
11	C	510	PEE	C17-C18-C19-C20
11	P	407	PEE	C36-C37-C38-C39
11	P	407	PEE	C1-C2-C3-O3
18	D	502	CDL	CB3-CB4-CB6-OB8
11	P	411	PEE	C1-C2-C3-O3
11	C	507	PEE	C4-O4P-P-O3P
11	A	501	PEE	O3P-C1-C2-O2
18	D	502	CDL	OA6-CA4-CA6-OA8
18	D	502	CDL	CB2-C1-CA2-OA2
18	D	502	CDL	CA2-C1-CB2-OB2
11	R	502	PEE	O5-C30-O3-C3
11	C	509	PEE	C11-C12-C13-C14
11	R	502	PEE	C17-C18-C19-C20
11	R	502	PEE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
11	P	407	PEE	C12-C13-C14-C15
11	C	505	PEE	C12-C13-C14-C15
18	D	502	CDL	CA3-CA4-CA6-OA8
11	C	505	PEE	O3P-C1-C2-O2
11	P	409	PEE	O3P-C1-C2-O2
11	P	401	PEE	C11-C12-C13-C14
11	P	409	PEE	C13-C14-C15-C16
11	R	502	PEE	C12-C13-C14-C15
11	A	501	PEE	C4-O4P-P-O3P
18	D	502	CDL	CB3-OB5-PB2-OB2
11	E	502	PEE	C4-O4P-P-O3P
11	C	509	PEE	C4-O4P-P-O1P
11	R	502	PEE	C1-O3P-P-O1P
11	C	507	PEE	C1-O3P-P-O1P
11	P	407	PEE	C4-O4P-P-O2P
18	D	502	CDL	CA3-OA5-PA1-OA3
11	C	505	PEE	C1-O3P-P-O1P
18	T	101	CDL	CA2-OA2-PA1-OA3
11	P	409	PEE	C4-O4P-P-O2P
18	G	101	CDL	CA2-OA2-PA1-OA3
18	G	101	CDL	CB2-OB2-PB2-OB3
18	G	101	CDL	CB3-OB5-PB2-OB4
18	Q	502	CDL	CA3-OA5-PA1-OA3
11	E	502	PEE	C10-C11-C12-C13
11	A	501	PEE	O3P-C1-C2-C3
11	P	409	PEE	O3P-C1-C2-C3
18	G	101	CDL	OA5-CA3-CA4-CA6
15	C	506	MES	C7-C8-S-O3S
11	P	410	PEE	C16-C17-C18-C19
15	C	506	MES	C7-C8-S-O1S
15	C	506	MES	C7-C8-S-O2S
11	C	505	PEE	C16-C17-C18-C19
11	E	502	PEE	C15-C16-C17-C18
11	E	502	PEE	C34-C35-C36-C37
12	C	501	HEM	C3A-C2A-CAA-CBA
12	P	402	HEM	C3A-C2A-CAA-CBA
18	T	101	CDL	OB6-CB4-CB6-OB8
11	P	409	PEE	O5-C30-O3-C3
11	P	409	PEE	C41-C42-C43-C44
19	P	406	BOG	C3'-C4'-C5'-C6'
11	P	409	PEE	C31-C30-O3-C3
11	E	502	PEE	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
11	R	502	PEE	C4-O4P-P-O3P
18	D	502	CDL	CA2-OA2-PA1-OA5
11	C	505	PEE	C4-O4P-P-O3P
11	P	409	PEE	C1-O3P-P-O4P
18	G	101	CDL	CA3-OA5-PA1-OA2
11	P	411	PEE	C4-O4P-P-O3P
11	P	407	PEE	C23-C24-C25-C26
11	A	501	PEE	O5-C30-O3-C3
11	P	409	PEE	C44-C45-C46-C47
11	A	501	PEE	C31-C30-O3-C3
11	E	502	PEE	C18-C19-C20-C21
11	P	407	PEE	C16-C17-C18-C19
11	P	407	PEE	O3P-C1-C2-C3
18	T	101	CDL	OA5-CA3-CA4-CA6
11	R	502	PEE	C33-C34-C35-C36
11	R	502	PEE	C24-C25-C26-C27
11	P	410	PEE	C11-C12-C13-C14
11	C	507	PEE	O3P-C1-C2-C3
11	C	509	PEE	C35-C36-C37-C38
11	P	407	PEE	O3P-C1-C2-O2
18	T	101	CDL	OA5-CA3-CA4-OA6
11	E	502	PEE	O2-C2-C3-O3
11	P	407	PEE	C21-C22-C23-C24
11	P	409	PEE	C1-C2-O2-C10
11	P	407	PEE	C15-C16-C17-C18
14	C	504	U10	C2-C3-O3-C3M
11	R	502	PEE	C15-C16-C17-C18
11	R	502	PEE	C1-C2-C3-O3
18	T	101	CDL	CB3-CB4-CB6-OB8
11	E	502	PEE	O3P-C1-C2-O2
11	C	505	PEE	C11-C12-C13-C14
11	C	505	PEE	O2-C10-C11-C12
11	E	502	PEE	O3-C30-C31-C32
11	C	505	PEE	C31-C32-C33-C34
11	P	409	PEE	C36-C37-C38-C39
18	D	502	CDL	CA2-OA2-PA1-OA3
11	P	411	PEE	C4-O4P-P-O1P
11	P	409	PEE	O3-C30-C31-C32
11	P	409	PEE	C3-C2-O2-C10
11	C	505	PEE	O3-C30-C31-C32
11	E	502	PEE	O5-C30-C31-C32
18	D	502	CDL	OB7-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
11	C	505	PEE	O4-C10-C11-C12
11	P	409	PEE	O5-C30-C31-C32
11	C	505	PEE	O5-C30-C31-C32

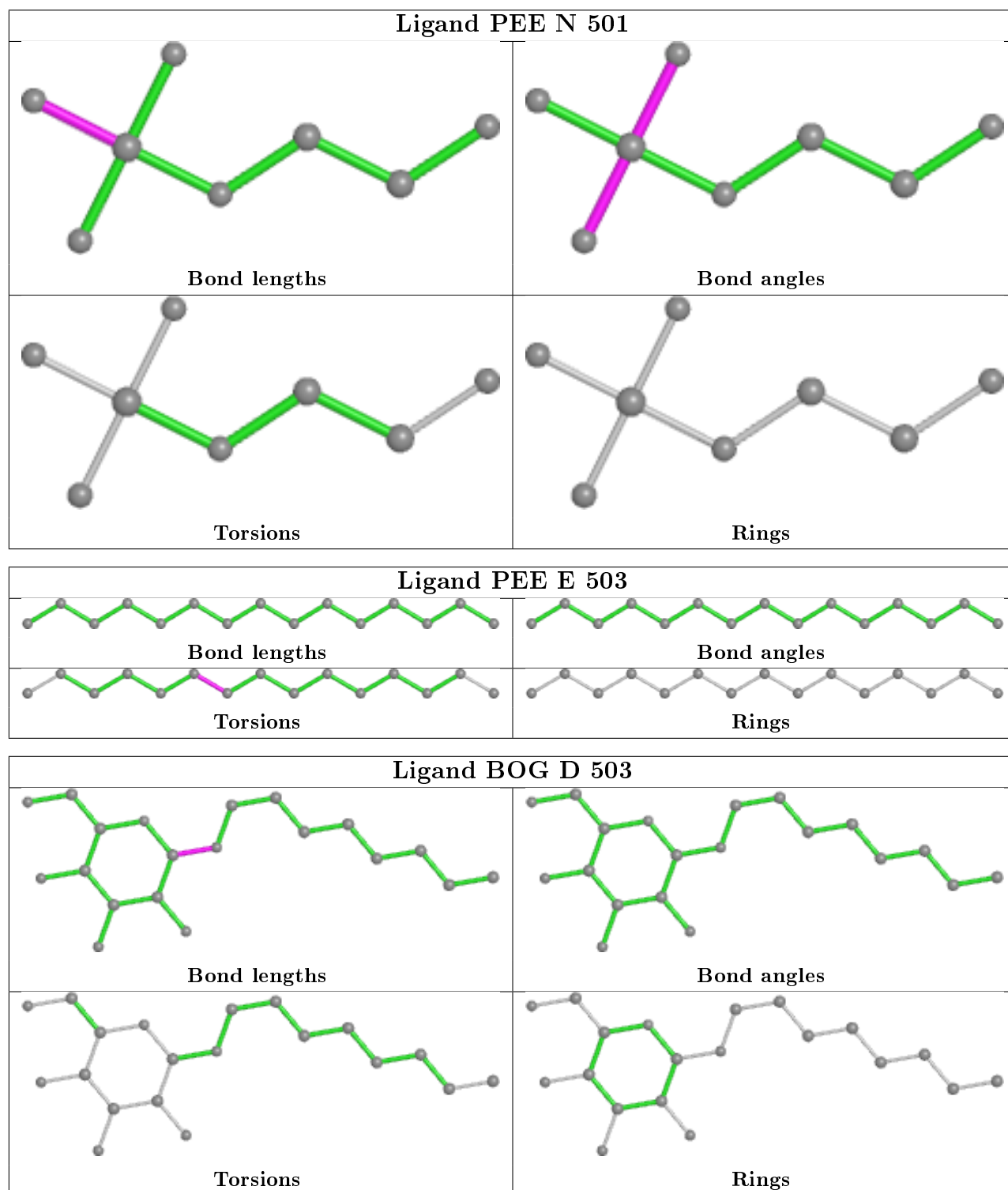
There are no ring outliers.

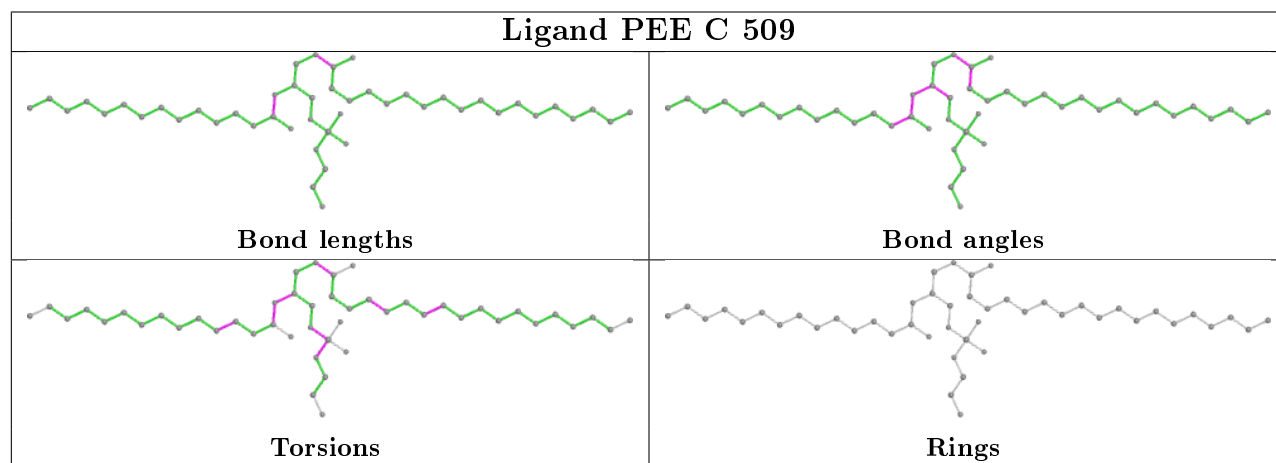
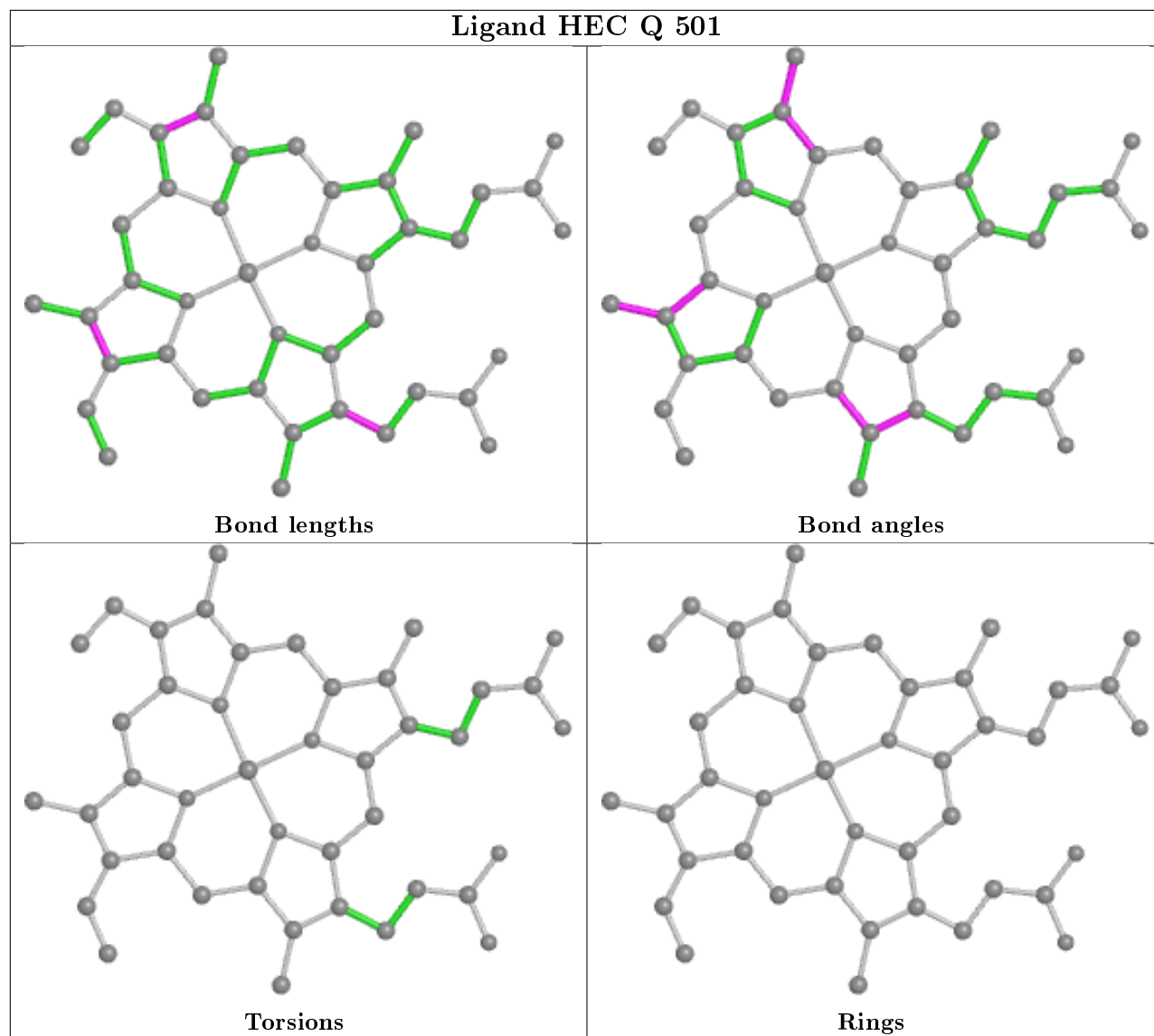
23 monomers are involved in 48 short contacts:

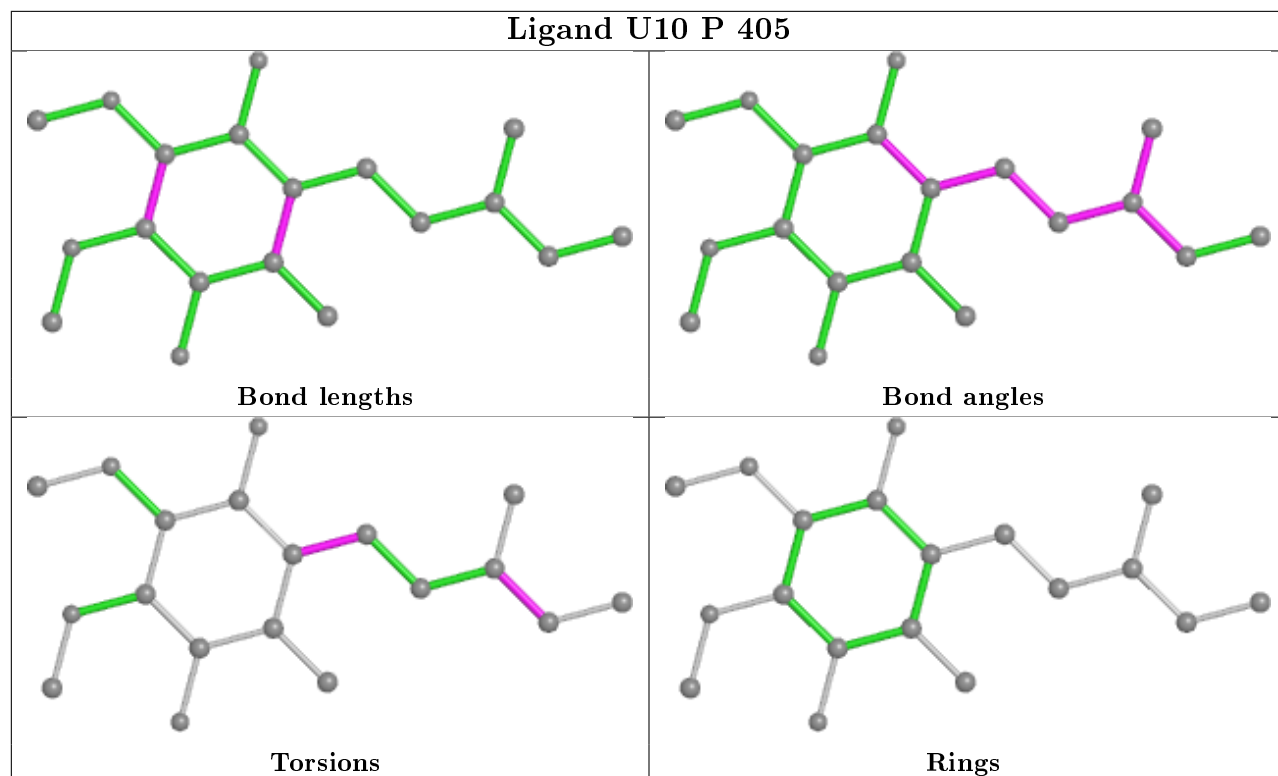
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	E	503	PEE	2	0
11	C	509	PEE	2	0
14	P	405	U10	3	0
11	A	501	PEE	1	0
11	P	401	PEE	1	0
11	R	502	PEE	5	0
11	P	407	PEE	2	0
18	D	502	CDL	1	0
12	C	502	HEM	3	0
12	C	501	HEM	4	0
16	P	408	GOL	1	0
19	P	406	BOG	3	0
18	T	101	CDL	3	0
13	C	503	Y52	2	0
11	P	409	PEE	3	0
18	G	101	CDL	1	0
16	C	508	GOL	1	0
13	P	404	Y52	1	0
14	C	504	U10	1	0
11	P	411	PEE	1	0
12	P	402	HEM	5	0
12	P	403	HEM	3	0
11	E	502	PEE	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

