



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:35 pm BST

PDB ID : 4D6T  
Title : Cytochrome bc1 bound to the 4(1H)-pyridone GW844520  
Authors : Capper, M.J.; O'Neill, P.M.; Fisher, N.; Strange, R.W.; Moss, D.; Ward, S.A.;  
Berry, N.G.; Lawrenson, A.S.; Hasnain, S.S.; Biagini, G.A.; Antonyuk, S.V.  
Deposited on : 2014-11-14  
Resolution : 3.57 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](mailto: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.

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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 : 2.11  
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) : 2.11

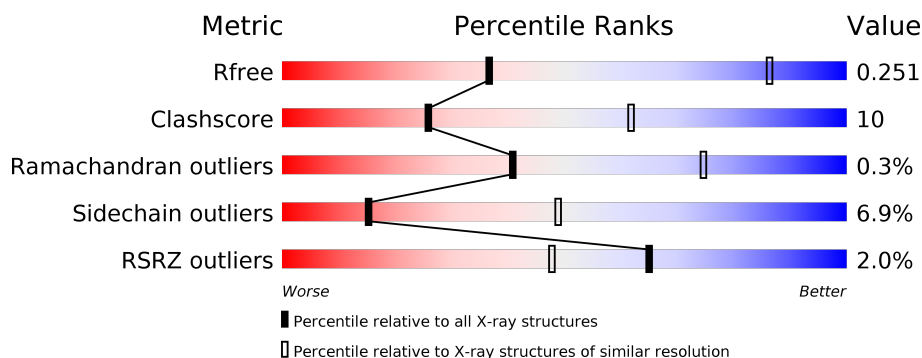
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.57 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	1094 (3.66-3.50)
Clashscore	141614	1181 (3.66-3.50)
Ramachandran outliers	138981	1143 (3.66-3.50)
Sidechain outliers	138945	1143 (3.66-3.50)
RSRZ outliers	127900	1012 (3.66-3.50)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	480	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>16%</div> <div>• 8%</div> </div> </div>
1	N	480	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>15%</div> <div>•• 8%</div> </div> </div>
2	B	453	<div> <div>6%</div> <div> <div></div> <div>71%</div> <div>19%</div> <div>• 7%</div> </div> </div>
3	C	379	<div> <div></div> <div> <div></div> <div>75%</div> <div>19%</div> <div>••</div> </div> </div>
3	P	379	<div> <div></div> <div> <div></div> <div>77%</div> <div>17%</div> <div>••</div> </div> </div>
4	D	265	<div> <div>%</div> <div> <div></div> <div>76%</div> <div>13%</div> <div>• 9%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	Q	265	
5	E	274	
5	I	274	
5	R	274	
6	F	111	
6	S	111	
7	G	82	
7	T	82	
8	H	91	
8	U	91	
9	J	64	
9	W	64	
10	O	453	
11	V	274	

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
14	PO4	F	501	-	-	-	X
14	PO4	N	501	-	-	-	X
14	PO4	S	501	-	-	-	X
15	PEE	C	505	X	-	-	-
15	PEE	D	506	X	-	-	-
15	PEE	P	505	X	-	-	-
15	PEE	Q	506	X	-	-	-
18	FES	R	501	-	-	X	-
19	GOL	R	502	-	-	-	X

## 2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 31051 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 CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	444	Total	C	N	O	S	0	0	0
			3439	2148	607	664	20			
1	N	444	Total	C	N	O	S	0	0	0
			3432	2142	607	663	20			

- Molecule 2 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	422	Total	C	N	O	S	0	0	0
			3164	1988	561	608	7			

- Molecule 3 is a protein called CYTOCHROME B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	374	Total	C	N	O	S	0	0	0
			2968	1993	463	494	18			
3	P	370	Total	C	N	O	S	0	0	0
			2936	1973	456	489	18			

- Molecule 4 is a protein called CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	240	Total	C	N	O	S	0	0	0
			1912	1222	329	346	15			
4	Q	241	Total	C	N	O	S	0	0	0
			1918	1225	330	348	15			

- Molecule 5 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	73	Total	C	N	O	S	0	0	0
			549	341	92	114	2			
5	I	21	Total	C	N	O	S	0	0	0
			157	97	31	28	1			
5	R	196	Total	C	N	O	S	0	0	0
			1518	957	263	290	8			

- Molecule 6 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	0	0
			860	547	154	157	2			
6	S	99	Total	C	N	O	S	0	0	0
			869	553	156	158	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	56	ASP	ASN	conflict	UNP P00129
S	56	ASP	ASN	conflict	UNP P00129

- Molecule 7 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	80	Total	C	N	O	S	0	0	0
			677	439	127	110	1			
7	T	74	Total	C	N	O	S	0	0	0
			624	408	117	98	1			

- Molecule 8 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 6, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	65	Total	C	N	O	S	0	0	0
			529	321	96	107	5			
8	U	66	Total	C	N	O	S	0	0	0
			538	327	98	108	5			

- Molecule 9 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	J	58	Total	C	N	O	0	0	0
			482	317	83	82			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	W	59	Total	C	N	O	0	0	0
			487	320	84	83			

- Molecule 10 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	O	419	Total	C	N	O	S	0	0	0
			3140	1972	555	606	7			

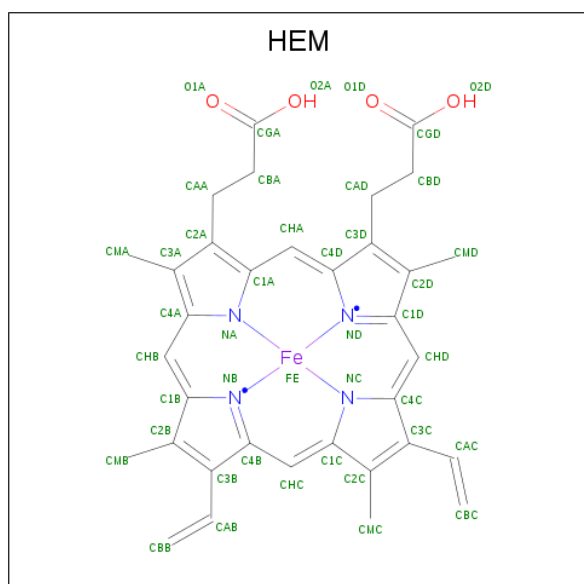
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	305	GLU	GLN	conflict	UNP P23004

- Molecule 11 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL.

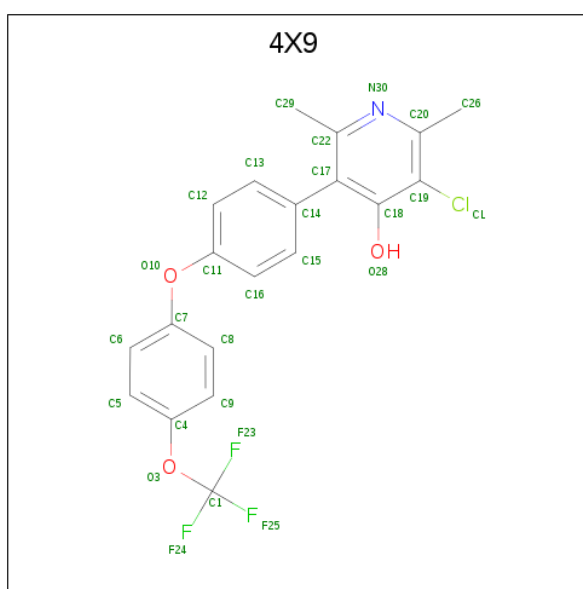
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	V	17	Total	C	N	O	0	0	0
			127	81	24	22			

- Molecule 12 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

- Molecule 13 is 3-chloro-2,6-dimethyl-5-{4-[4-(trifluoromethoxy)phenoxy]phenyl}pyridin-4-ol (three-letter code: 4X9) (formula: C<sub>20</sub>H<sub>15</sub>ClF<sub>3</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total	C	Cl	F	N	O	0
			28	20	1	3	1	3	0
13	P	1	Total	C	Cl	F	N	O	0
			28	20	1	3	1	3	0

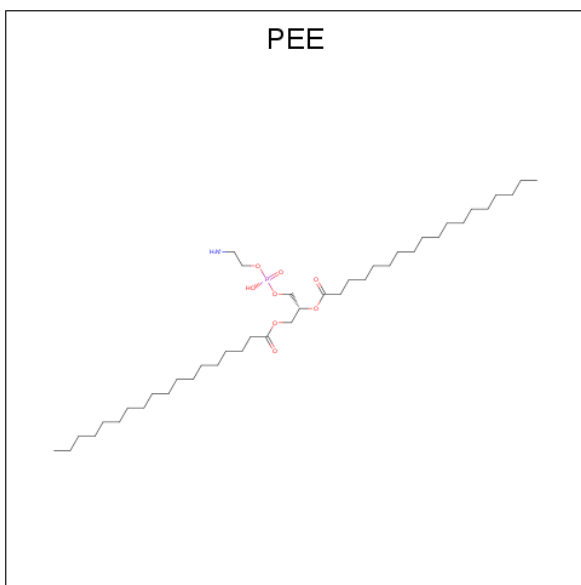
- Molecule 14 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total	O	P	0	0
			5	4	1		
14	D	1	Total	O	P	0	0
			5	4	1		
14	D	1	Total	O	P	0	0
			5	4	1		
14	D	1	Total	O	P	0	0
			5	4	1		
14	E	1	Total	O	P	0	0
			5	4	1		
14	F	1	Total	O	P	0	0
			5	4	1		
14	N	1	Total	O	P	0	0
			5	4	1		
14	N	1	Total	O	P	0	0
			5	4	1		
14	Q	1	Total	O	P	0	0
			5	4	1		
14	Q	1	Total	O	P	0	0
			5	4	1		
14	S	1	Total	O	P	0	0
			5	4	1		

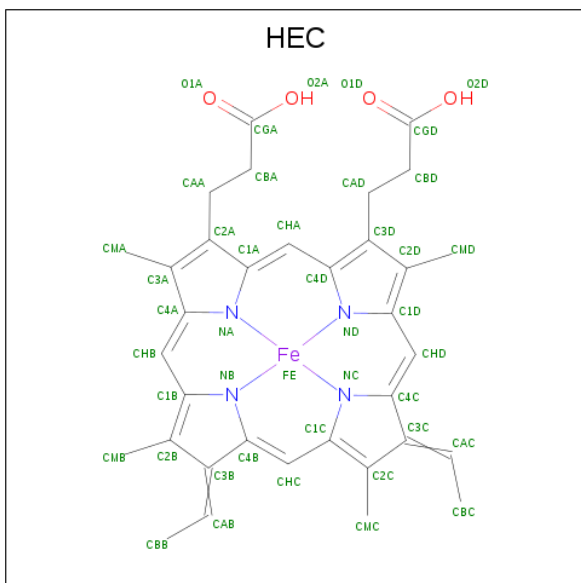
- Molecule 15 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula:  $C_{41}H_{83}NO_8P$ ).





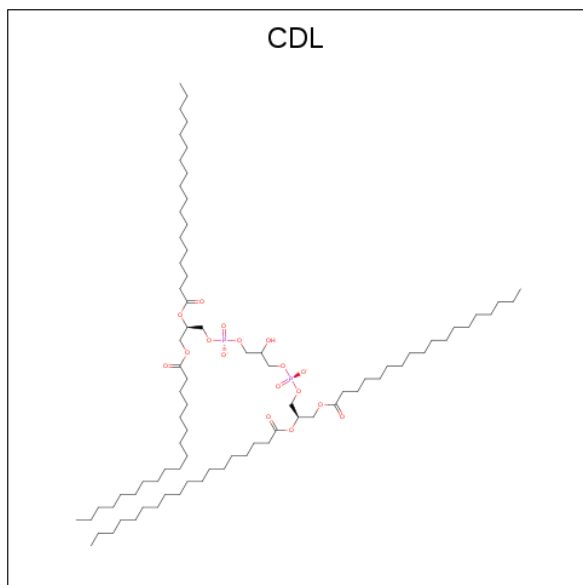
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total 49	C 39	N 1	O 8	P 1	0	0
15	D	1	Total 26	C 16	N 1	O 8	P 1	0	0
15	P	1	Total 49	C 39	N 1	O 8	P 1	0	0
15	Q	1	Total 51	C 41	N 1	O 8	P 1	0	0

- Molecule 16 is HEME C (three-letter code: HEC) (formula:  $\text{C}_{34}\text{H}_{34}\text{FeN}_4\text{O}_4$ ).



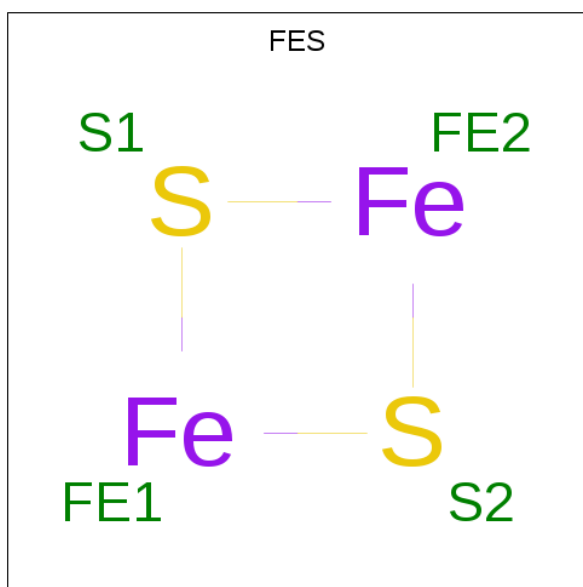
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
16	Q	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



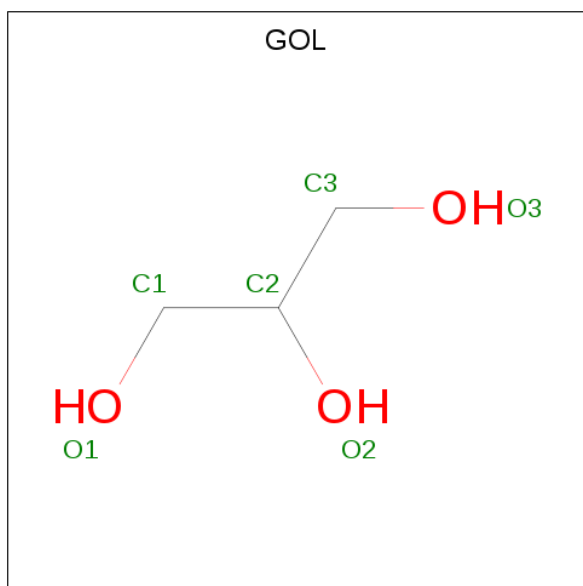
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	D	1	Total	C	O	P	0	0
			39	24	13	2		
17	G	1	Total	C	O	P	0	0
			44	25	17	2		
17	Q	1	Total	C	O	P	0	0
			39	24	13	2		
17	T	1	Total	C	O	P	0	0
			49	30	17	2		

- Molecule 18 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $Fe_2S_2$ ).