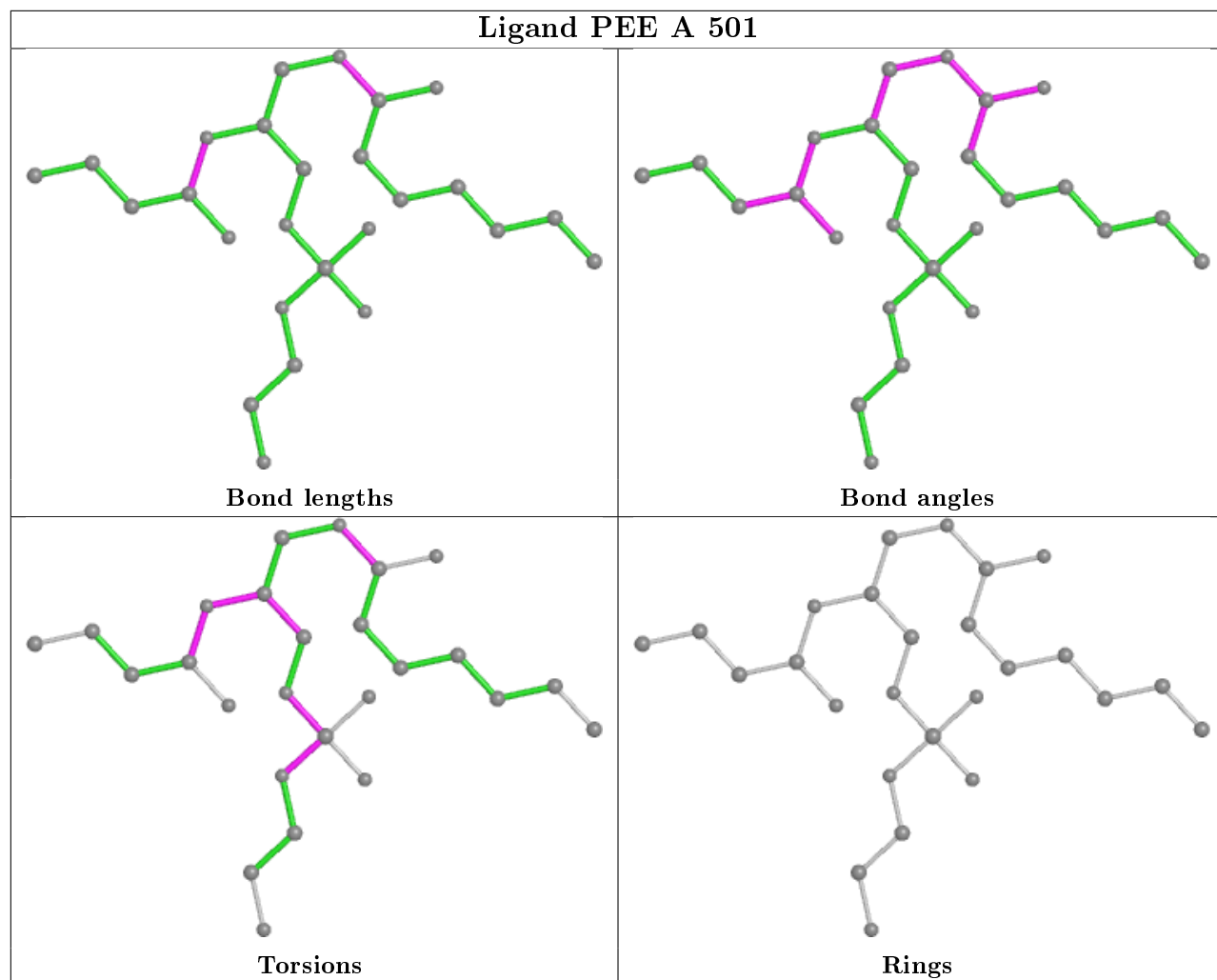
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