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

- Molecule 19 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).

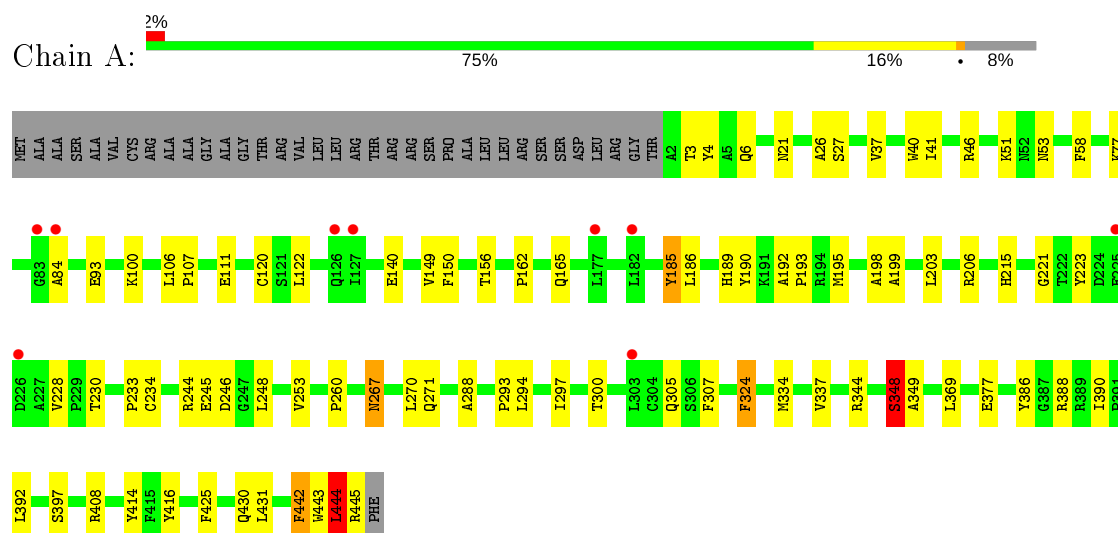


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	R	1	Total	C	O	0	0
			6	3	3		

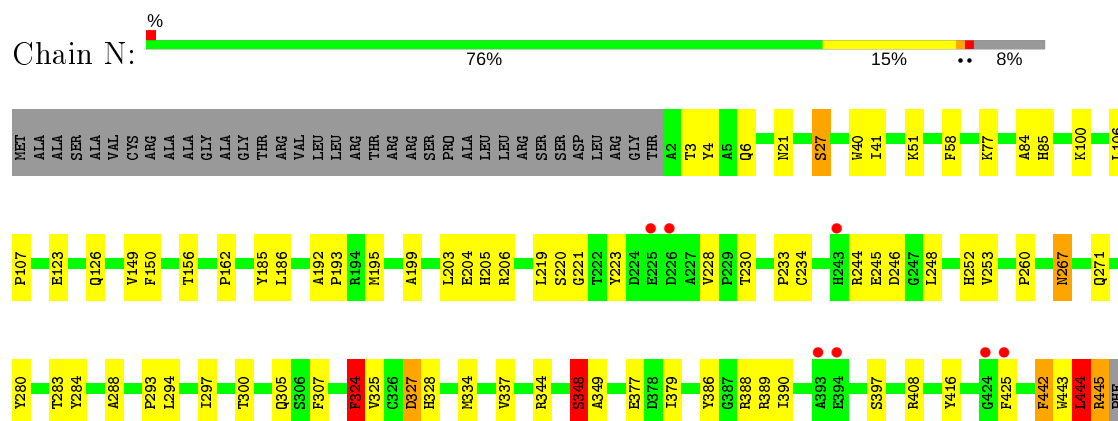
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

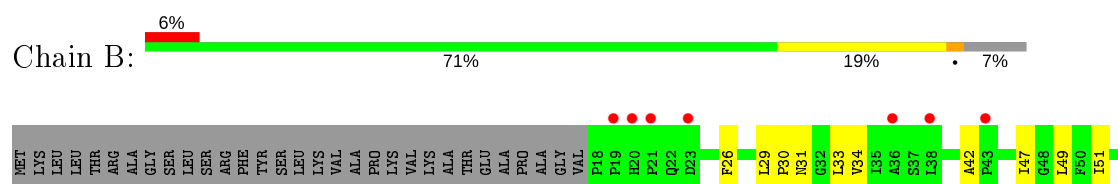
#### • Molecule 1: CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL

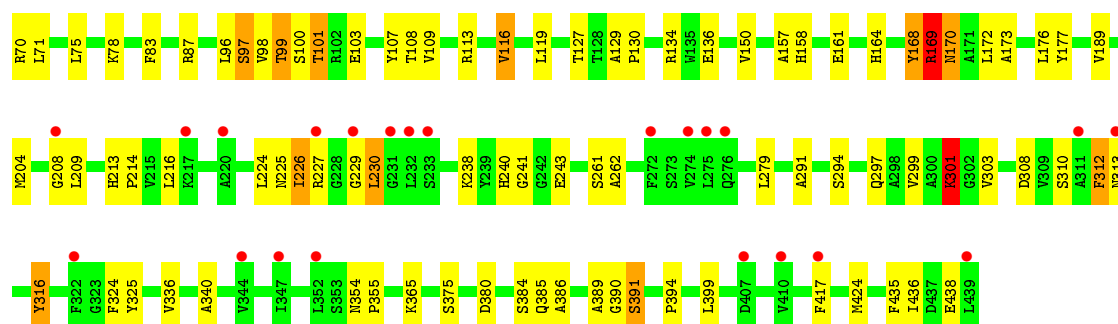


#### • Molecule 1: CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL



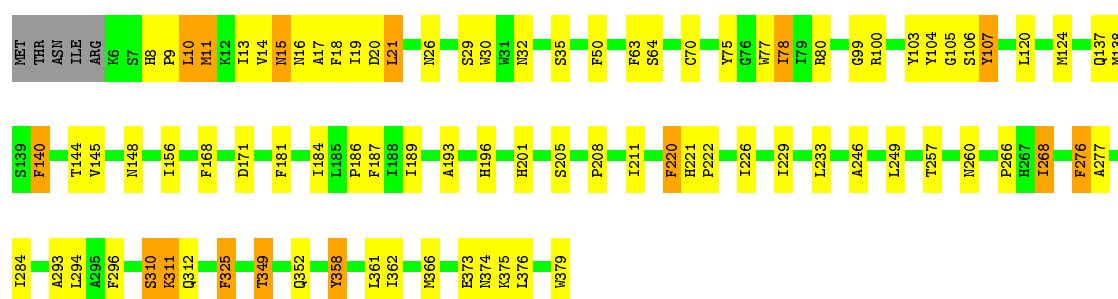
#### • Molecule 2: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL