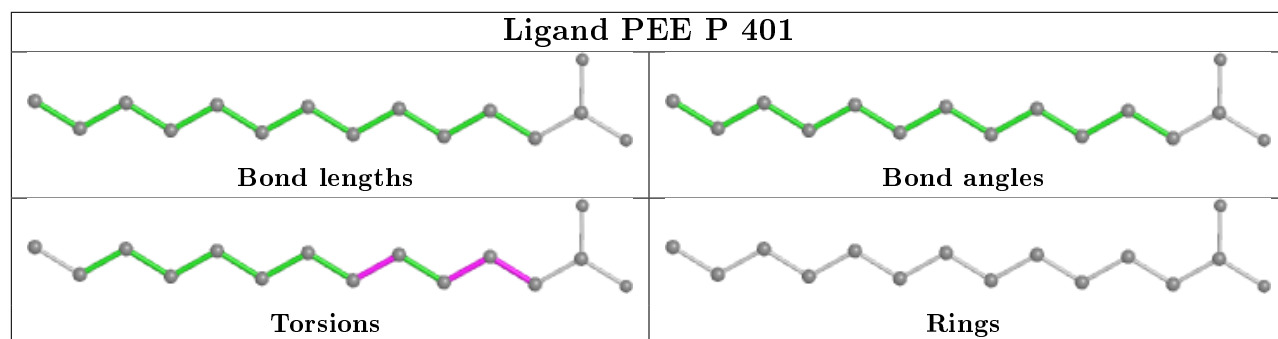




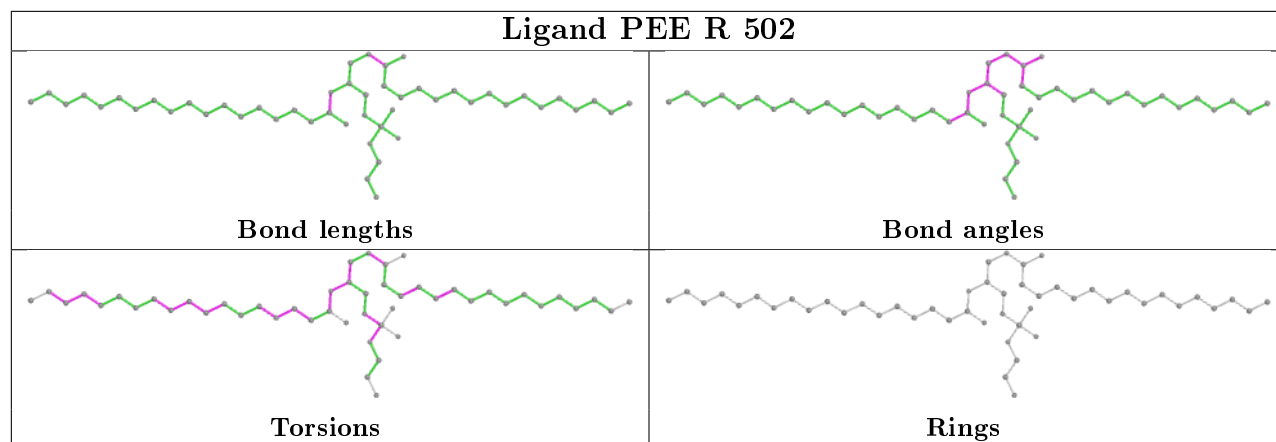
Ligand PEE A 501



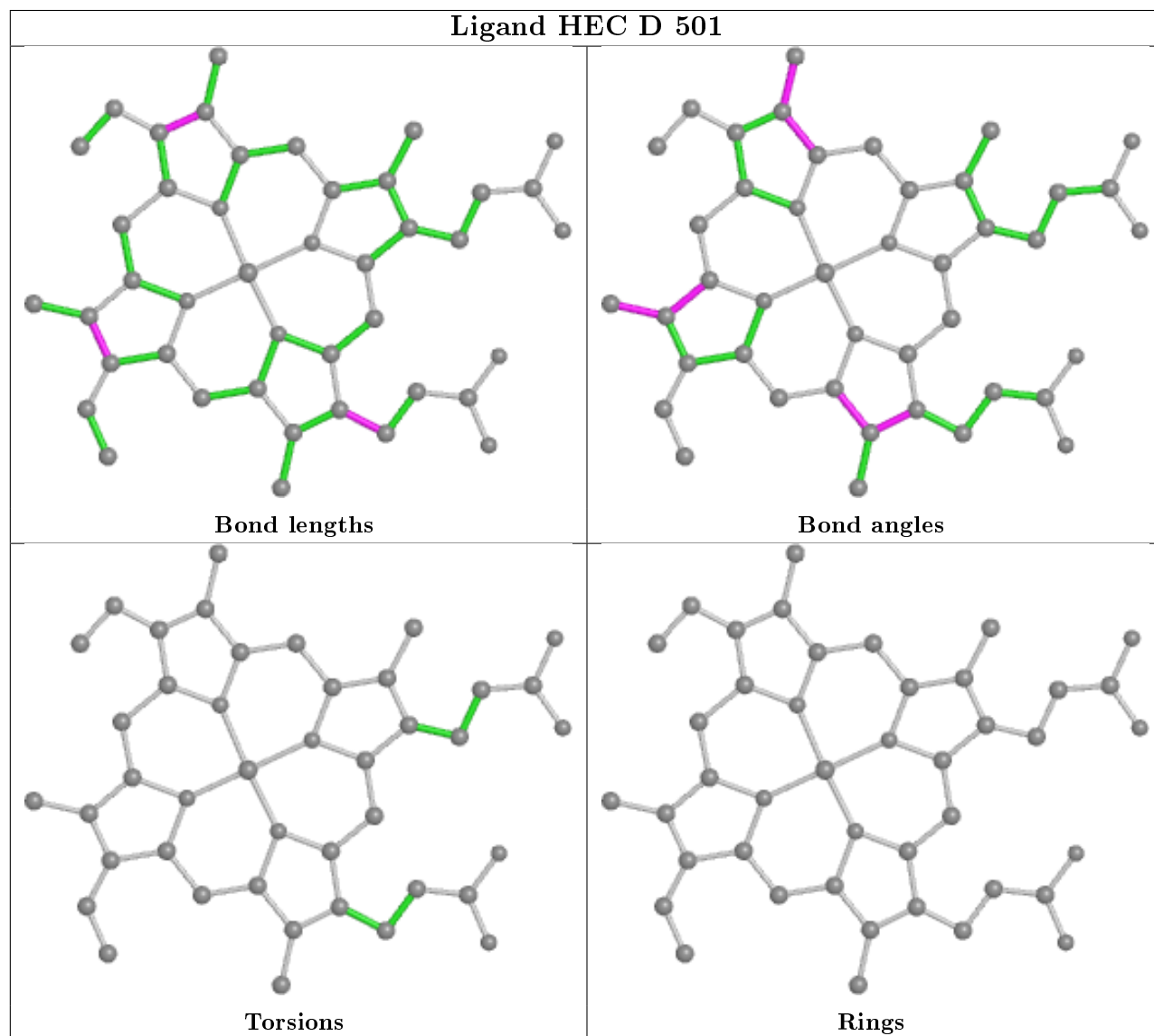
Ligand PEE P 401



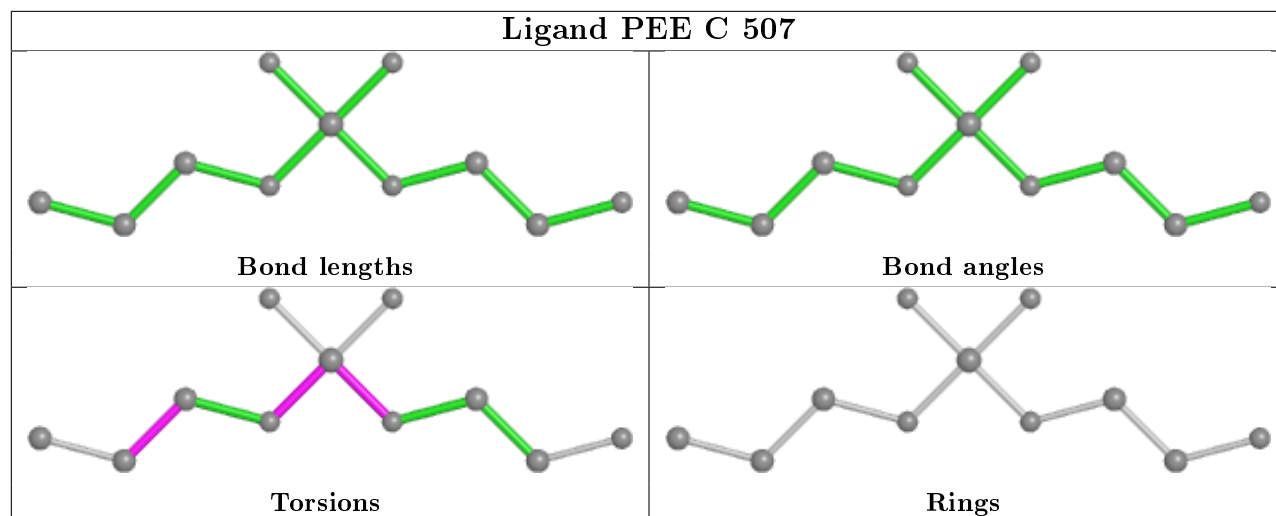
Ligand PEE R 502



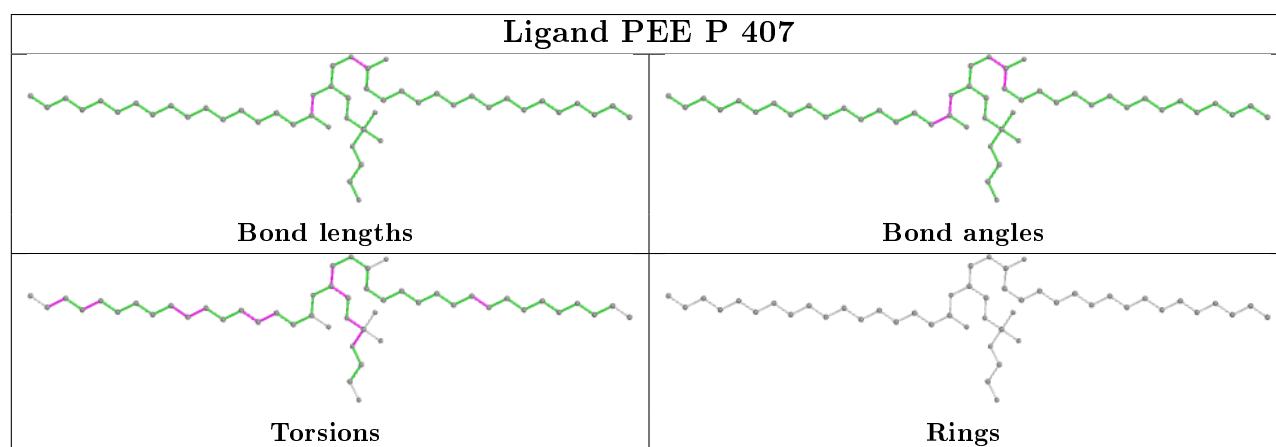
Ligand HEC D 501



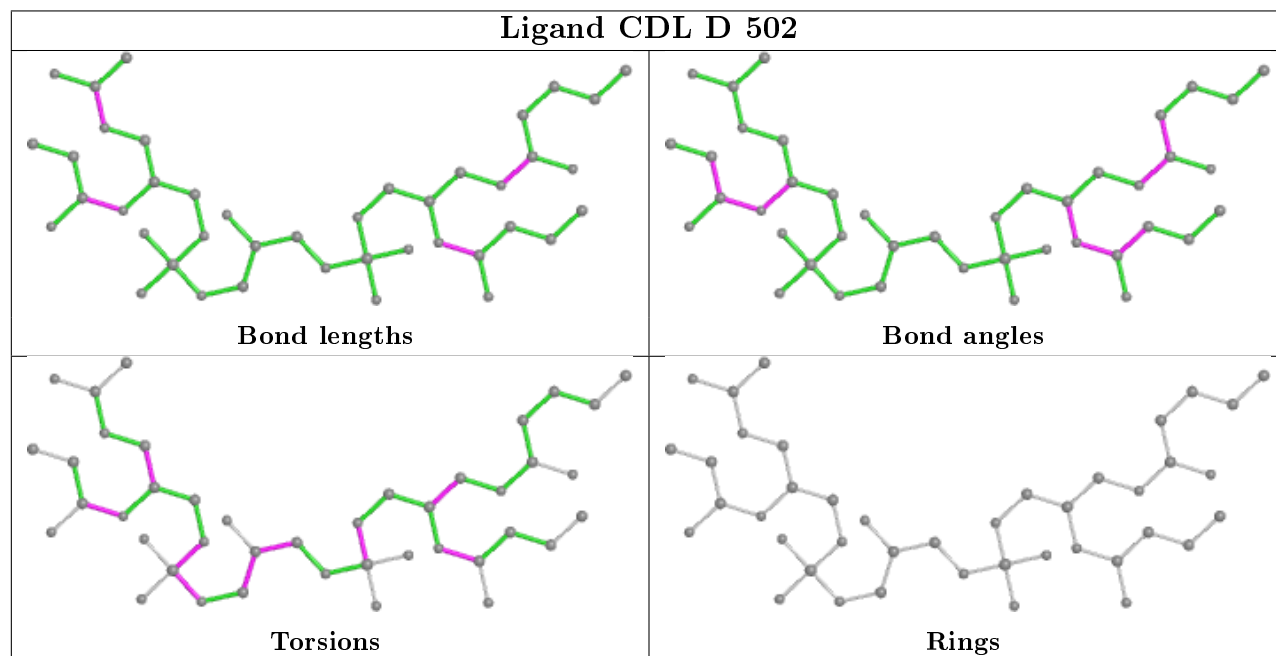
Ligand PEE C 507

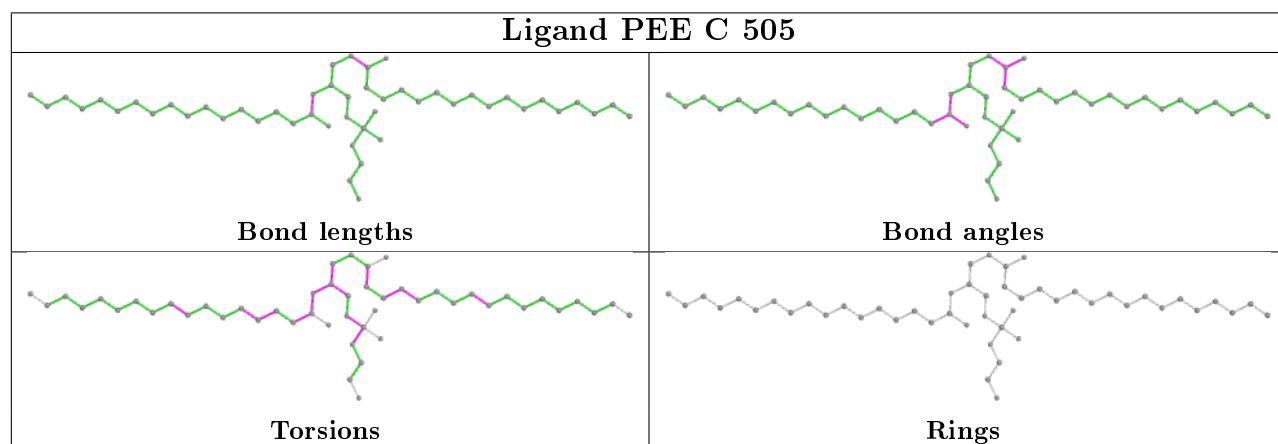
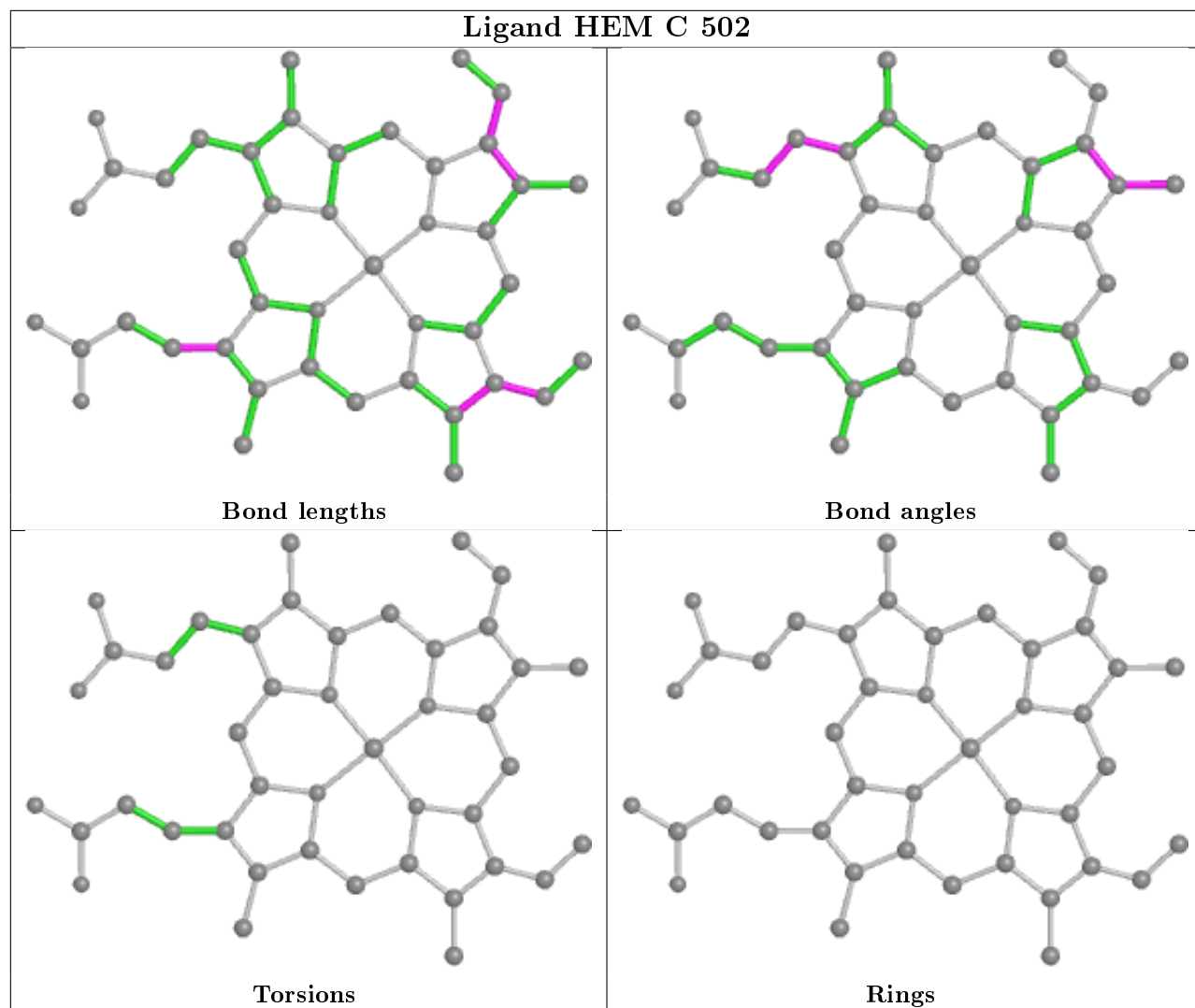


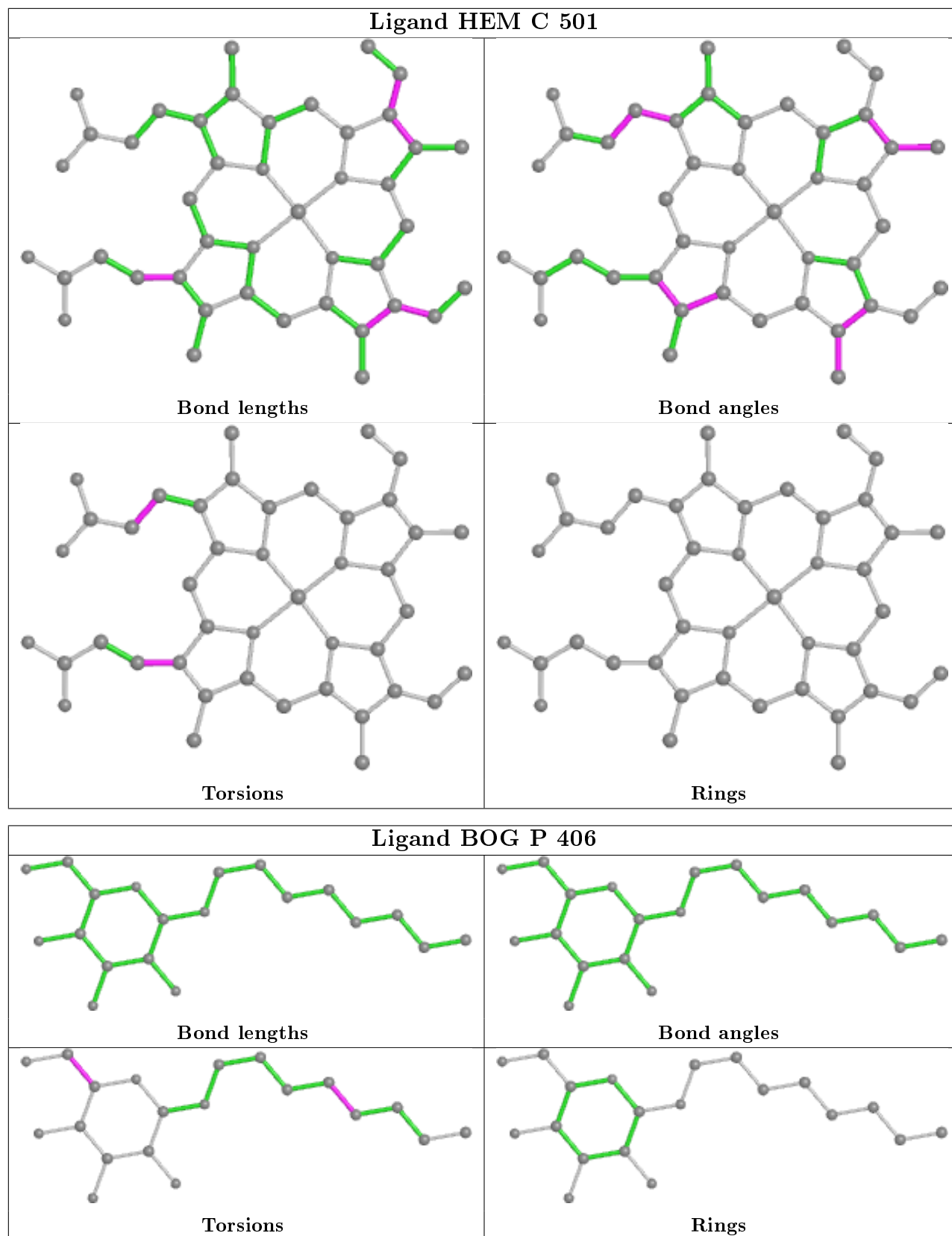
Ligand PEE P 407



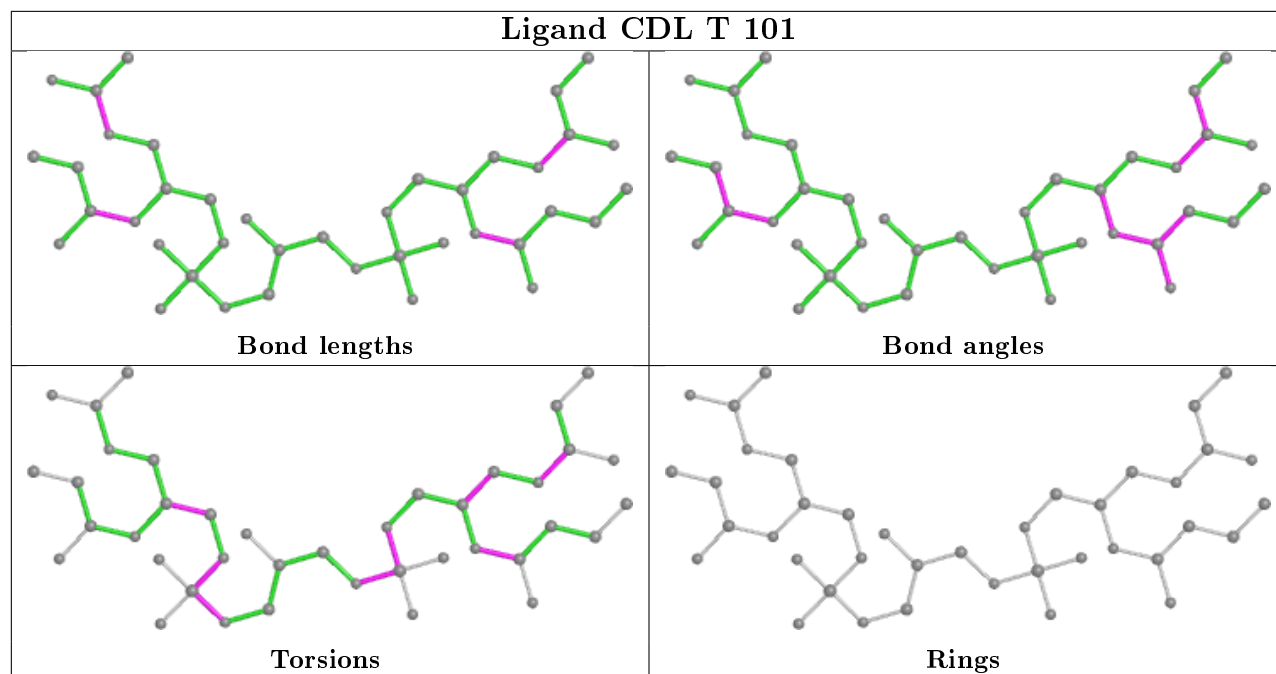
Ligand CDL D 502



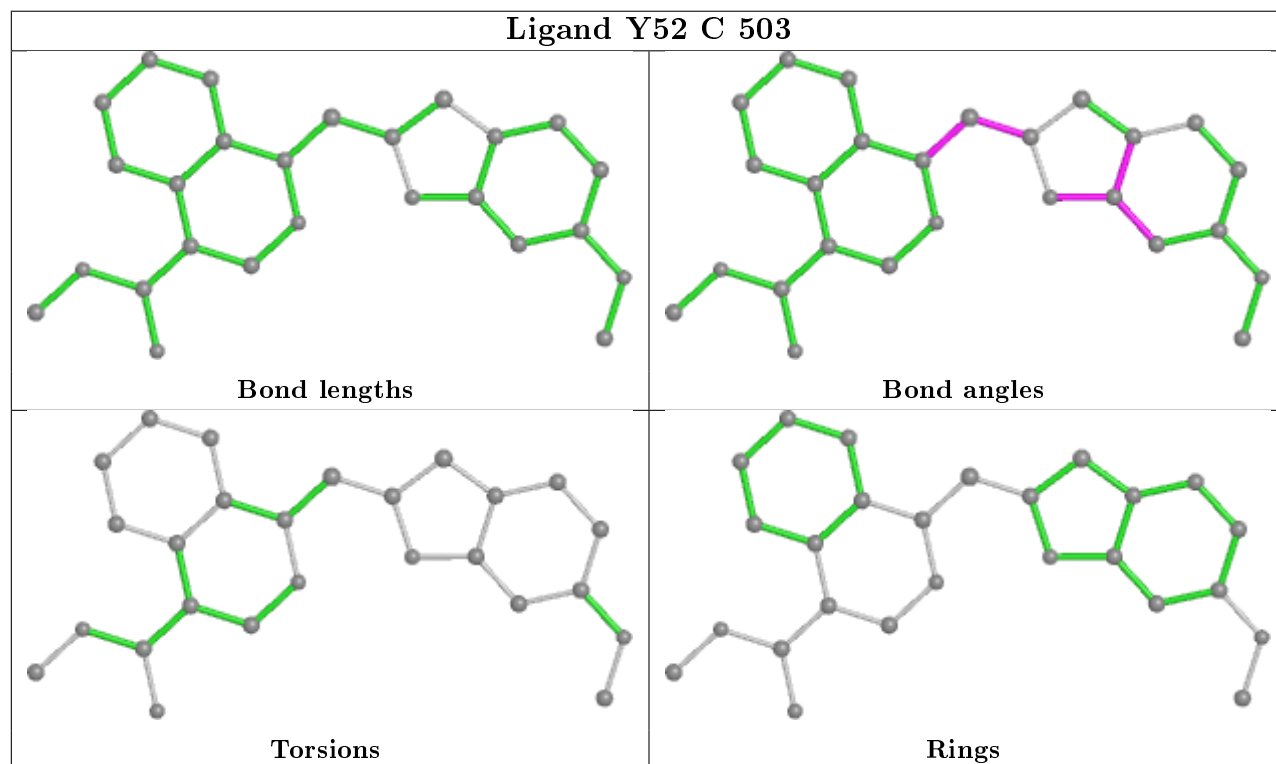


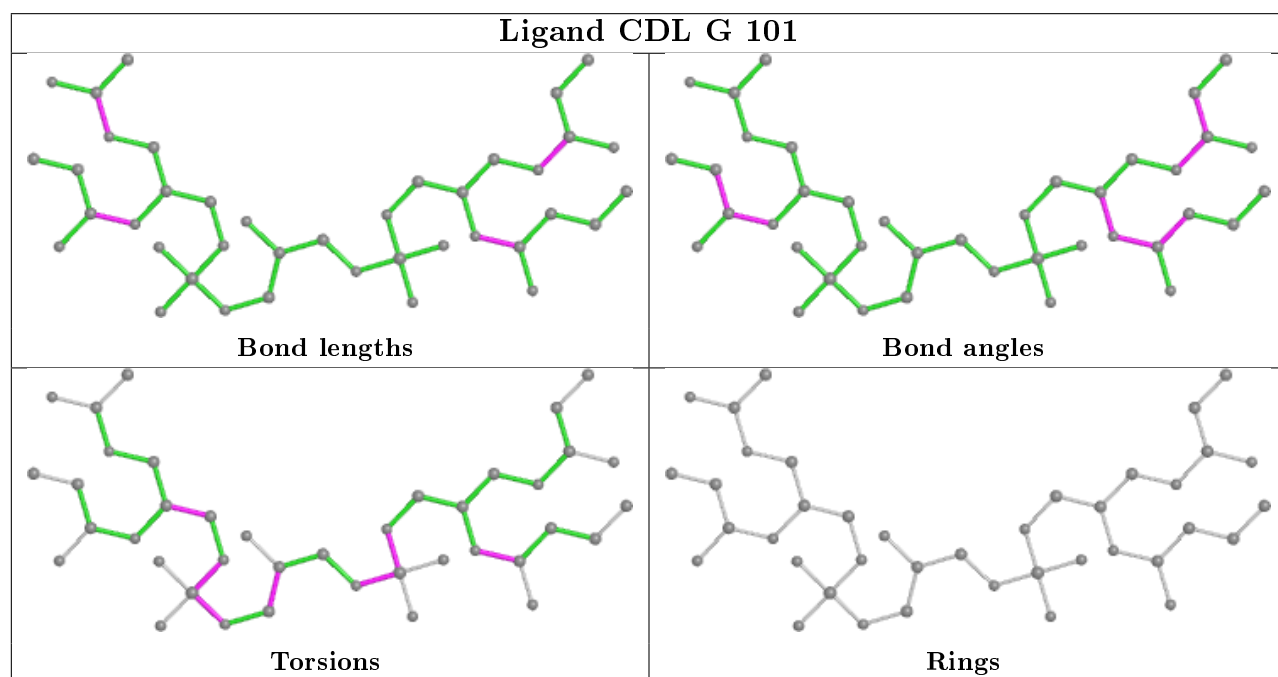
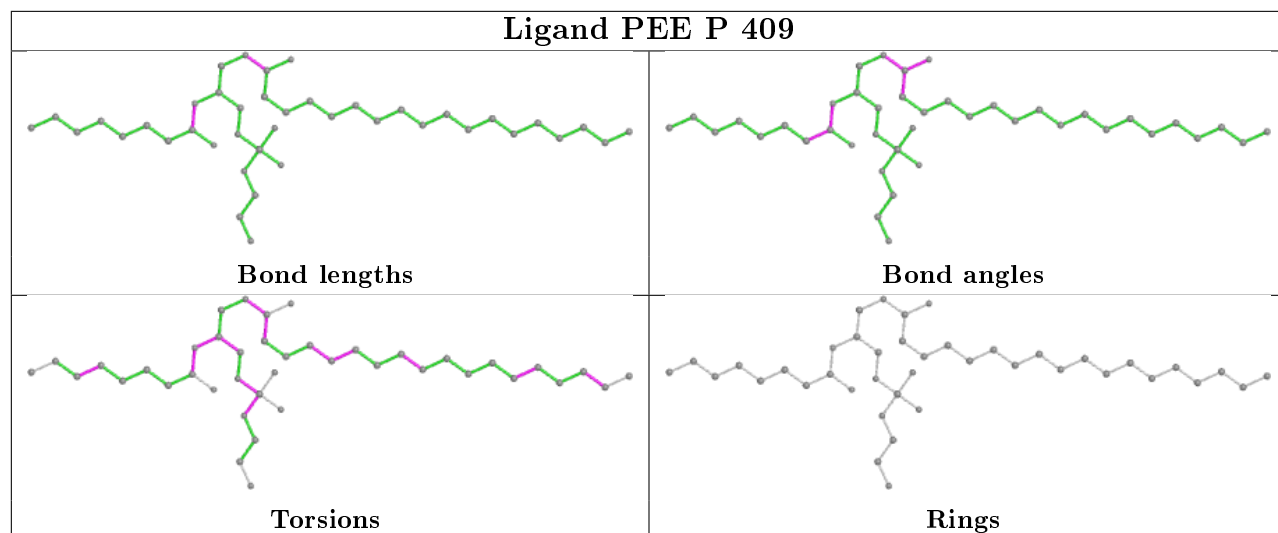


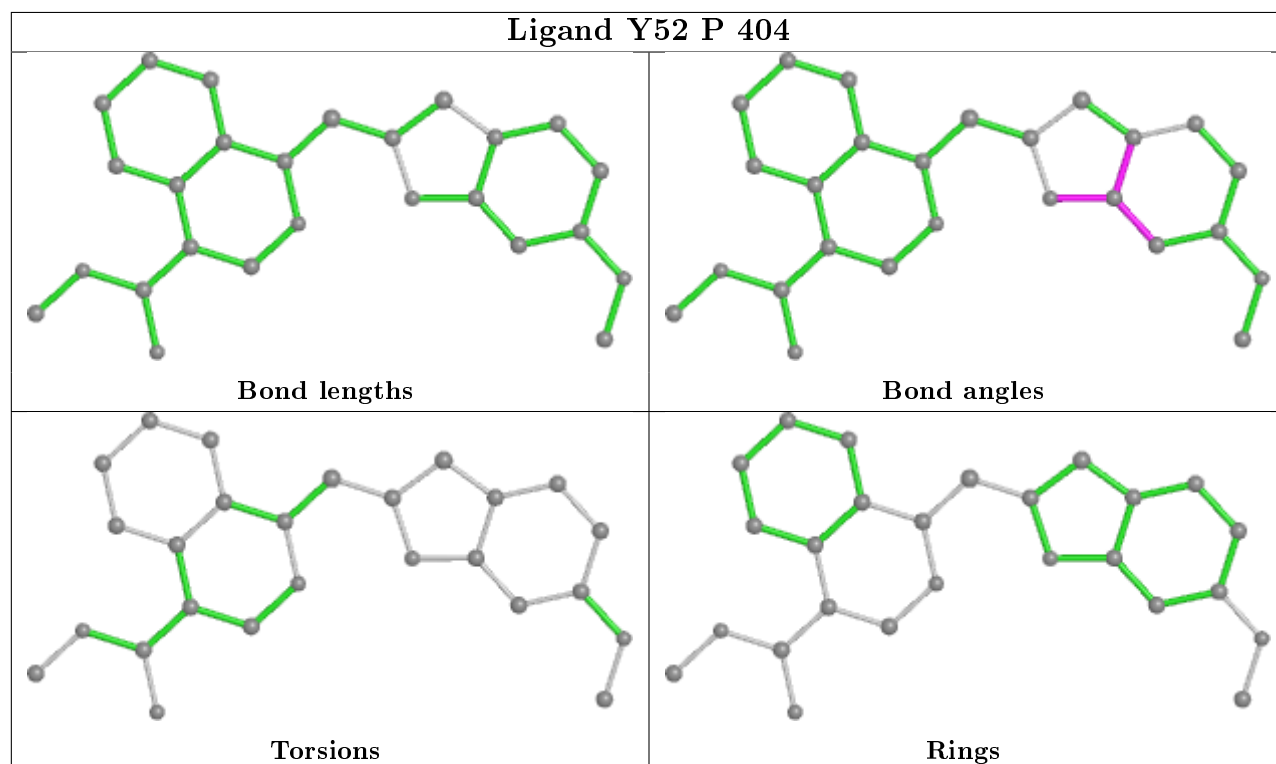
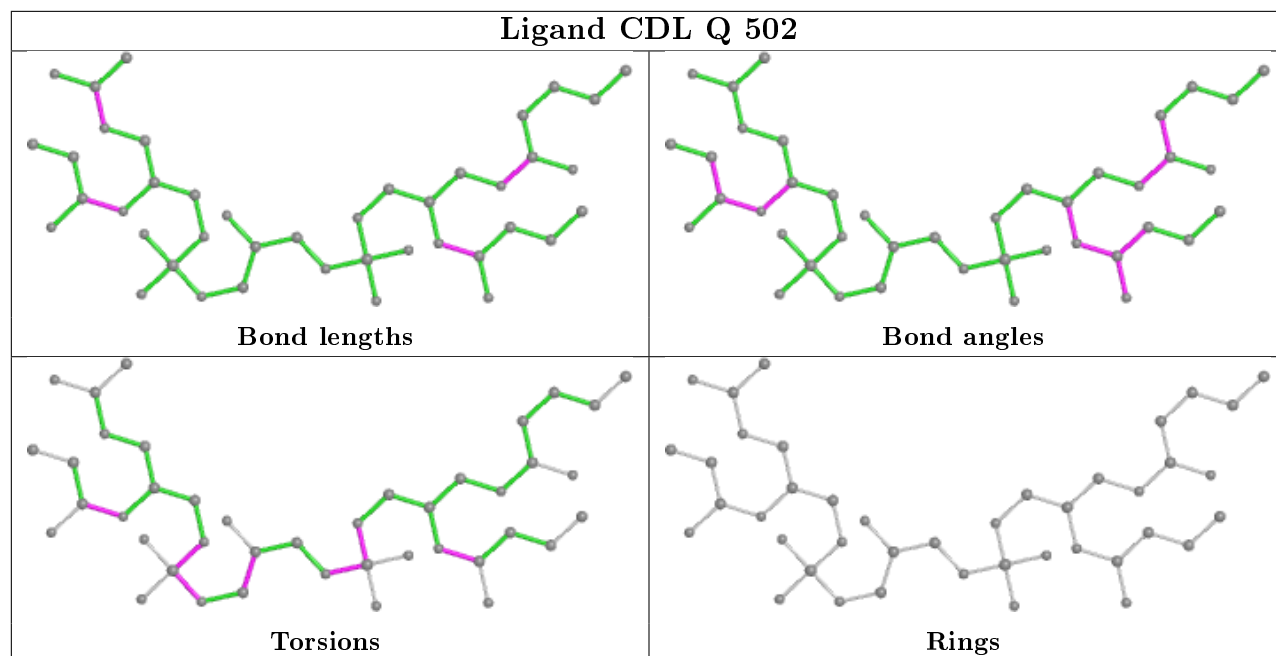
Ligand CDL T 101

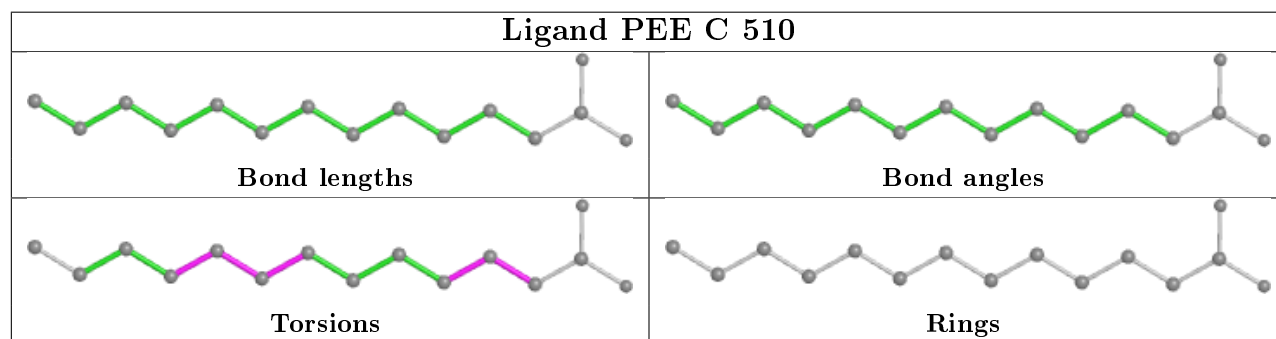
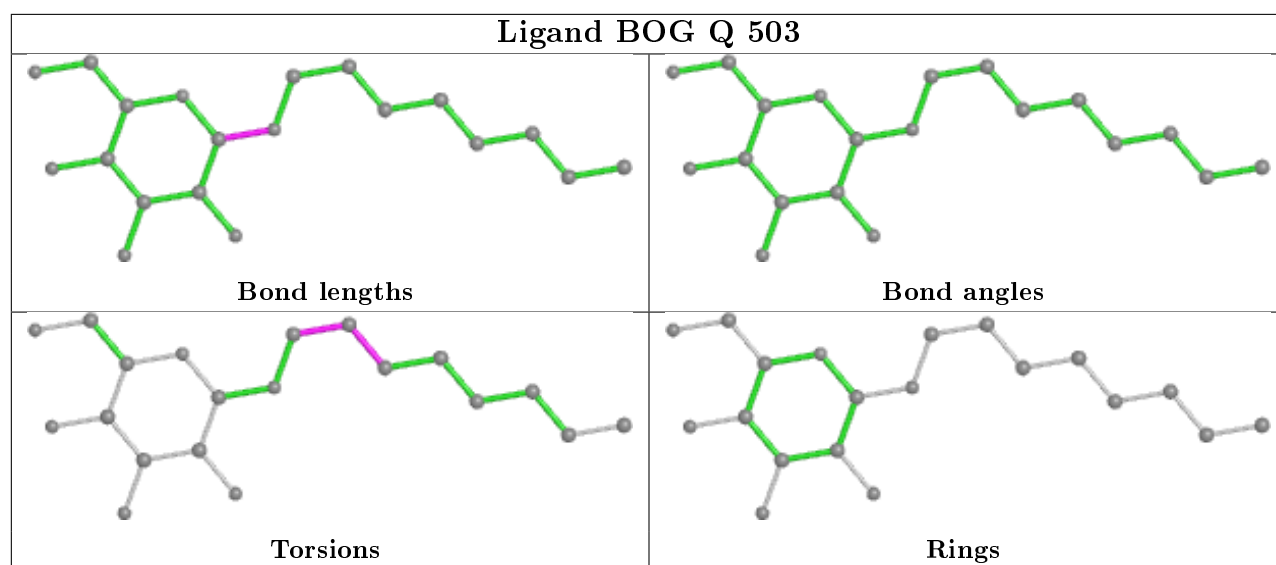
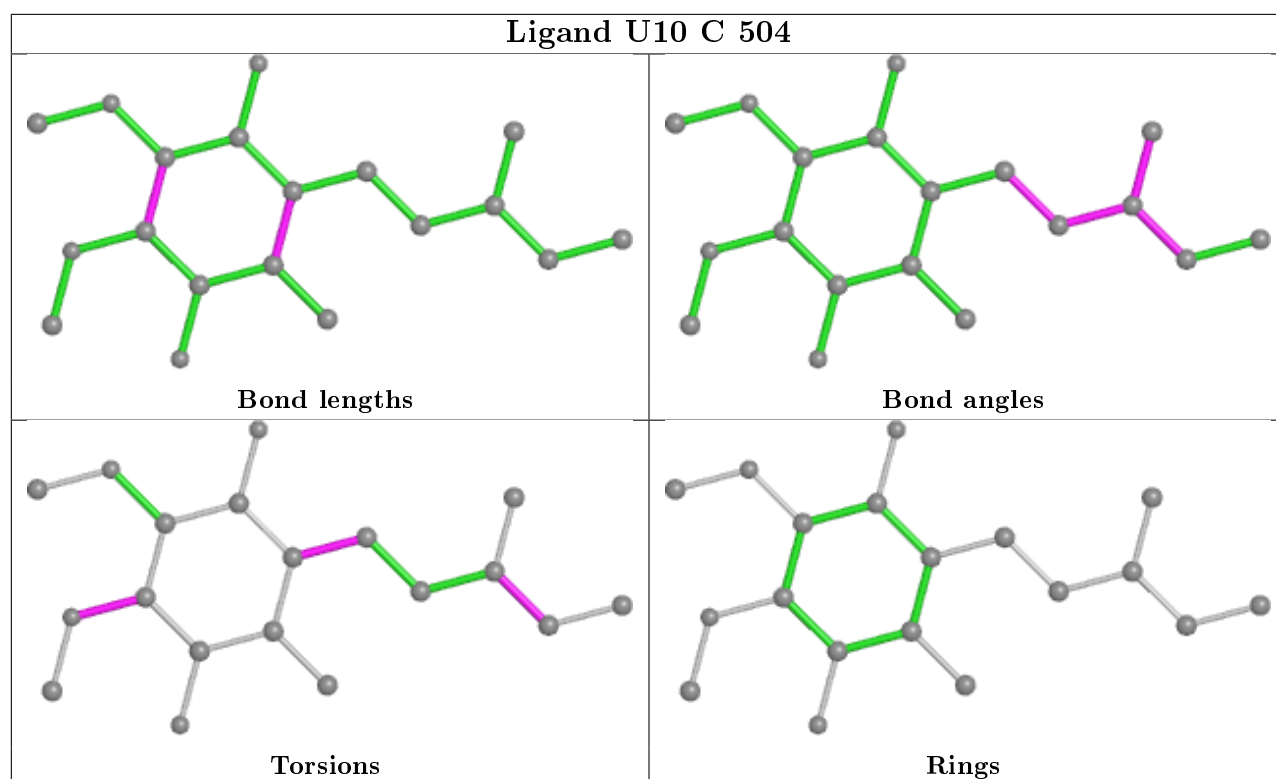