• Molecule 3: CYTOCHROME B

Chain C: 75% 19%



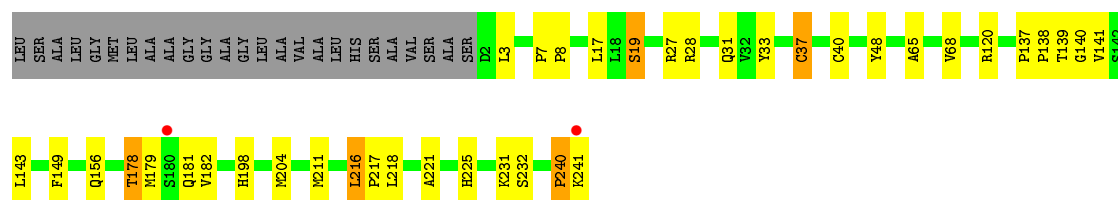
• Molecule 3: CYTOCHROME B

Chain P: 77% 17%

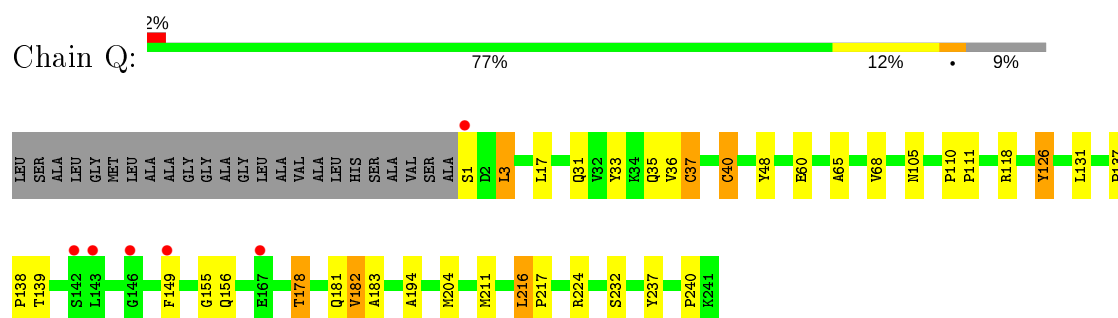


• Molecule 4: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL

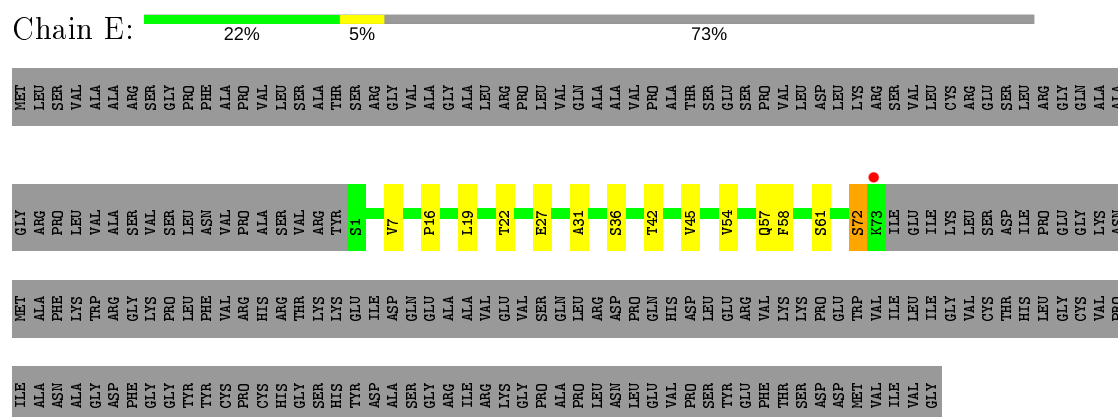
Chain D: % 76% 13% 9%



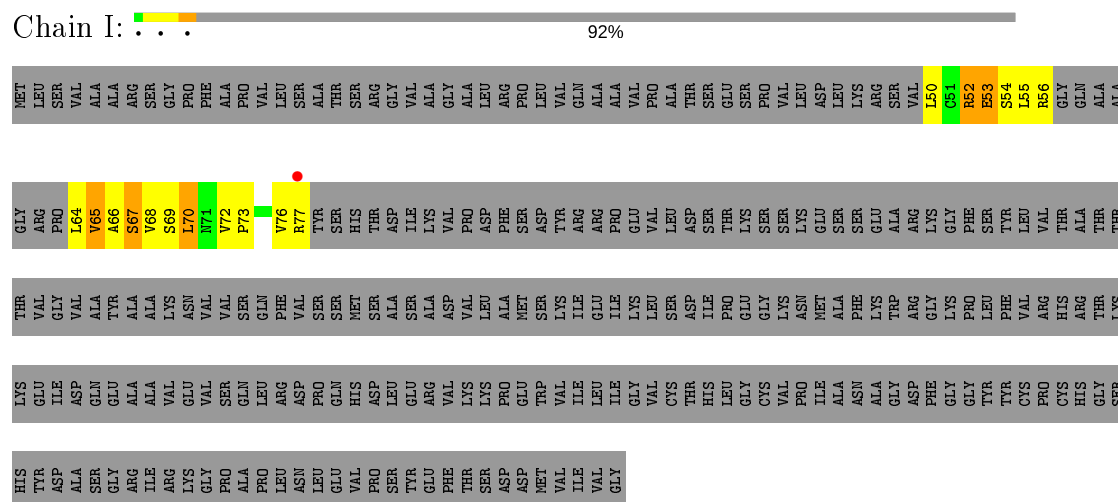
• Molecule 4: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL



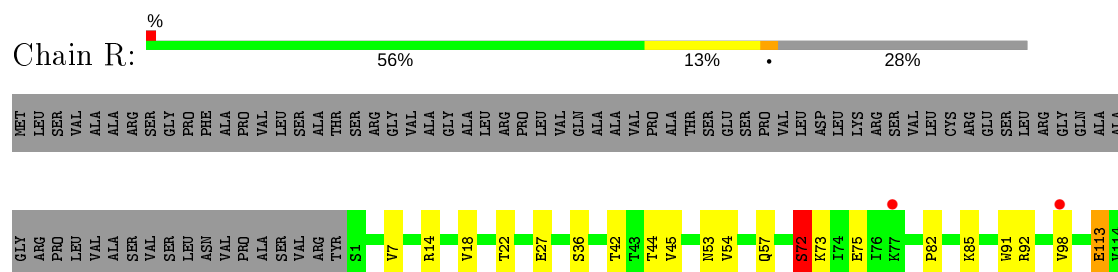
- Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