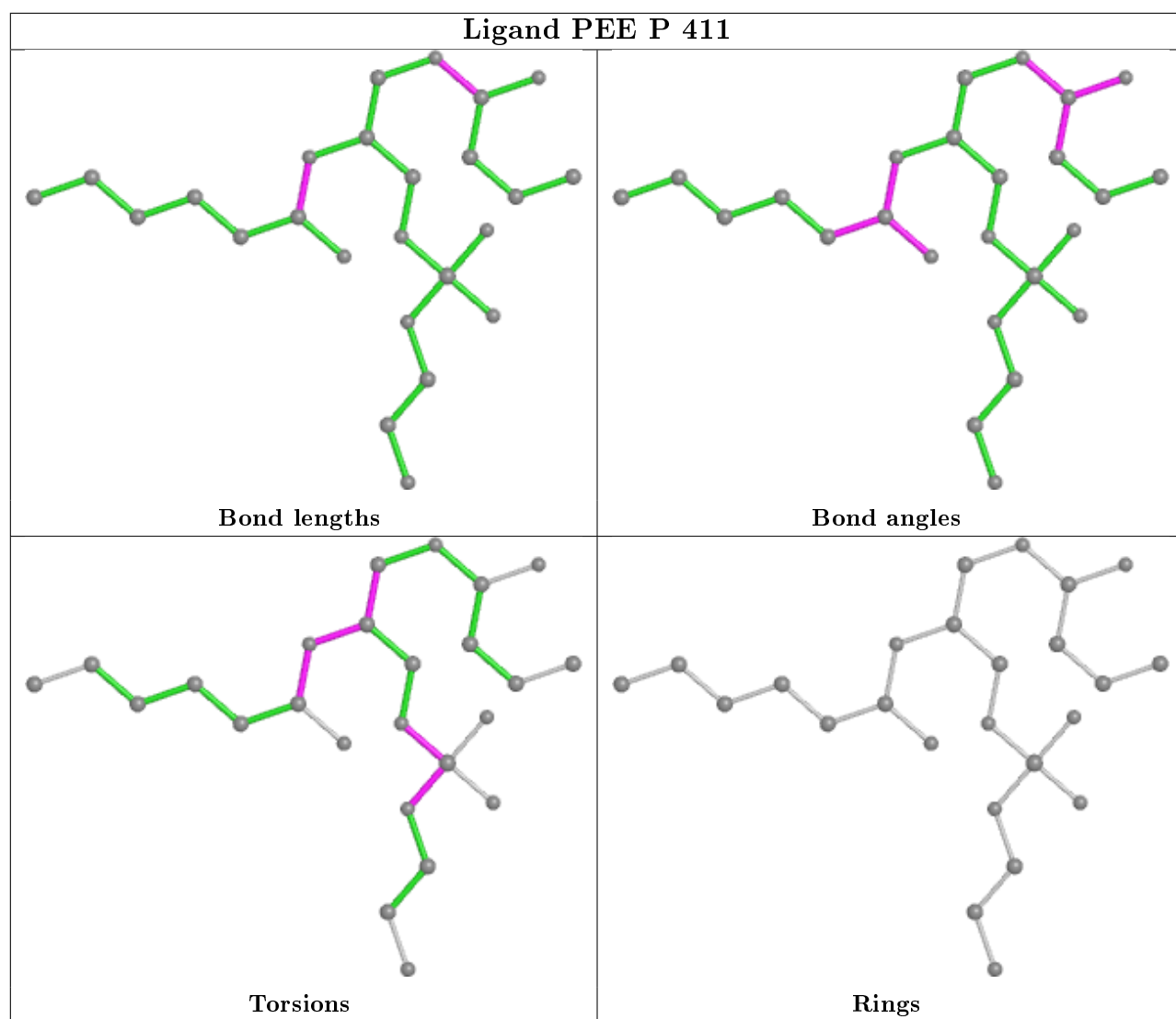
Ligand Y52 C 503

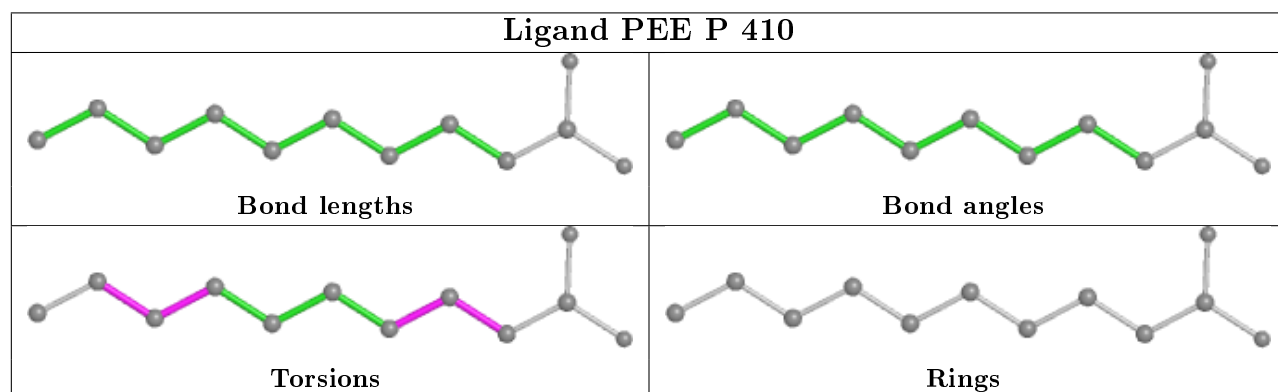
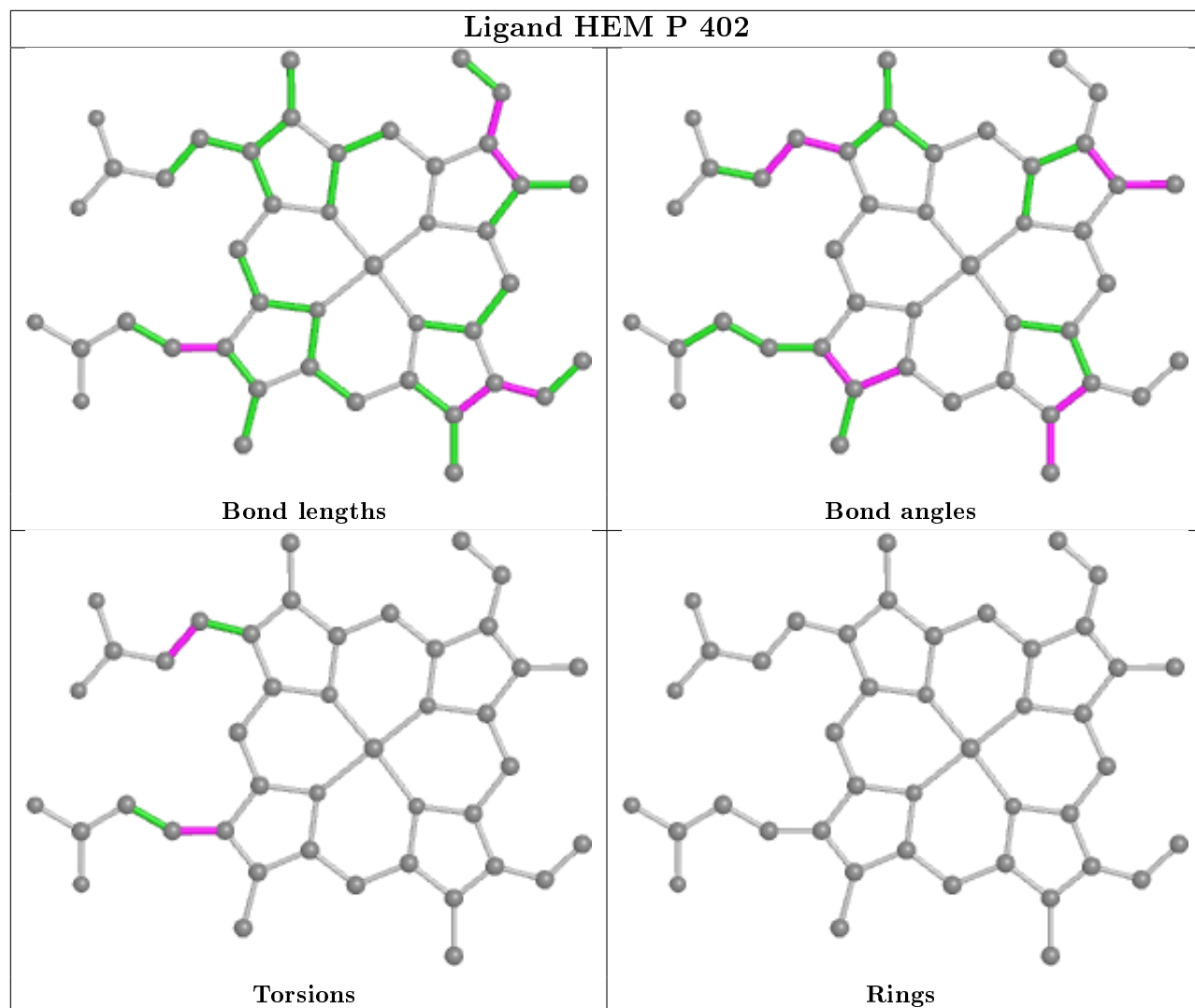


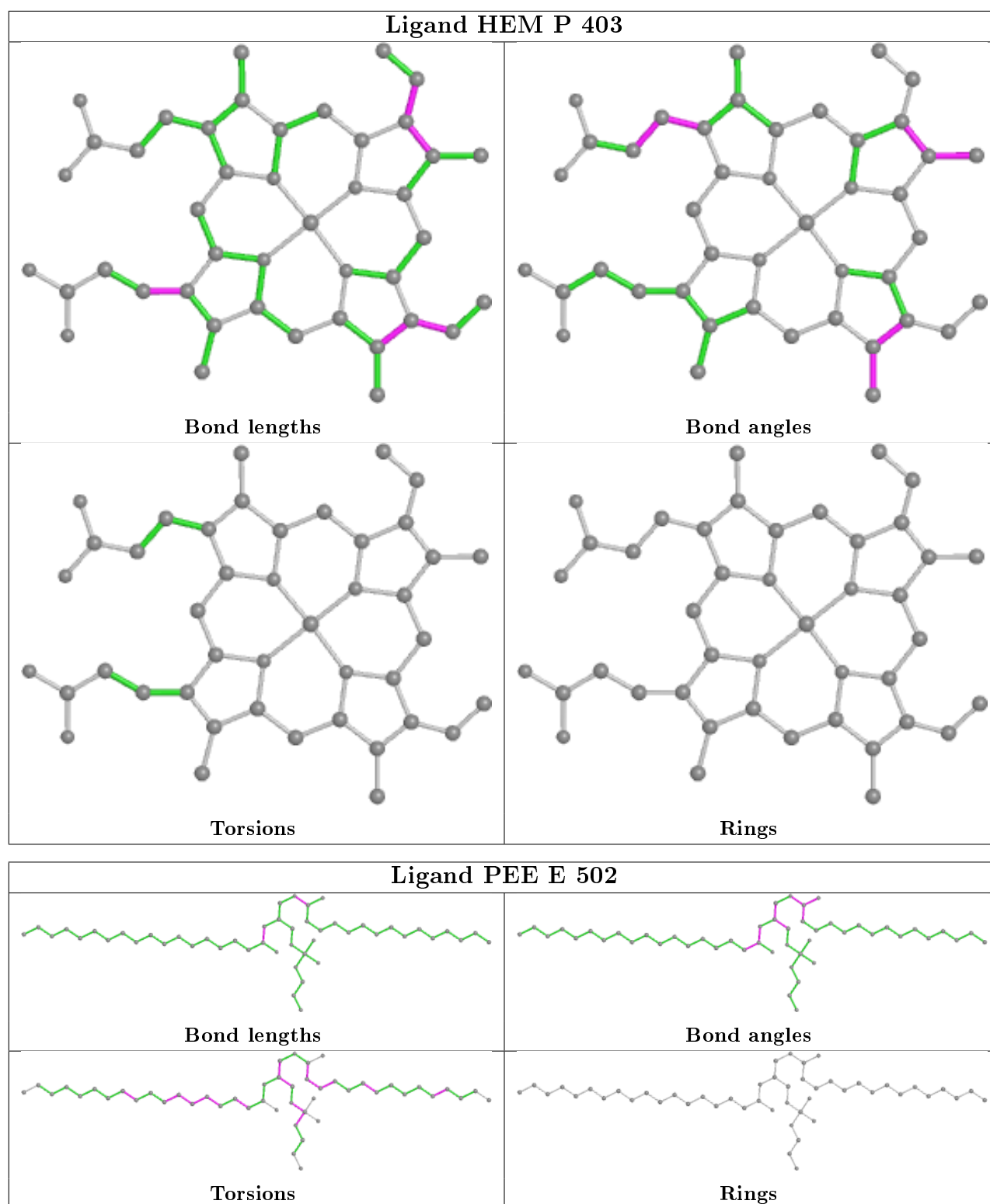












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	443/446 (99%)	0.05	8 (1%) 68 58	28, 53, 78, 101	0
1	N	442/446 (99%)	0.15	9 (2%) 65 54	36, 57, 81, 99	0
2	B	421/441 (95%)	0.24	7 (1%) 70 60	47, 67, 102, 123	0
2	O	422/441 (95%)	0.17	8 (1%) 66 57	35, 63, 86, 104	0
3	C	379/380 (99%)	-0.17	4 (1%) 80 73	22, 33, 70, 102	0
3	P	379/380 (99%)	0.03	2 (0%) 91 87	27, 51, 78, 104	0
4	D	241/241 (100%)	-0.14	3 (1%) 79 70	25, 37, 73, 95	0
4	Q	241/241 (100%)	0.14	5 (2%) 63 53	39, 59, 85, 117	0
5	E	196/196 (100%)	1.61	75 (38%) 0 0	28, 114, 166, 182	9 (4%)
5	R	196/196 (100%)	1.00	41 (20%) 1 1	36, 81, 131, 141	8 (4%)
6	F	101/110 (91%)	-0.17	0 100 100	25, 37, 53, 78	0
6	S	101/110 (91%)	0.22	2 (1%) 65 54	46, 59, 86, 102	0
7	G	80/81 (98%)	0.18	1 (1%) 77 68	28, 45, 73, 89	0
7	T	79/81 (97%)	0.65	9 (11%) 5 4	40, 70, 122, 127	0
8	H	68/77 (88%)	0.14	1 (1%) 73 64	35, 50, 68, 101	0
8	U	68/77 (88%)	1.45	20 (29%) 0 0	66, 91, 113, 117	0
9	I	30/76 (39%)	1.01	7 (23%) 0 1	55, 77, 116, 120	0
9	V	30/76 (39%)	1.22	7 (23%) 0 1	47, 78, 119, 130	0
10	J	61/61 (100%)	0.81	6 (9%) 7 6	34, 46, 79, 129	0
10	W	60/61 (98%)	0.74	3 (5%) 28 18	41, 55, 92, 117	0
All	All	4038/4218 (95%)	0.26	218 (5%) 25 16	22, 56, 107, 182	17 (0%)

All (218) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	E	163	SER	14.2
5	R	163	SER	7.5
5	E	162	GLY	7.4
10	J	62	SER	7.2
5	E	172	ARG	6.6
5	E	115	SER	6.6
5	E	82	PRO	6.3
10	J	64	GLU	6.2
5	E	84	GLY	6.0
5	E	120	PRO	5.9
5	E	121	GLN	5.6
5	R	102	THR	5.6
5	E	85	LYS	5.5
5	E	157	TYR	5.3
5	E	102	THR	5.3
9	I	51	CYS	5.2
5	R	125	ASP	5.1
5	E	83	GLU	5.1
5	R	114	VAL	5.0
5	E	117	LEU	5.0
9	V	57	GLY	5.0
9	V	51	CYS	5.0
5	E	171	ILE	4.9
5	E	104	ALA	4.8
5	E	107	ASN	4.7
5	E	176	ALA	4.7
5	E	106	ILE	4.6
5	R	117	LEU	4.4
5	E	103	GLN	4.4
5	E	174	GLY	4.2
5	R	157	TYR	4.2
5	E	150	SER	4.2
5	E	114	VAL	4.2
5	R	165	TYR	4.1
8	U	50	THR	4.0
8	U	44	VAL	4.0
5	R	120	PRO	4.0
5	E	173	LYS	4.0
5	E	116	LYS	3.9
5	E	126	ARG	3.8
10	J	63	GLU	3.8
8	U	13	LEU	3.8
5	E	164	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
5	E	119	ASP	3.8
3	P	156	TYR	3.8
5	E	123	ASP	3.8
5	E	112	VAL	3.7
5	E	152	ASP	3.7
8	U	39	LEU	3.7
5	R	171	ILE	3.7
7	T	77	TYR	3.7
5	E	99	ARG	3.7
5	E	179	ASN	3.7
1	A	218	GLY	3.6
5	E	113	ASP	3.6
5	E	178	TYR	3.6
9	I	57	GLY	3.6
5	R	162	GLY	3.6
5	E	167	ALA	3.6
5	E	140	THR	3.6
5	E	118	ARG	3.5
5	E	175	PRO	3.5
5	R	113	ASP	3.5
5	R	164	HIS	3.5
5	E	125	ASP	3.5
1	N	217	SER	3.5
5	E	146	PRO	3.5
10	J	61	ALA	3.4
5	R	177	PRO	3.4
5	E	168	SER	3.4
5	E	149	ASN	3.4
3	C	8	SER	3.4
7	T	80	ASP	3.3
5	E	165	TYR	3.3
5	R	115	SER	3.3
5	R	124	LEU	3.3
1	A	217	SER	3.3
3	P	371	GLY	3.3
5	E	151	GLY	3.3
5	E	79	SER	3.2
5	E	158	CYS	3.2
5	R	119	ASP	3.2
8	U	46	SER	3.2
9	I	52	ARG	3.2
9	V	50	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
5	R	122	HIS	3.2
5	E	187	PHE	3.1
5	E	156	TYR	3.1
5	E	81	ILE	3.1
9	I	53	GLU	3.1
6	S	13	MET	3.0
5	R	156	TYR	3.0
5	E	191	ASP	3.0
5	R	170	ARG	3.0
5	R	158	CYS	3.0
8	U	35	GLU	3.0
5	E	108	GLN	3.0
5	R	112	VAL	3.0
5	R	155	GLY	3.0
5	R	84	GLY	3.0
2	B	31	ASN	3.0
8	U	37	LEU	3.0
5	E	177	PRO	3.0
9	V	48	PRO	3.0
5	E	190	ASP	2.9
9	V	54	SER	2.9
9	V	52	ARG	2.9
5	R	127	VAL	2.9
5	R	140	THR	2.9
5	R	172	ARG	2.9
2	B	230	ALA	2.9
2	B	226	ILE	2.9
5	E	185	TYR	2.9
5	E	122	HIS	2.9
5	R	105	GLU	2.8
8	U	41	ASP	2.8
2	B	227	ARG	2.8
1	N	68	LYS	2.8
2	B	229	GLY	2.8
8	U	52	GLU	2.8
8	U	28	GLU	2.7
9	I	54	SER	2.7
2	O	355	GLU	2.7
5	E	184	THR	2.7
5	E	105	GLU	2.7
7	T	78	GLU	2.7
10	W	4	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
5	E	76	ILE	2.7
8	U	45	SER	2.6
5	E	100	HIS	2.6
5	E	109	GLU	2.6
4	D	80	LEU	2.6
5	E	192	LEU	2.6
5	R	118	ARG	2.6
5	R	82	PRO	2.6
5	E	148	ALA	2.6
10	J	33	ARG	2.6
5	R	174	GLY	2.6
5	R	167	ALA	2.5
5	E	132	TRP	2.5
1	N	66	GLY	2.5
5	E	86	ASN	2.5
5	E	101	ARG	2.5
6	S	11	ARG	2.5
5	E	153	PHE	2.5
1	N	69	LYS	2.5
5	R	152	ASP	2.5
5	E	141	HIS	2.5
1	N	71	PRO	2.4
5	E	124	LEU	2.4
9	I	48	PRO	2.4
5	R	85	LYS	2.4
4	Q	1	GLY	2.4
1	N	178	THR	2.4
8	U	11	GLU	2.4
10	W	60	GLU	2.4
2	O	296	TYR	2.4
9	V	49	LEU	2.4
5	E	154	GLY	2.4
8	U	40	CYS	2.4
1	A	219	VAL	2.3
7	T	74	PRO	2.3
8	U	49	HIS	2.3
1	A	226	ASP	2.3
10	W	63	GLU	2.3
1	A	4	TYR	2.3
4	Q	81	PHE	2.3
5	R	100	HIS	2.3
4	D	79	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
7	G	80	ASP	2.3
3	C	285	ILE	2.3
1	A	223	TYR	2.3
5	R	176	ALA	2.3
1	A	69	LYS	2.2
1	N	404	ALA	2.2
5	E	194	VAL	2.2
5	E	143	GLY	2.2
1	A	222	THR	2.2
8	U	23	HIS	2.2
4	Q	82	MET	2.2
5	R	83	GLU	2.2
2	O	19	PRO	2.2
3	C	156	TYR	2.2
4	Q	77	ASN	2.2
5	R	187	PHE	2.2
5	R	109	GLU	2.2
8	H	11	GLU	2.2
8	U	43	ARG	2.2
5	E	110	ALA	2.2
2	O	350	GLY	2.2
7	T	2	ILE	2.2
5	R	143	GLY	2.2
1	N	204	SER	2.2
5	E	111	GLU	2.2
8	U	12	GLU	2.2
8	U	33	ALA	2.1
2	O	222	GLN	2.1
2	O	349	GLN	2.1
5	R	121	GLN	2.1
7	T	68	ARG	2.1
7	T	75	ALA	2.1
7	T	79	ASN	2.1
2	O	218	GLN	2.1
5	E	186	GLN	2.1
1	N	67	THR	2.1
5	E	188	VAL	2.1
10	J	60	GLU	2.1
8	U	27	THR	2.1
9	I	56	SER	2.1
4	D	78	GLY	2.1
8	U	26	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
5	R	103	GLN	2.1
4	Q	79	GLU	2.1
2	B	228	SER	2.1
2	O	200	THR	2.0
3	C	155	PRO	2.0
7	T	66	PHE	2.0
2	B	80	ALA	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FME	C	1	9/11	0.70	0.41	72,88,96,99	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	PEE	N	501	8/51	0.72	0.28	57,79,96,112	0
11	PEE	A	501	26/51	0.72	0.33	27,87,106,123	0
11	PEE	P	409	41/51	0.72	0.34	54,69,112,128	0
18	CDL	Q	502	42/100	0.73	0.36	40,99,121,136	0
11	PEE	P	411	25/51	0.74	0.41	36,60,75,80	25
11	PEE	C	509	47/51	0.76	0.32	22,48,88,107	0
11	PEE	R	502	49/51	0.76	0.39	33,64,79,88	0
11	PEE	C	507	11/51	0.76	0.38	25,51,62,63	11
11	PEE	P	401	15/51	0.78	0.37	41,58,88,89	0
19	BOG	P	406	20/20	0.79	0.27	39,74,96,98	0

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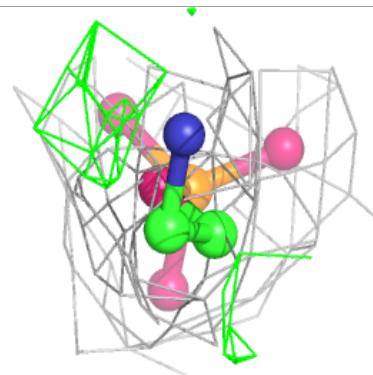
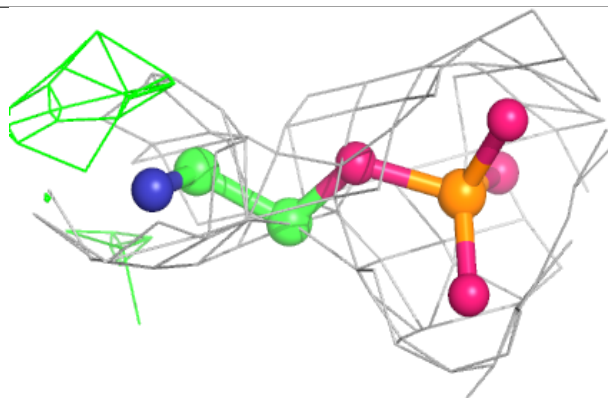
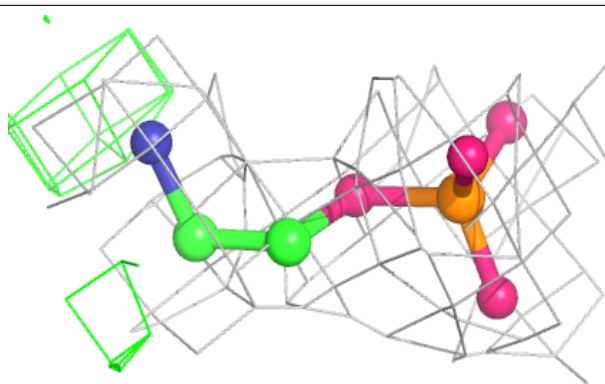
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	U10	P	405	19/63	0.80	0.39	60,75,88,91	0
18	CDL	T	101	40/100	0.81	0.32	44,85,97,98	0
11	PEE	E	503	15/51	0.81	0.33	22,49,63,68	0
11	PEE	E	502	48/51	0.81	0.33	36,55,80,86	0
18	CDL	D	502	42/100	0.83	0.30	46,80,99,127	0
15	MES	C	506	12/12	0.85	0.33	45,69,109,122	0
11	PEE	P	410	12/51	0.86	0.26	30,37,46,47	0
14	U10	C	504	19/63	0.86	0.32	45,59,67,70	0
11	PEE	P	407	49/51	0.86	0.28	45,68,84,89	0
18	CDL	G	101	40/100	0.86	0.27	24,56,69,73	0
11	PEE	C	510	15/51	0.87	0.25	25,54,81,84	0
19	BOG	D	503	20/20	0.88	0.31	29,46,54,57	0
16	GOL	C	508	6/6	0.91	0.24	34,35,38,43	0
11	PEE	C	505	49/51	0.91	0.22	22,43,54,57	0
19	BOG	Q	503	20/20	0.92	0.24	34,54,62,63	0
16	GOL	P	408	6/6	0.93	0.26	42,43,49,51	0
13	Y52	P	404	27/27	0.95	0.22	38,46,58,63	0
12	HEM	C	501	43/43	0.96	0.23	18,24,32,35	0
20	FES	R	501	4/4	0.96	0.13	71,84,92,107	0
17	HEC	D	501	43/43	0.96	0.21	26,34,40,42	0
17	HEC	Q	501	43/43	0.96	0.23	44,51,63,71	0
12	HEM	P	402	43/43	0.96	0.26	26,32,43,53	0
12	HEM	P	403	43/43	0.96	0.25	27,33,50,53	0
13	Y52	C	503	27/27	0.96	0.18	25,33,45,51	0
12	HEM	C	502	43/43	0.97	0.24	19,24,32,37	0
20	FES	E	501	4/4	0.98	0.11	92,103,103,106	4

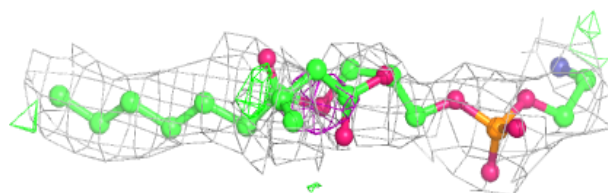
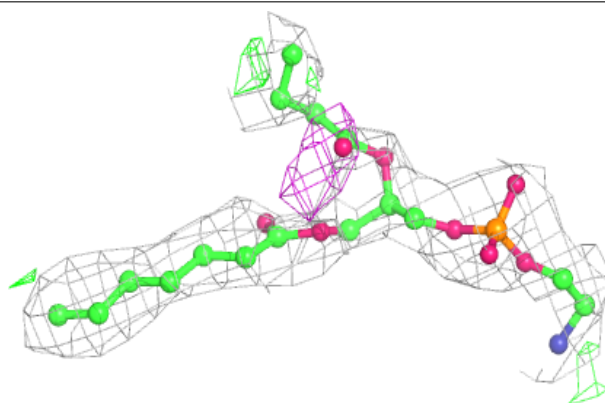
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PEE N 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

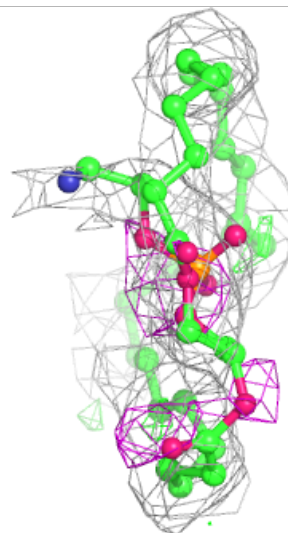
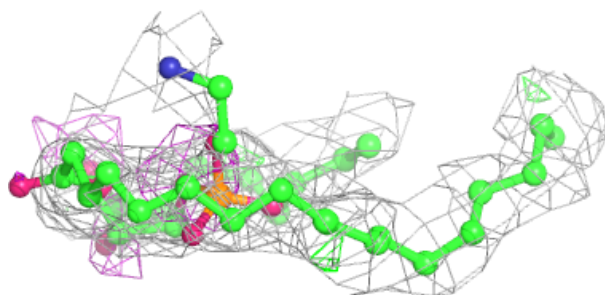
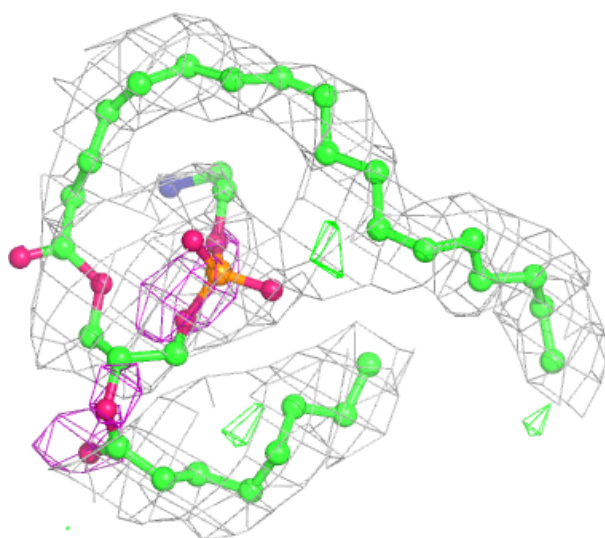
**Electron density around PEE A 501:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



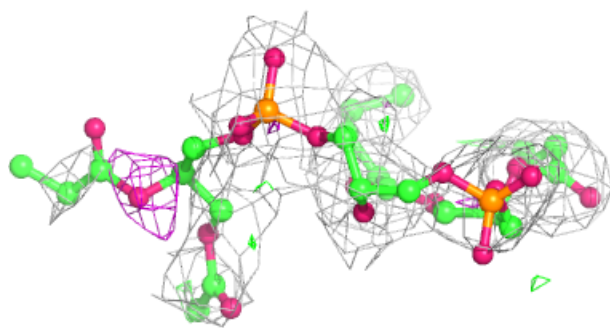
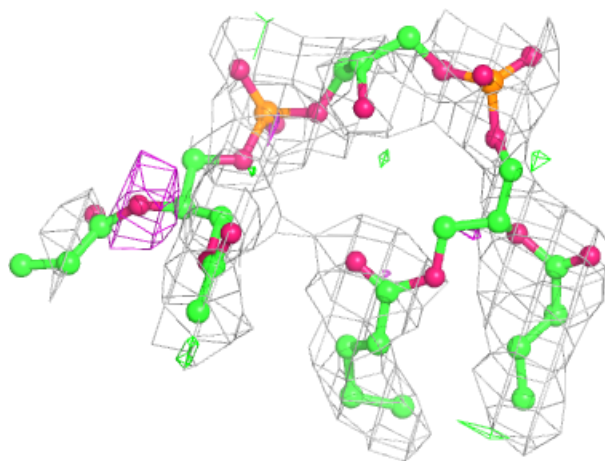
Electron density around PEE P 409:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



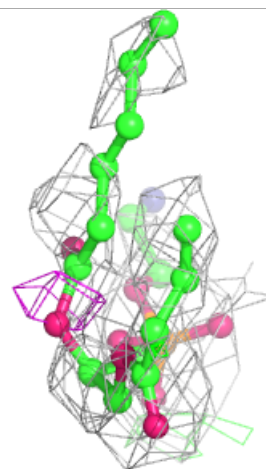
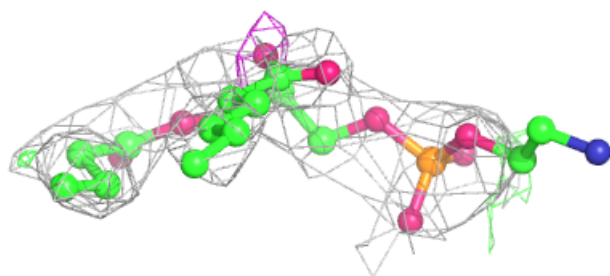
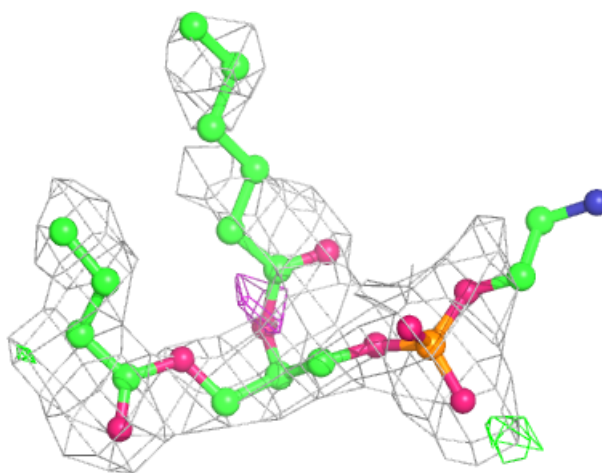
Electron density around CDL Q 502:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



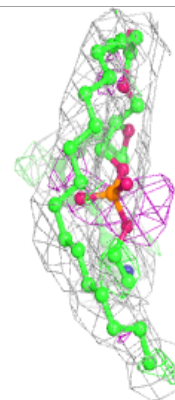
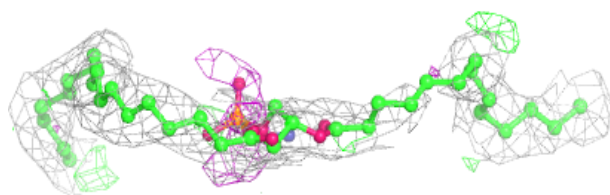
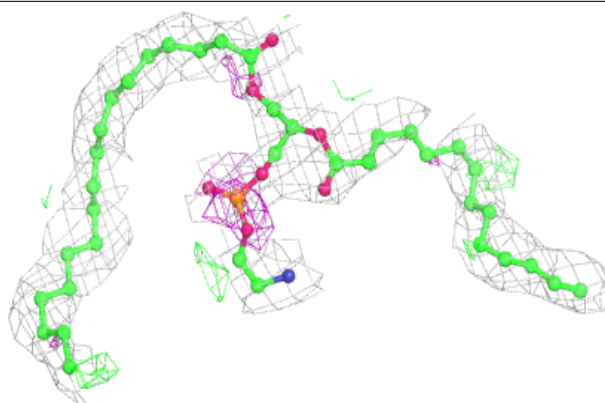
Electron density around PEE P 411:

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and green (positive)

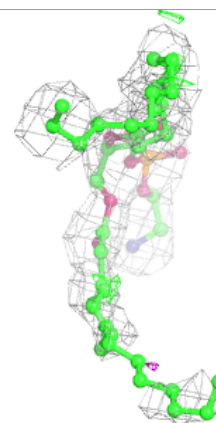
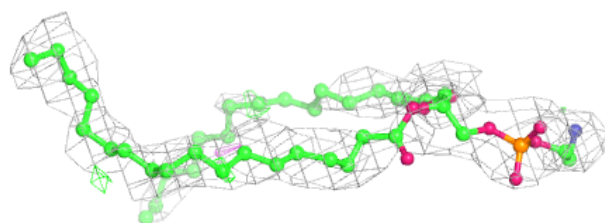
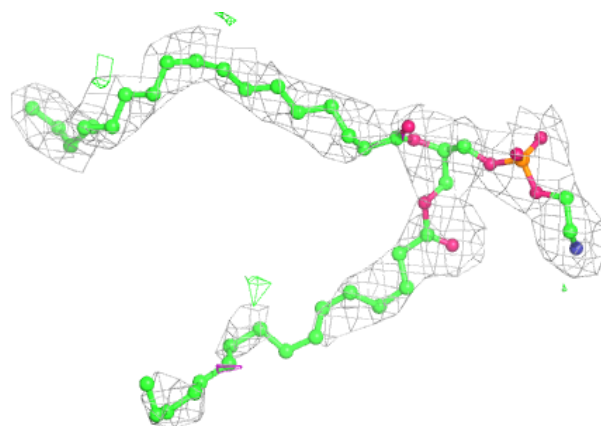


Electron density around PEE C 509:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

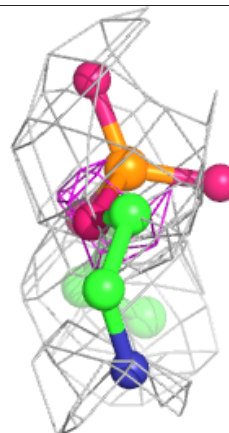
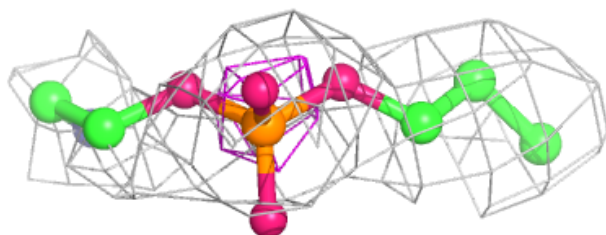
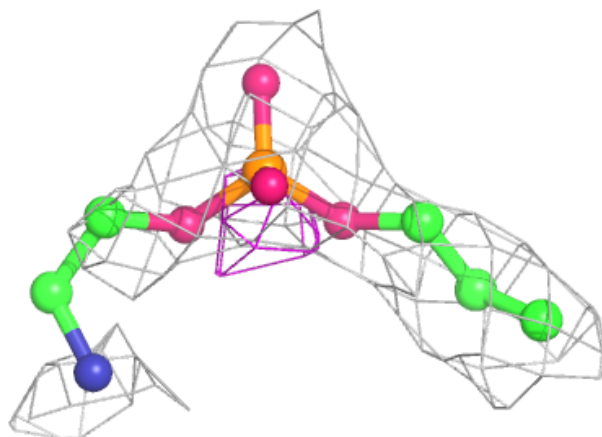
**Electron density around PEE R 502:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

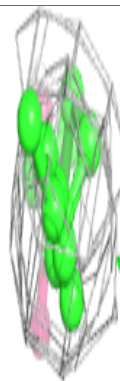
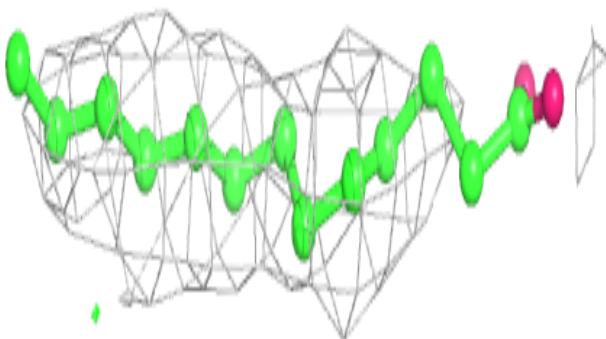
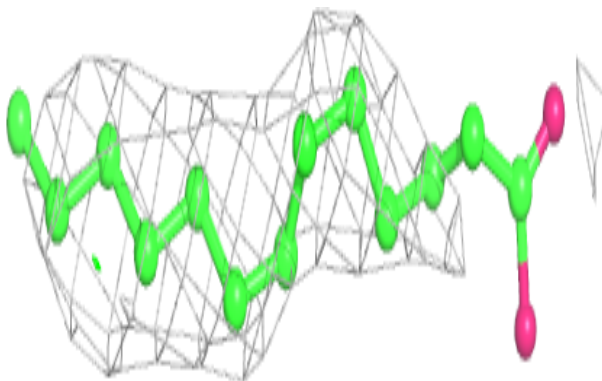


Electron density around PEE C 507:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

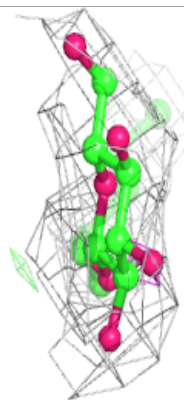
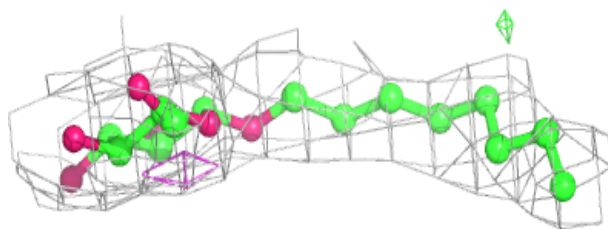
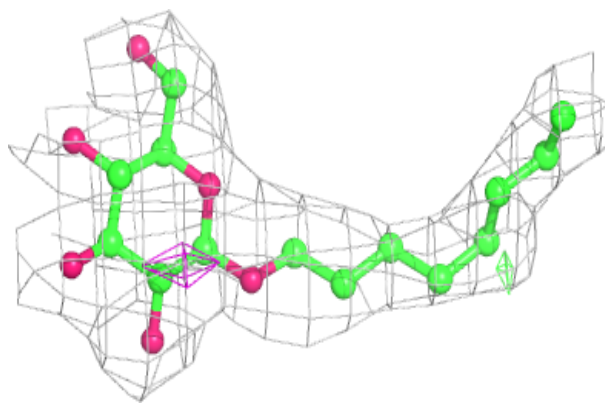
**Electron density around PEE P 401:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