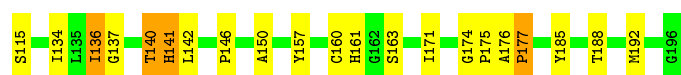


● Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

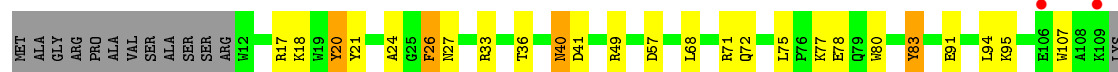


- Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL





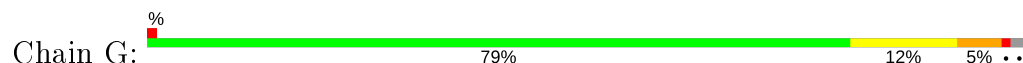
• Molecule 6: CYTOCHROME B-C1 COMPLEX SUBUNIT 7



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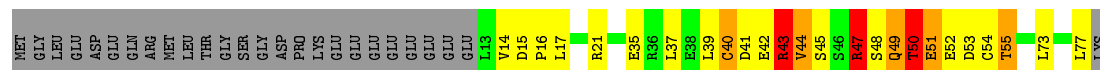
• Molecule 7: CYTOCHROME B-C1 COMPLEX SUBUNIT 8



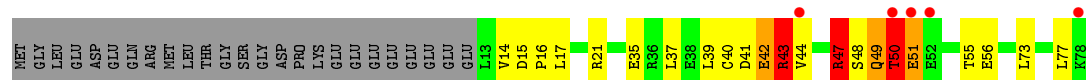
• Molecule 7: CYTOCHROME B-C1 COMPLEX SUBUNIT 8



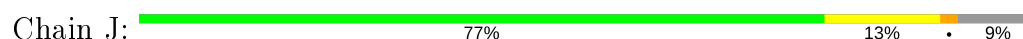
• Molecule 8: CYTOCHROME B-C1 COMPLEX SUBUNIT 6, MITOCHONDRIAL



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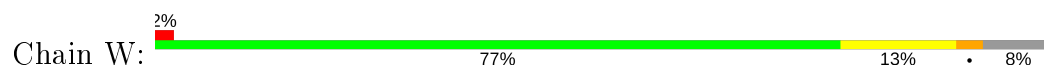


• Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT 9

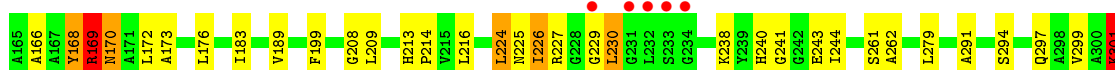
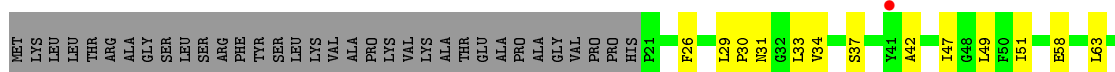




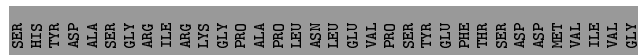
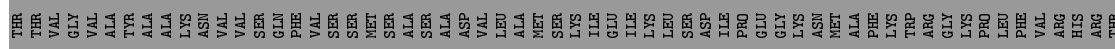
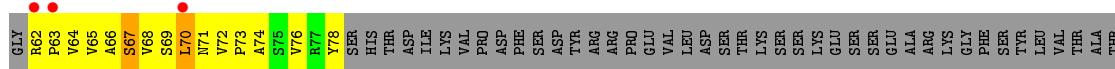
- Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT 9



- Molecule 10: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL



- Molecule 11: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.90Å 129.90Å 722.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.57 49.81 – 3.57	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-3.57) 99.9 (49.81-3.57)	Depositor EDS
$R_{merge}$	0.24	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.86 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.206 , 0.252 0.207 , 0.251	Depositor DCC
$R_{free}$ test set	3953 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	122.6	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 79.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.064 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	31051	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CDL, PO4, FES, 4X9, HEC, HEM, PEE

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	0.46	1/3511 (0.0%)	0.69	5/4766 (0.1%)
1	N	0.42	0/3503	0.70	7/4755 (0.1%)
2	B	0.69	3/3224 (0.1%)	0.80	10/4375 (0.2%)
3	C	0.50	0/3065	0.68	0/4196
3	P	0.48	1/3031 (0.0%)	0.67	0/4150
4	D	0.42	0/1971	0.62	0/2676
4	Q	0.42	0/1977	0.61	0/2684
5	E	0.41	0/557	0.62	0/752
5	I	0.57	0/156	1.24	2/209 (1.0%)
5	R	0.43	0/1552	0.78	7/2100 (0.3%)
6	F	0.46	0/879	0.68	0/1180
6	S	0.47	0/888	0.65	0/1191
7	G	0.52	1/699 (0.1%)	1.26	6/946 (0.6%)
7	T	0.49	0/645	0.74	0/873
8	H	2.11	7/534 (1.3%)	1.96	8/718 (1.1%)
8	U	1.48	6/543 (1.1%)	2.09	10/729 (1.4%)
9	J	0.42	0/495	0.59	0/667
9	W	0.43	0/500	0.60	0/675
10	O	0.50	2/3197 (0.1%)	0.95	12/4336 (0.3%)
11	V	0.58	0/129	0.86	0/177
All	All	0.59	21/31056 (0.1%)	0.82	67/42155 (0.2%)

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
1	N	0	1
2	B	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	G	0	1
8	H	0	1
8	U	0	3
10	O	0	2
All	All	0	11

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	169	ARG	CZ-NH2	28.39	1.70	1.33
8	H	43	ARG	CZ-NH1	26.86	1.68	1.33
8	H	47	ARG	CZ-NH2	25.79	1.66	1.33
8	U	47	ARG	CZ-NH2	25.71	1.66	1.33
8	H	43	ARG	NE-CZ	23.73	1.64	1.33
10	O	169	ARG	NE-CZ	15.59	1.53	1.33
1	A	408	ARG	CZ-NH2	13.97	1.51	1.33
2	B	169	ARG	CZ-NH1	-11.66	1.17	1.33
8	U	43	ARG	CZ-NH2	-10.62	1.19	1.33
8	U	43	ARG	CZ-NH1	9.93	1.46	1.33
8	H	47	ARG	CD-NE	9.43	1.62	1.46
8	U	43	ARG	NE-CZ	8.60	1.44	1.33
10	O	169	ARG	CZ-NH1	7.78	1.43	1.33
2	B	169	ARG	NE-CZ	6.49	1.41	1.33
8	H	42	GLU	CD-OE2	6.18	1.32	1.25
8	H	47	ARG	CZ-NH1	-5.94	1.25	1.33
8	U	50	THR	CB-CG2	5.50	1.70	1.52
3	P	220	PHE	CG-CD1	-5.38	1.30	1.38
8	H	40	CYS	CB-SG	5.23	1.91	1.82
8	U	42	GLU	CD-OE2	5.08	1.31	1.25
7	G	74	PRO	N-CD	5.01	1.54	1.47

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	U	47	ARG	NE-CZ-NH2	-37.30	101.65	120.30
8	H	47	ARG	NE-CZ-NH2	33.38	136.99	120.30
7	G	75	ALA	N-CA-CB	-19.29	83.10	110.10
8	U	43	ARG	NH1-CZ-NH2	-18.82	98.69	119.40
10	O	169	ARG	NH1-CZ-NH2	-17.91	99.70	119.40
8	U	43	ARG	NE-CZ-NH1	17.41	129.00	120.30
10	O	169	ARG	NE-CZ-NH2	17.25	128.93	120.30
8	H	43	ARG	NE-CZ-NH2	-16.30	112.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	43	ARG	NE-CZ-NH1	15.84	128.22	120.30
10	O	169	ARG	NE-CZ-NH1	15.61	128.10	120.30
2	B	390	GLY	N-CA-C	15.33	151.42	113.10
10	O	390	GLY	N-CA-C	15.25	151.24	113.10
8	H	47	ARG	NH1-CZ-NH2	-14.99	102.92	119.40
7	G	74	PRO	N-CA-C	14.66	150.22	112.10
10	O	301	LYS	CB-CA-C	-14.42	81.56	110.40
8	U	47	ARG	NH1-CZ-NH2	13.47	134.21	119.40
10	O	168	TYR	CB-CA-C	-12.57	85.27	110.40
10	O	301	LYS	N-CA-C	12.53	144.84	111.00
2	B	301	LYS	N-CA-C	12.14	143.79	111.00
8	U	43	ARG	CB-CG-CD	-11.76	81.03	111.60
2	B	391	SER	N-CA-CB	11.69	128.03	110.50
10	O	169	ARG	N-CA-CB	-11.51	89.89	110.60
2	B	169	ARG	NE-CZ-NH1	11.35	125.97	120.30
8	U	43	ARG	CD-NE-CZ	-11.17	107.97	123.60
10	O	391	SER	N-CA-CB	11.11	127.16	110.50
2	B	301	LYS	CB-CA-C	-11.09	88.22	110.40
7	G	77	TYR	C-N-CA	10.54	148.06	121.70
10	O	169	ARG	N-CA-C	10.10	138.26	111.00
7	G	74	PRO	CB-CA-C	-9.99	87.02	112.00
8	H	50	THR	CB-CA-C	-9.80	85.15	111.60
1	A	349	ALA	N-CA-CB	9.42	123.29	110.10
5	R	142	LEU	N-CA-C	-8.95	86.83	111.00
2	B	169	ARG	NE-CZ-NH2	-8.92	115.84	120.30
8	U	50	THR	CB-CA-C	-8.37	89.01	111.60
5	R	141	HIS	CB-CA-C	-8.23	93.95	110.40
5	I	53	GLU	N-CA-C	8.15	133.00	111.00
2	B	169	ARG	N-CA-CB	-8.15	95.94	110.60
1	N	349	ALA	N-CA-CB	8.13	121.48	110.10
8	H	43	ARG	CB-CG-CD	-7.93	90.97	111.60
5	R	72	SER	N-CA-C	7.88	132.29	111.00
5	R	142	LEU	N-CA-CB	7.80	126.00	110.40
1	A	348	SER	CB-CA-C	7.54	124.42	110.10
8	H	43	ARG	N-CA-CB	-7.47	97.14	110.60
1	A	349	ALA	N-CA-C	-7.33	91.20	111.00
8	H	47	ARG	CD-NE-CZ	7.25	133.74	123.60
7	G	77	TYR	N-CA-C	7.24	130.54	111.00
5	I	52	ARG	CB-CA-C	6.95	124.29	110.40
1	N	349	ALA	N-CA-C	-6.93	92.29	111.00
1	A	348	SER	N-CA-C	-6.65	93.04	111.00
10	O	301	LYS	C-N-CA	6.42	135.79	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	LYS	C-N-CA	6.40	135.75	122.30
7	G	73	ASN	C-N-CD	6.03	141.06	128.40
8	U	43	ARG	NE-CZ-NH2	5.98	123.29	120.30
1	N	445	ARG	NE-CZ-NH2	-5.96	117.32	120.30
5	R	73	LYS	N-CA-CB	5.89	121.20	110.60
5	R	72	SER	CB-CA-C	-5.87	98.94	110.10
10	O	169	ARG	CD-NE-CZ	-5.80	115.47	123.60
1	N	348	SER	N-CA-C	-5.67	95.68	111.00
2	B	169	ARG	NH1-CZ-NH2	-5.67	113.16	119.40
1	N	408	ARG	CB-CG-CD	-5.57	97.13	111.60
1	A	408	ARG	CG-CD-NE	5.51	123.37	111.80
1	N	348	SER	CB-CA-C	5.45	120.45	110.10
8	U	42	GLU	OE1-CD-OE2	5.44	129.83	123.30
8	U	47	ARG	NE-CZ-NH1	-5.42	117.59	120.30
2	B	168	TYR	CB-CA-C	-5.19	100.02	110.40
5	R	73	LYS	N-CA-C	-5.07	97.32	111.00
1	N	324	PHE	CB-CG-CD1	5.00	124.30	120.80

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	444	LEU	Peptide
2	B	169	ARG	Sidechain
2	B	301	LYS	Peptide
7	G	77	TYR	Peptide
8	H	50	THR	Peptide
1	N	444	LEU	Peptide
10	O	169	ARG	Sidechain
10	O	301	LYS	Peptide
8	U	43	ARG	Sidechain
8	U	47	ARG	Sidechain
8	U	50	THR	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	3439	0	3337	45	0
1	N	3432	0	3330	42	0
2	B	3164	0	3144	80	0
3	C	2968	0	3028	82	0
3	P	2936	0	2996	71	0
4	D	1912	0	1861	42	0
4	Q	1918	0	1870	38	0
5	E	549	0	547	9	0
5	I	157	0	171	27	0
5	R	1518	0	1504	27	0
6	F	860	0	849	24	1
6	S	869	0	862	24	0
7	G	677	0	672	9	0
7	T	624	0	630	8	0
8	H	529	0	512	45	0
8	U	538	0	522	23	1
9	J	482	0	483	8	0
9	W	487	0	487	9	0
10	O	3140	0	3121	104	0
11	V	127	0	135	40	0
12	C	86	0	60	10	0
12	P	86	0	60	10	0
13	C	28	0	14	6	0
13	P	28	0	14	5	0
14	C	5	0	0	0	0
14	D	15	0	0	0	0
14	E	5	0	0	0	0
14	F	5	0	0	0	0
14	N	10	0	0	0	0
14	Q	10	0	0	0	0
14	S	5	0	0	0	0
15	C	49	0	72	1	0
15	D	26	0	26	0	0
15	P	49	0	72	1	0
15	Q	51	0	82	3	0
16	D	43	0	32	12	0
16	Q	43	0	32	10	0
17	D	39	0	39	0	0
17	G	44	0	32	0	0
17	Q	39	0	39	1	0
17	T	49	0	42	1	0
18	R	4	0	0	3	0
19	R	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	31051	0	30685	645	1

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 10.