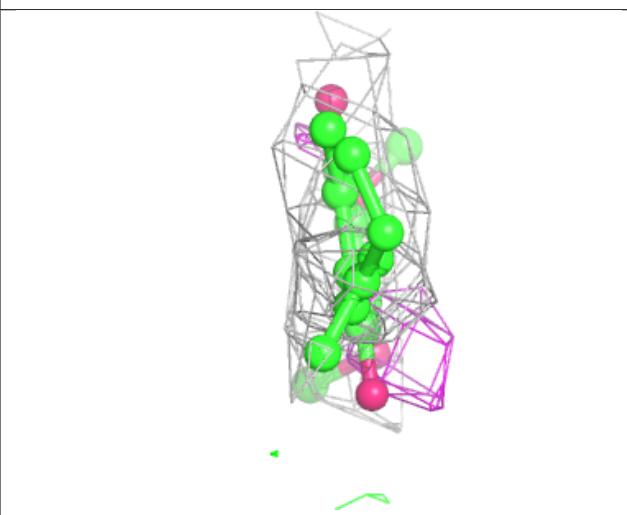
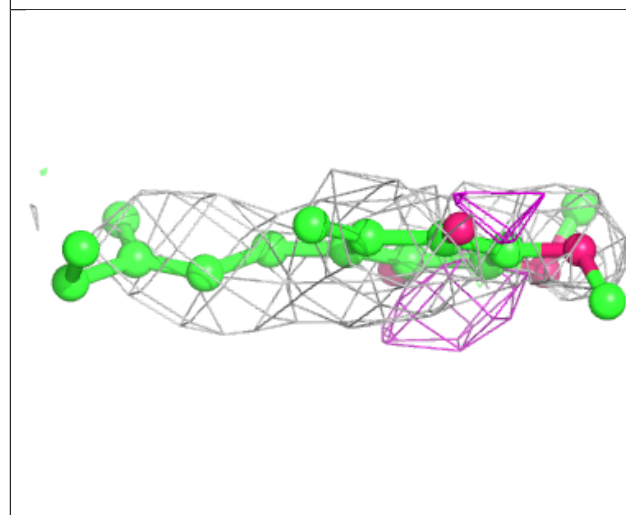
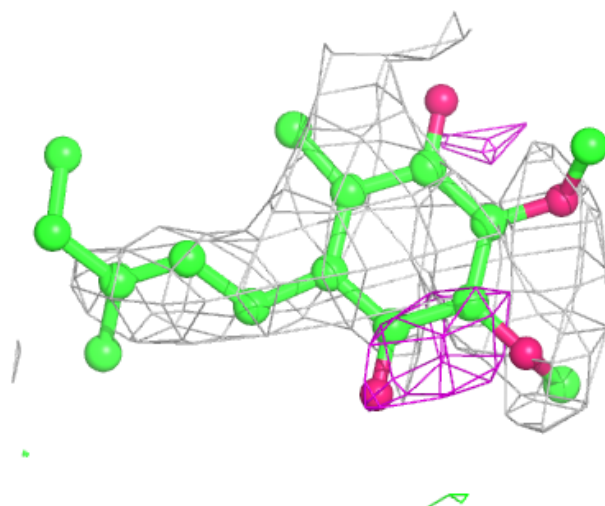
Electron density around BOG P 406:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



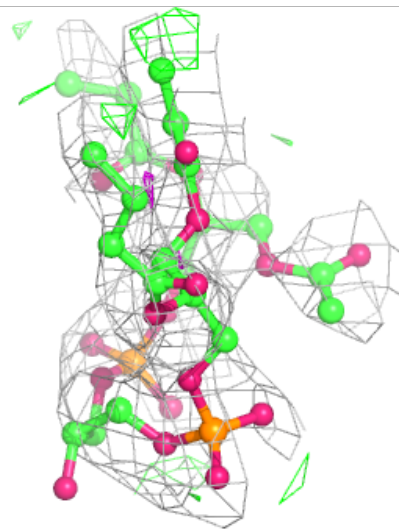
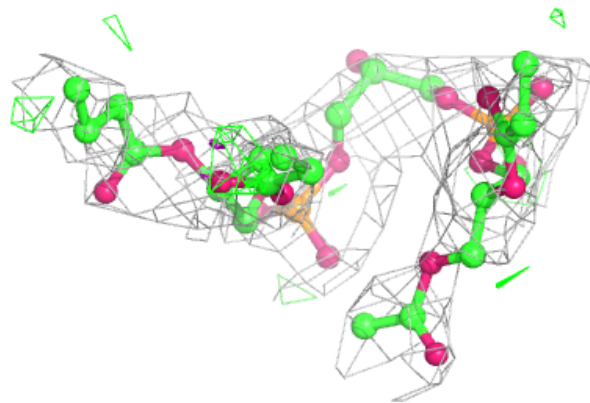
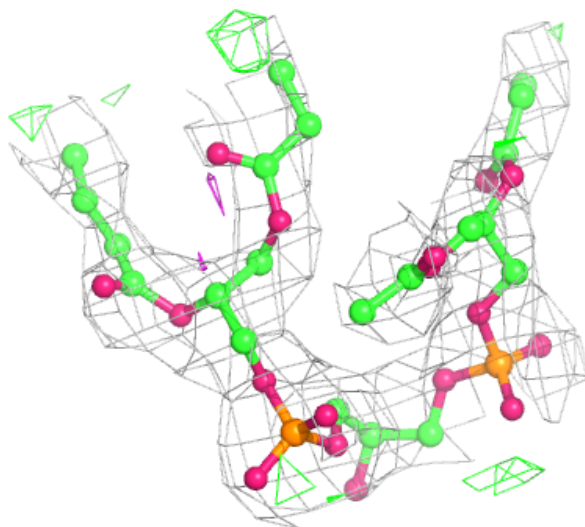
Electron density around U10 P 405:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



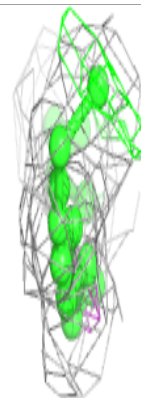
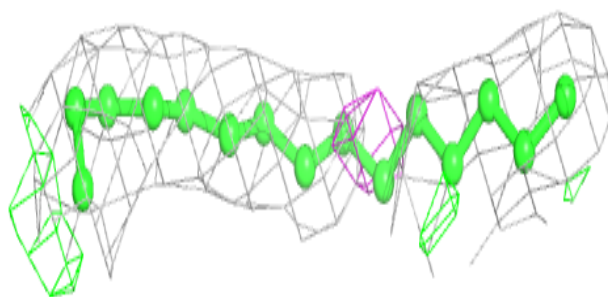
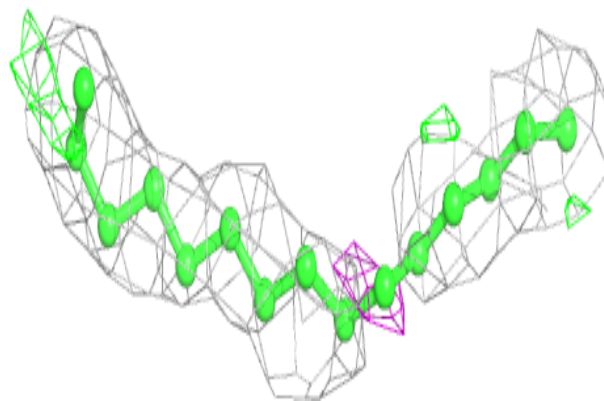
Electron density around CDL T 101:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

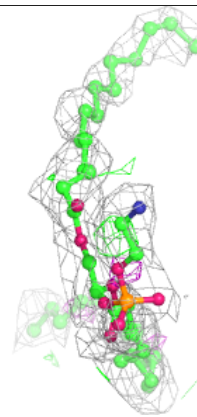
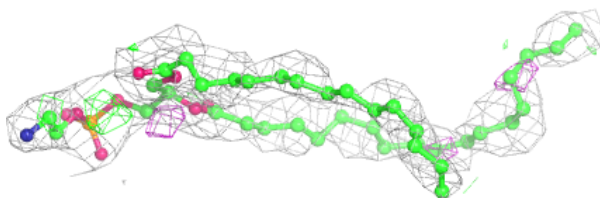
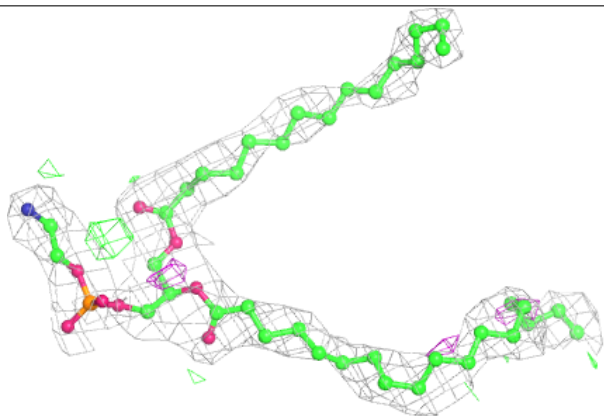


Electron density around PEE E 503:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

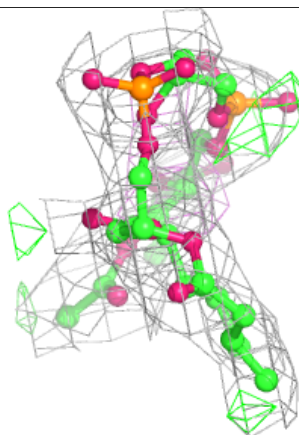
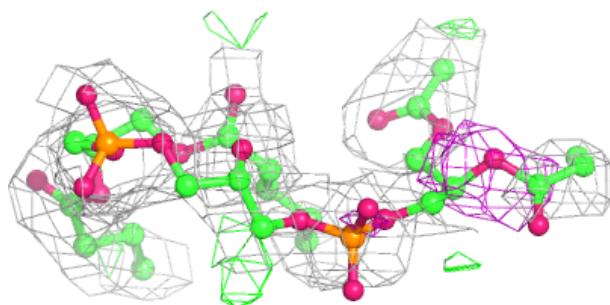
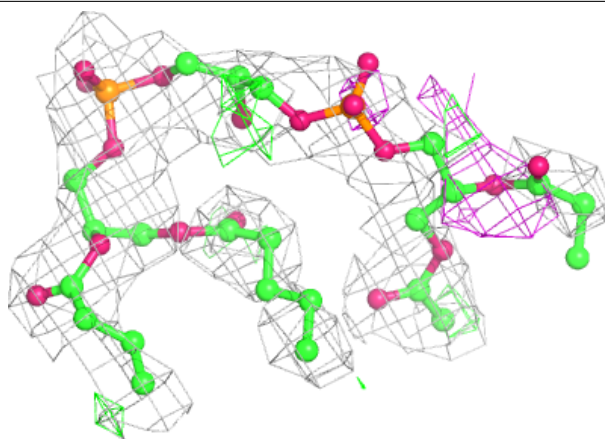
**Electron density around PEE E 502:**

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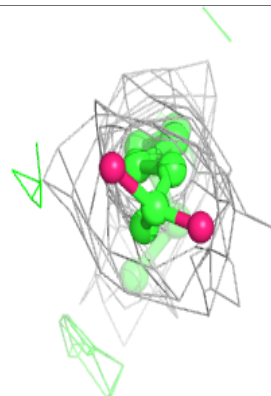
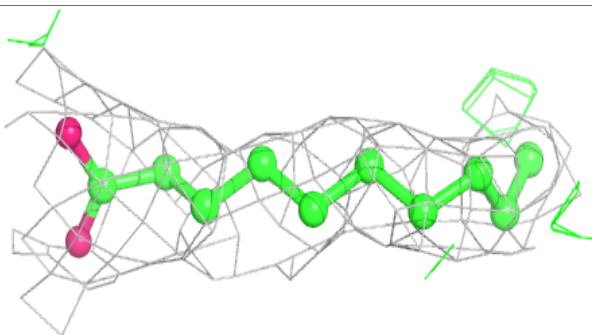
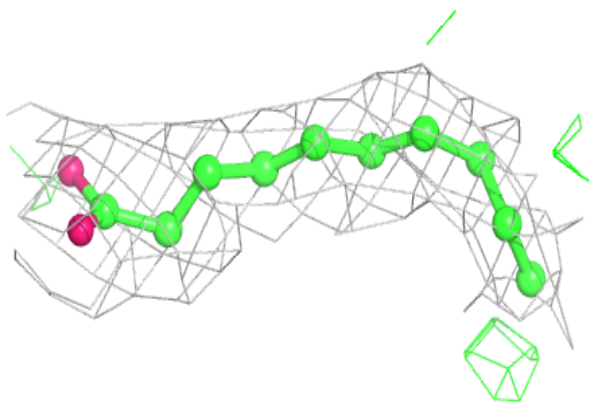


Electron density around CDL D 502:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

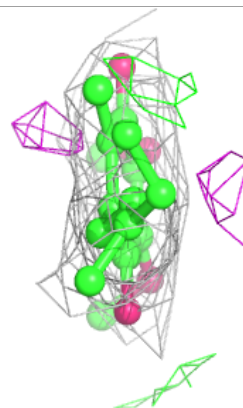
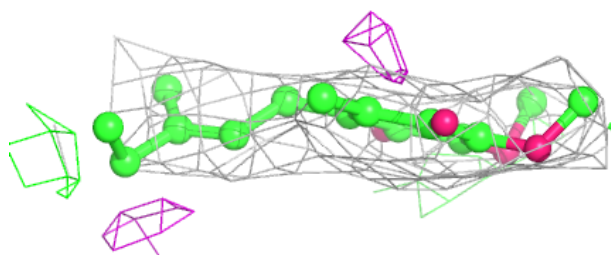
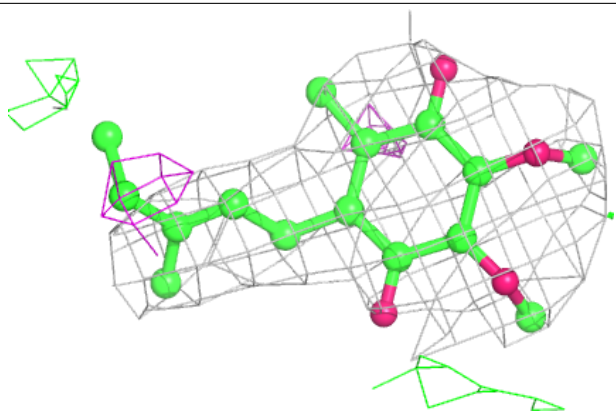
**Electron density around PEE P 410:**

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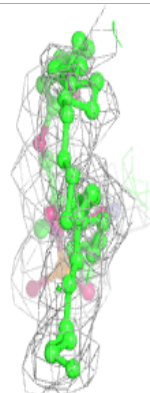
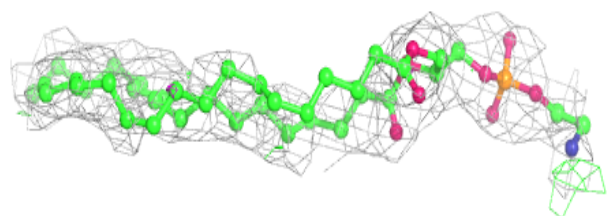
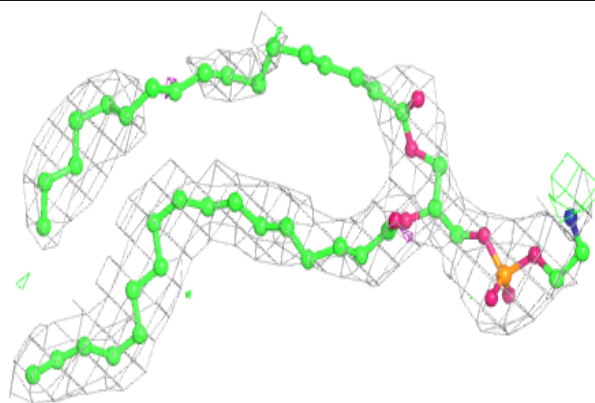


Electron density around U10 C 504:

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and green (positive)

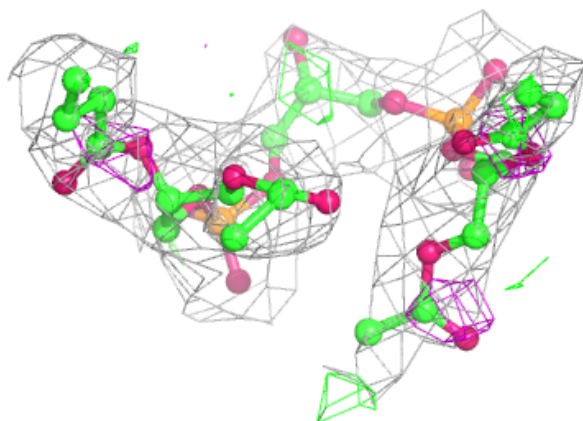
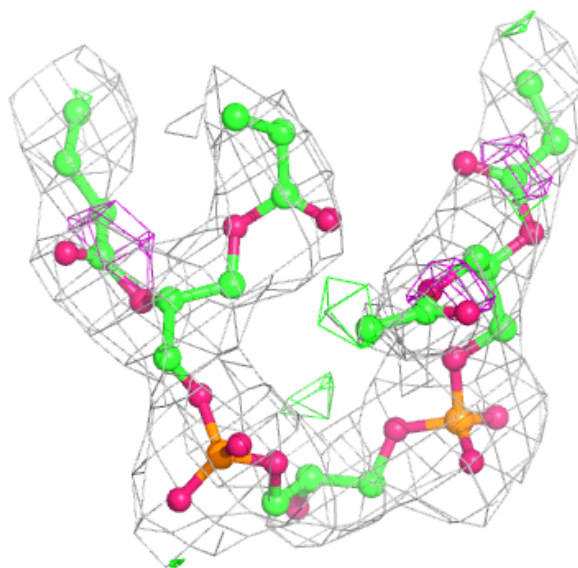
**Electron density around PEE P 407:**

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and green (positive)



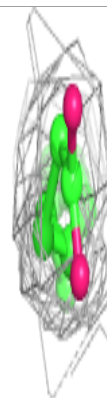
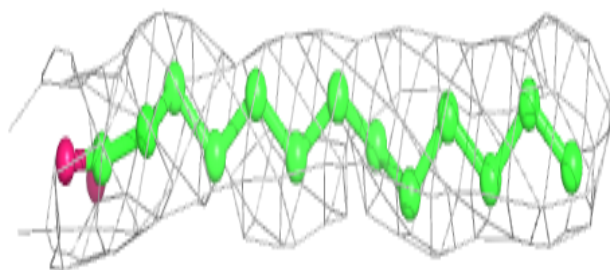
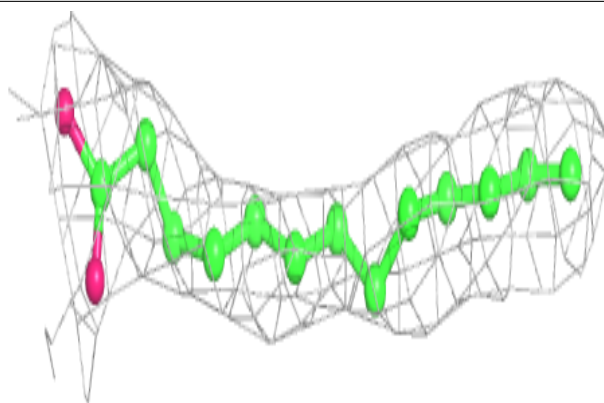
Electron density around CDL G 101:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