All (645) 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)
8:H:43:ARG:NH1	8:H:43:ARG:CZ	1.68	1.56
2:B:169:ARG:NH2	2:B:169:ARG:CZ	1.70	1.49
8:H:47:ARG:CD	8:H:50:THR:HG21	1.35	1.44
8:H:47:ARG:CD	8:H:50:THR:CG2	2.07	1.32
8:H:47:ARG:HD2	8:H:50:THR:CG2	1.62	1.28
4:D:139:THR:OG1	8:H:41:ASP:OD1	1.55	1.22
8:H:44:VAL:CG2	8:H:47:ARG:HH21	1.53	1.20
10:O:168:TYR:O	10:O:173:ALA:HB2	1.41	1.17
1:N:284:TYR:CE1	11:V:73:PRO:HB3	1.80	1.16
8:H:47:ARG:HD2	8:H:50:THR:HG22	1.28	1.15
8:H:44:VAL:HG22	8:H:47:ARG:HH21	1.10	1.12
4:Q:139:THR:OG1	8:U:41:ASP:OD1	1.68	1.08
10:O:89:ILE:HD12	11:V:70:LEU:HD22	1.36	1.03
4:Q:37:CYS:SG	16:Q:501:HEC:CAB	2.48	1.02
8:H:47:ARG:CZ	8:H:50:THR:OG1	1.88	1.01
1:A:344:ARG:O	1:A:348:SER:O	1.79	1.01
8:U:37:LEU:O	8:U:41:ASP:HB2	1.61	1.01
10:O:85:ILE:HG22	11:V:70:LEU:HD13	1.43	0.99
4:D:40:CYS:SG	16:D:501:HEC:HBC3	2.02	0.99
10:O:90:GLU:HG2	11:V:71:ASN:OD1	1.64	0.97
2:B:168:TYR:HD2	2:B:172:LEU:HB2	1.27	0.96
8:H:37:LEU:O	8:H:41:ASP:HB2	1.64	0.96
8:H:44:VAL:HG22	8:H:47:ARG:NH2	1.80	0.94
10:O:168:TYR:HD2	10:O:172:LEU:HB2	1.33	0.93
3:C:376:LEU:HD12	6:F:20:TYR:HD2	1.33	0.93
1:N:344:ARG:O	1:N:348:SER:O	1.86	0.91
2:B:99:THR:CG2	5:I:67:SER:OG	2.19	0.91
8:U:43:ARG:O	8:U:47:ARG:HG2	1.72	0.89
10:O:85:ILE:HG22	11:V:70:LEU:CD1	2.02	0.89
4:Q:1:SER:HA	4:Q:155:GLY:HA2	1.54	0.88
4:D:178:THR:HG21	8:H:16:PRO:HD2	1.57	0.87
8:U:43:ARG:O	8:U:47:ARG:CG	2.23	0.87
8:H:44:VAL:CG2	8:H:47:ARG:NH2	2.36	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:376:LEU:CD1	6:F:20:TYR:HD2	1.90	0.84
2:B:99:THR:HG22	5:I:67:SER:OG	1.77	0.84
4:Q:37:CYS:SG	16:Q:501:HEC:CBB	2.66	0.83
3:P:276:PHE:HD1	3:P:277:ALA:N	1.74	0.83
4:D:37:CYS:SG	16:D:501:HEC:CAB	2.66	0.83
8:H:44:VAL:HG23	8:H:47:ARG:HH21	1.44	0.83
10:O:90:GLU:CG	11:V:71:ASN:OD1	2.26	0.83
3:C:376:LEU:HD12	6:F:20:TYR:CD2	2.14	0.82
3:C:276:PHE:HD1	3:C:277:ALA:N	1.78	0.82
2:B:168:TYR:CD2	2:B:172:LEU:HB2	2.14	0.81
10:O:169:ARG:HH21	10:O:238:LYS:HG2	1.45	0.81
8:H:50:THR:OG1	8:H:51:GLU:N	2.10	0.80
8:H:47:ARG:HH12	8:H:50:THR:C	1.85	0.80
10:O:168:TYR:CD2	10:O:172:LEU:HB2	2.17	0.80
8:U:50:THR:OG1	8:U:51:GLU:N	2.05	0.80
10:O:169:ARG:NH2	10:O:238:LYS:HG2	1.97	0.79
4:D:40:CYS:SG	16:D:501:HEC:CBC	2.69	0.79
3:C:145:VAL:HG21	3:C:268:ILE:HD12	1.64	0.79
8:H:47:ARG:NH1	8:H:50:THR:O	2.15	0.78
3:P:145:VAL:HG21	3:P:268:ILE:HD12	1.65	0.78
8:U:48:SER:C	8:U:49:GLN:HG2	2.04	0.78
4:D:37:CYS:SG	16:D:501:HEC:CBB	2.72	0.78
4:D:40:CYS:SG	16:D:501:HEC:CAC	2.71	0.78
12:C:502:HEM:HMC2	12:C:502:HEM:HBC2	1.64	0.77
4:D:140:GLY:HA3	8:H:53:ASP:HB3	1.64	0.76
4:D:37:CYS:SG	16:D:501:HEC:HBB3	2.25	0.76
10:O:89:ILE:HB	11:V:70:LEU:CD2	2.16	0.75
8:U:44:VAL:HG23	8:U:47:ARG:NH2	2.02	0.74
2:B:169:ARG:NH2	2:B:238:LYS:HG2	2.03	0.74
2:B:99:THR:HG23	5:I:67:SER:OG	1.87	0.74
4:D:120:ARG:NE	16:D:501:HEC:O1A	2.21	0.74
12:C:501:HEM:HBC2	12:C:501:HEM:HMC1	1.70	0.73
8:H:48:SER:C	8:H:49:GLN:HG2	2.09	0.73
5:I:53:GLU:HG3	5:I:53:GLU:O	1.88	0.73
13:P:503:4X9:C6	13:P:503:4X9:H16	2.18	0.72
7:G:77:TYR:O	7:G:80:ASP:O	2.07	0.72
10:O:89:ILE:CD1	11:V:70:LEU:HD22	2.16	0.72
6:F:20:TYR:HD1	6:F:20:TYR:O	1.73	0.72
2:B:78:LYS:HB2	2:B:129:ALA:HB1	1.72	0.71
3:C:106:SER:HB3	12:C:502:HEM:HBD2	1.71	0.71
8:H:43:ARG:O	8:H:47:ARG:HG2	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:438:GLU:OE2	10:O:169:ARG:NH1	2.23	0.71
12:P:501:HEM:HMC1	12:P:501:HEM:HBC2	1.71	0.71
2:B:227:ARG:HE	2:B:227:ARG:HA	1.55	0.70
2:B:168:TYR:O	2:B:173:ALA:HB2	1.92	0.70
3:C:205:SER:OG	13:C:503:4X9:H26B	1.91	0.70
1:N:253:VAL:HB	1:N:324:PHE:CE1	2.26	0.70
12:P:501:HEM:HBB2	12:P:501:HEM:HMB1	1.74	0.70