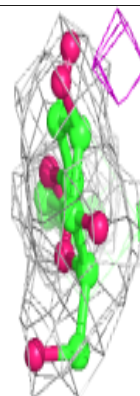
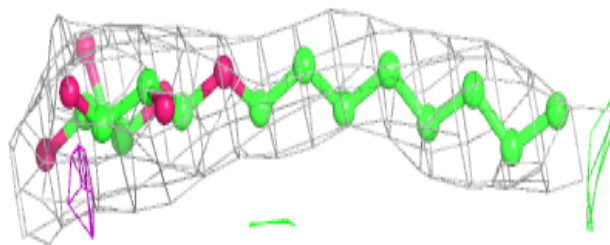
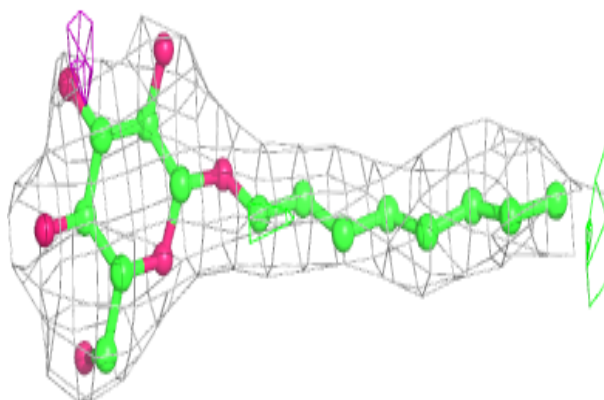


Electron density around PEE C 510:

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and green (positive)

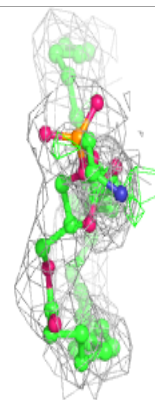
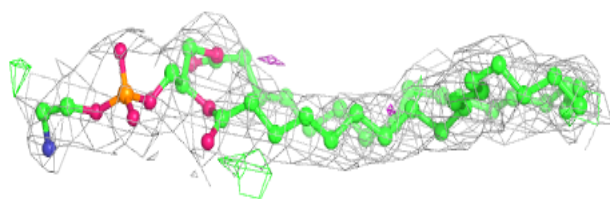
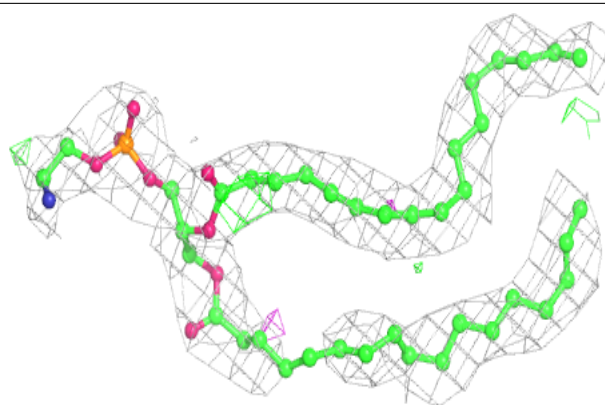
**Electron density around BOG D 503:**

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and green (positive)

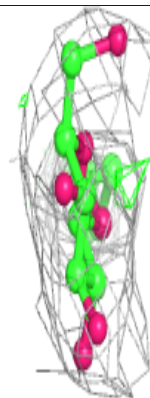
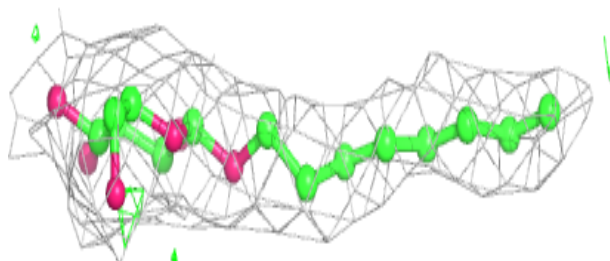
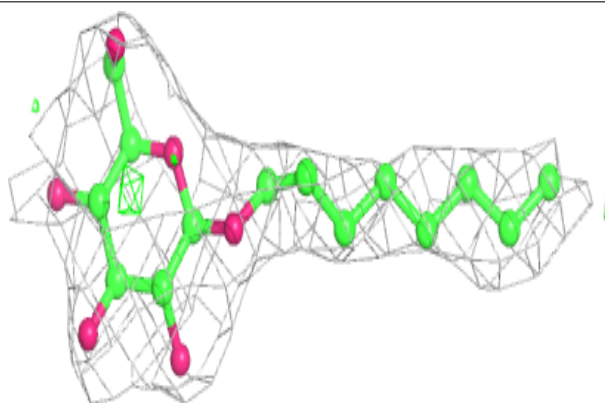


Electron density around PEE C 505:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

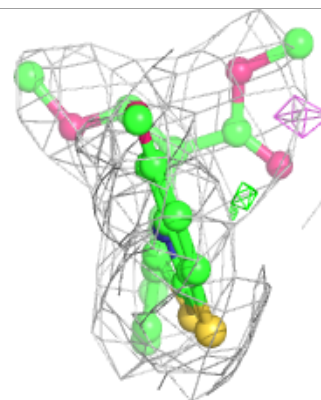
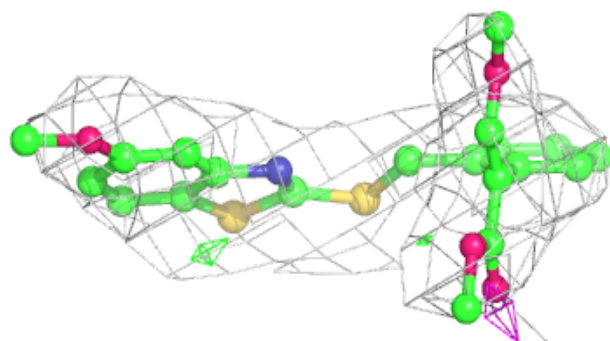
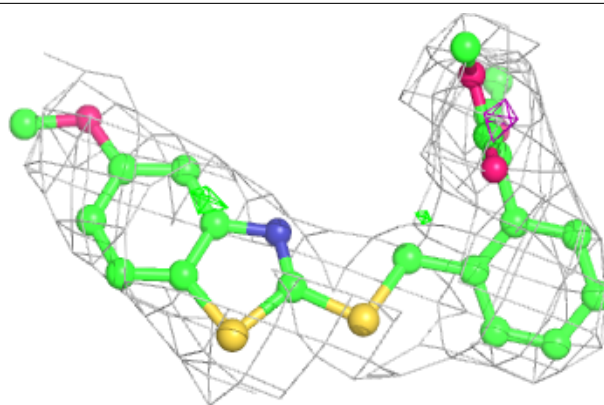
**Electron density around BOG Q 503:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



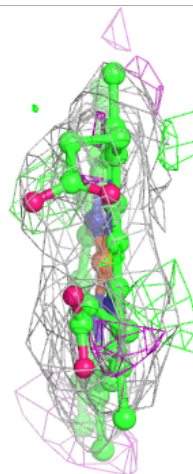
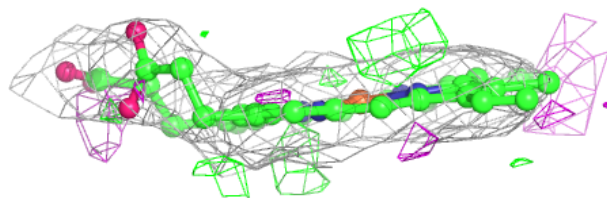
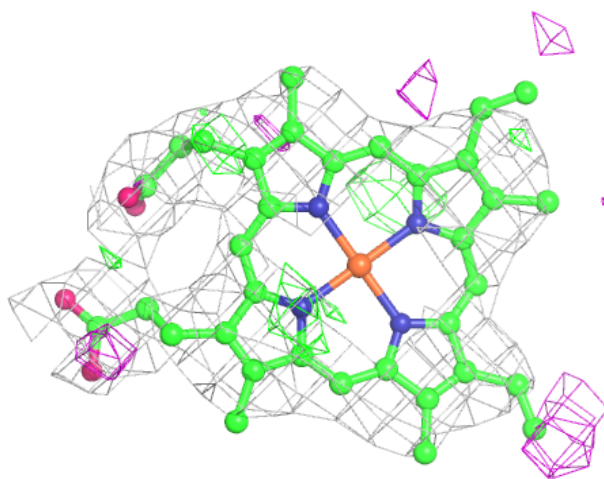
Electron density around Y52 P 404:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



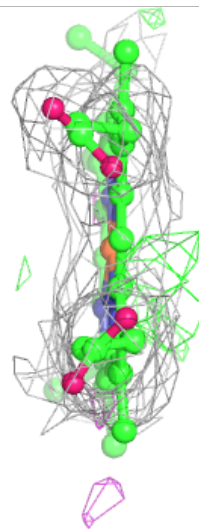
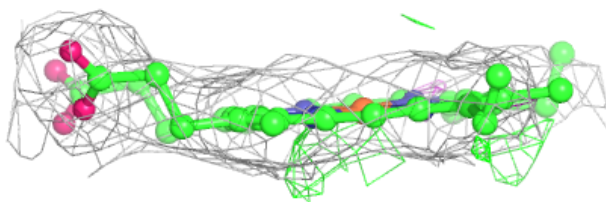
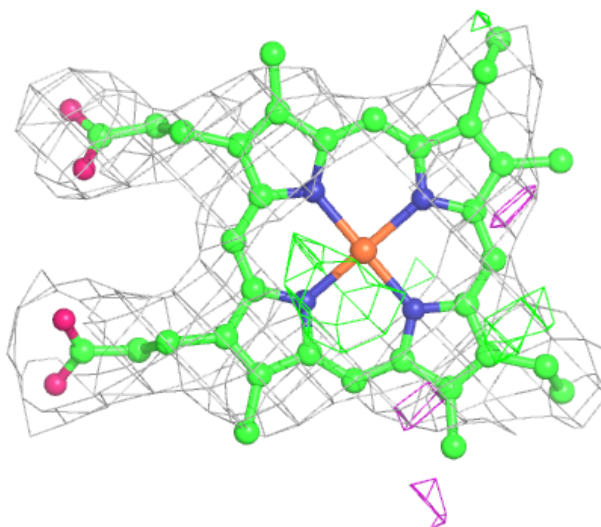
Electron density around HEM C 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



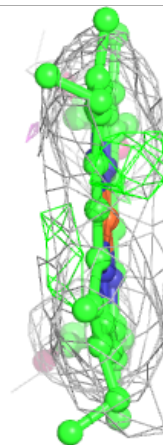
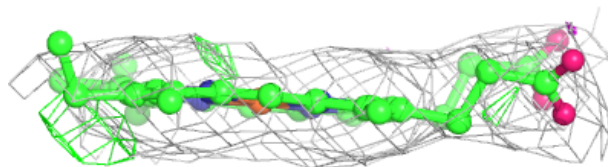
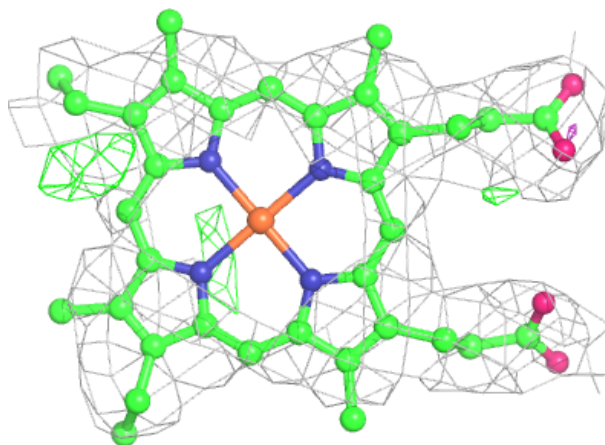
Electron density around HEC D 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



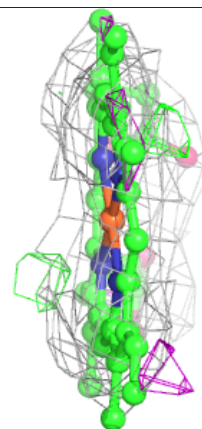
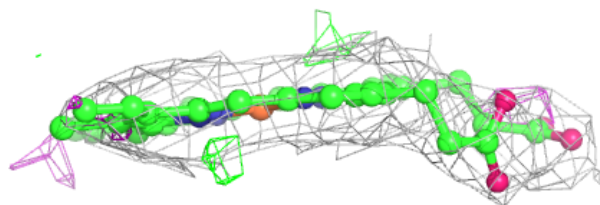
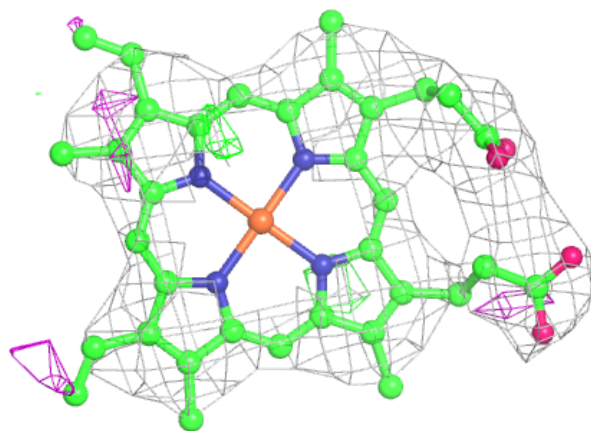
Electron density around HEC Q 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



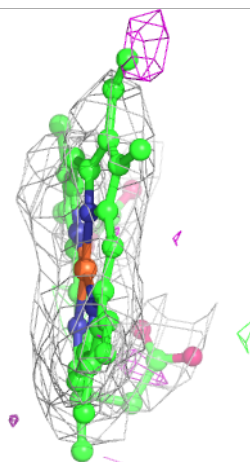
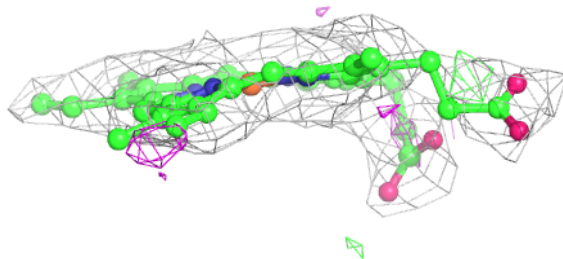
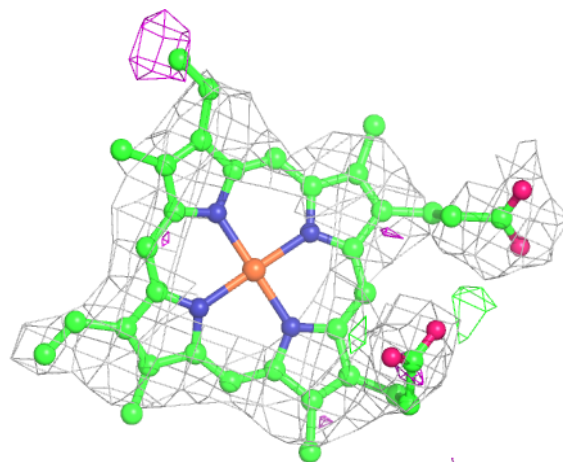
Electron density around HEM P 402:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



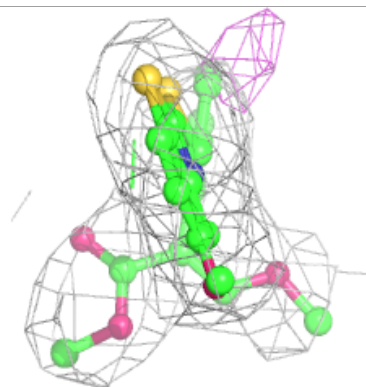
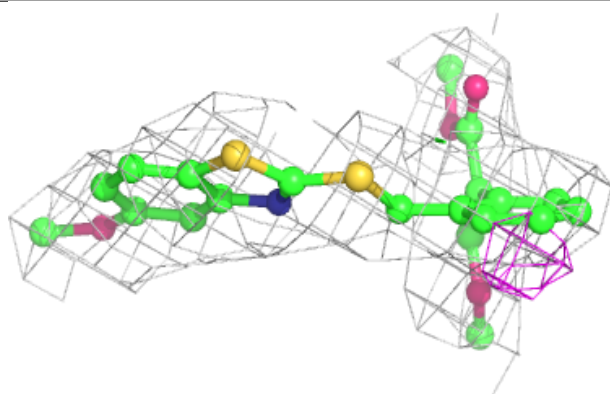
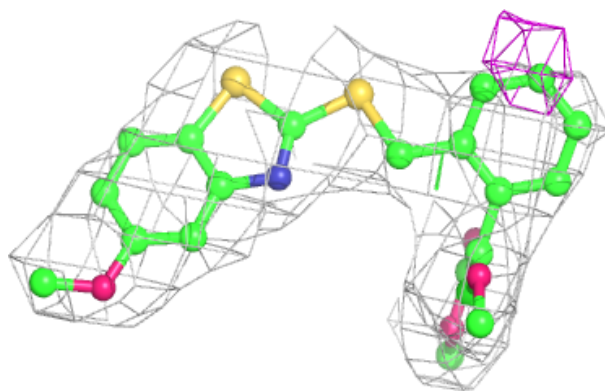
Electron density around HEM P 403:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



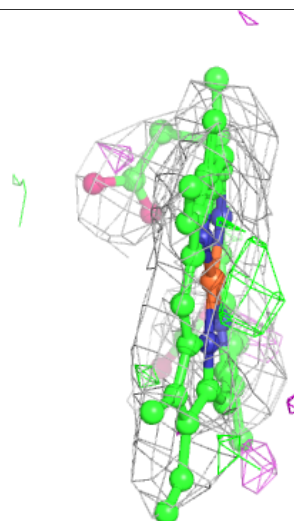
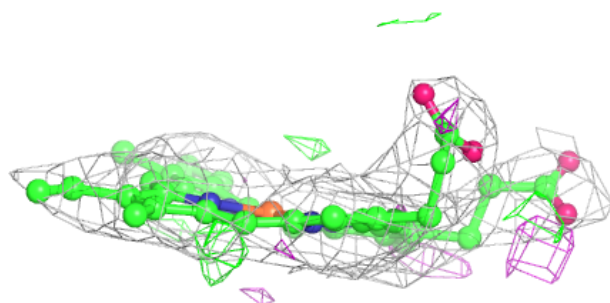
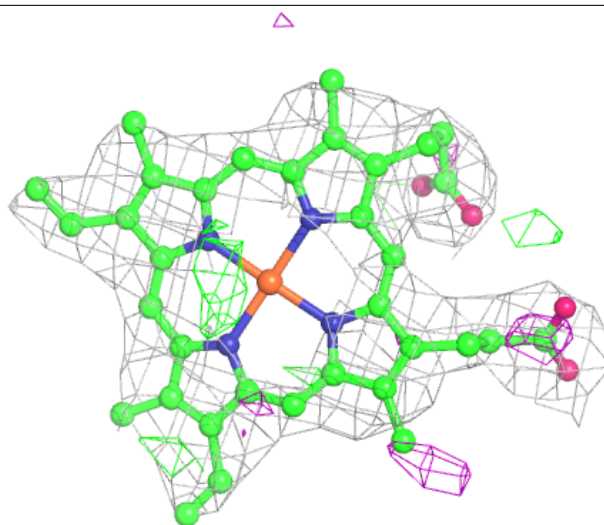
Electron density around Y52 C 503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.