5:R:98:VAL:O	5:R:98:VAL:HG23	1.92	0.70
8:H:40:CYS:HA	8:H:43:ARG:HG2	1.74	0.70
2:B:169:ARG:NH1	10:O:438:GLU:OE2	2.24	0.70
4:Q:40:CYS:SG	16:Q:501:HEC:HBC3	2.31	0.69
8:H:47:ARG:NH2	8:H:50:THR:OG1	2.23	0.69
10:O:168:TYR:O	10:O:173:ALA:CB	2.30	0.69
1:A:21:ASN:O	1:A:221:GLY:O	2.10	0.69
10:O:78:LYS:HB2	10:O:129:ALA:HB1	1.75	0.69
3:P:276:PHE:CD1	3:P:277:ALA:N	2.60	0.69
10:O:227:ARG:HA	10:O:227:ARG:HE	1.57	0.68
8:H:44:VAL:HA	8:H:47:ARG:HE	1.58	0.68
10:O:304:HIS:O	10:O:305:GLU:HG3	1.93	0.68
4:Q:37:CYS:SG	16:Q:501:HEC:HBB3	2.33	0.68
2:B:29:LEU:HD23	2:B:30:PRO:HD2	1.75	0.67
3:P:276:PHE:HD1	3:P:276:PHE:C	1.97	0.67
11:V:72:VAL:HG13	11:V:73:PRO:HD2	1.77	0.67
3:C:187:PHE:CZ	3:P:184:ILE:CD1	2.78	0.66
3:C:276:PHE:CD1	3:C:277:ALA:N	2.61	0.66
3:C:201:HIS:CE1	13:C:503:4X9:H29	2.30	0.65
2:B:170:ASN:ND2	2:B:170:ASN:H	1.93	0.65
6:F:20:TYR:HD1	6:F:20:TYR:C	1.99	0.65
11:V:72:VAL:HG12	11:V:73:PRO:O	1.95	0.65
3:P:78:ILE:HD11	4:Q:204:MET:CE	2.27	0.65
3:C:220:PHE:O	3:C:220:PHE:HD1	1.80	0.65
5:R:163:SER:HA	5:R:174:GLY:HA3	1.79	0.65
8:H:43:ARG:O	8:H:47:ARG:CG	2.45	0.65
8:H:44:VAL:HA	8:H:47:ARG:NE	2.12	0.65
11:V:70:LEU:O	11:V:70:LEU:HG	1.97	0.65
10:O:29:LEU:HD23	10:O:30:PRO:HD2	1.78	0.64
1:A:253:VAL:HB	1:A:324:PHE:CE1	2.33	0.64
3:P:276:PHE:C	3:P:276:PHE:CD1	2.71	0.64
1:N:21:ASN:O	1:N:221:GLY:O	2.16	0.64
6:F:20:TYR:CD1	6:F:20:TYR:C	2.71	0.64
1:N:324:PHE:CE2	1:N:334:MET:HB3	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:78:ILE:HD11	4:D:204:MET:CE	2.28	0.64
5:I:70:LEU:O	5:I:70:LEU:HG	1.96	0.64
5:R:175:PRO:HG2	18:R:501:FES:S1	2.38	0.63
6:F:20:TYR:HE1	6:F:24:ALA:HB2	1.64	0.63
6:S:40:ASN:C	6:S:40:ASN:OD1	2.35	0.63
3:C:379:TRP:CE2	6:F:33:ARG:HD3	2.34	0.63
5:I:72:VAL:HG12	5:I:73:PRO:O	1.99	0.62
3:P:220:PHE:CD1	3:P:224:TYR:HB2	2.34	0.62
4:D:178:THR:HG21	8:H:16:PRO:CD	2.29	0.62
11:V:62:ARG:O	11:V:78:TYR:HB3	2.00	0.62
10:O:98:VAL:O	11:V:67:SER:HA	2.00	0.62
3:C:168:PHE:HE2	5:R:72:SER:HB2	1.65	0.62
3:P:103:TYR:HB2	3:P:325:PHE:HE2	1.65	0.61
3:C:276:PHE:HD1	3:C:276:PHE:C	2.03	0.61
1:A:293:PRO:O	1:A:297:ILE:HG12	2.01	0.61
2:B:261:SER:OG	2:B:262:ALA:N	2.32	0.61
1:N:284:TYR:CE1	11:V:73:PRO:CB	2.71	0.61
10:O:170:ASN:ND2	10:O:170:ASN:H	1.96	0.61
2:B:169:ARG:CD	10:O:435:PHE:CZ	2.83	0.61
10:O:169:ARG:HH21	10:O:238:LYS:CG	2.12	0.61
1:N:253:VAL:HB	1:N:324:PHE:HE1	1.64	0.61
2:B:435:PHE:CZ	10:O:169:ARG:CD	2.84	0.61
3:P:376:LEU:HB2	6:S:20:TYR:HD2	1.64	0.61
12:C:501:HEM:HHC	12:C:501:HEM:HBB2	1.83	0.60
11:V:76:VAL:HG12	11:V:76:VAL:O	2.01	0.60
3:C:277:ALA:HB1	3:C:294:LEU:CD1	2.31	0.60
9:W:58:LYS:C	9:W:59:TYR:HD1	2.05	0.60
5:I:72:VAL:HG13	5:I:73:PRO:HD2	1.83	0.60
2:B:169:ARG:HD3	10:O:435:PHE:CE2	2.36	0.60
3:P:277:ALA:HB1	3:P:294:LEU:CD1	2.32	0.60
2:B:134:ARG:NH2	6:S:49:ARG:O	2.34	0.60
3:P:376:LEU:CB	6:S:20:TYR:HD2	2.15	0.60
1:A:324:PHE:CE2	1:A:334:MET:HB3	2.37	0.59
4:D:178:THR:CG2	8:H:15:ASP:HA	2.32	0.59
1:A:443:TRP:CD1	1:A:444:LEU:HD23	2.37	0.59
3:C:220:PHE:CD1	3:C:220:PHE:O	2.55	0.59
10:O:89:ILE:HB	11:V:70:LEU:HD23	1.83	0.59
5:R:161:HIS:HB2	18:R:501:FES:S1	2.43	0.59
4:D:33:TYR:HA	4:D:37:CYS:SG	2.43	0.58
2:B:279:LEU:HA	2:B:294:SER:HB3	1.85	0.58
4:Q:181:GLN:HB2	8:U:77:LEU:HD22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:40:CYS:HA	8:U:43:ARG:HG2	1.84	0.58
3:C:375:LYS:O	6:F:17:ARG:NH1	2.36	0.58
7:G:59:TYR:C	7:G:59:TYR:CD1	2.75	0.58
5:I:64:LEU:HD21	5:I:76:VAL:HG13	1.84	0.58
3:C:106:SER:HB3	12:C:502:HEM:CBD	2.33	0.57
2:B:98:VAL:O	5:I:68:VAL:O	2.22	0.57
3:C:120:LEU:HG	3:C:124:MET:HE2	1.86	0.57
3:C:361:LEU:O	3:C:366:MET:HG3	2.04	0.57
3:C:276:PHE:C	3:C:276:PHE:CD1	2.77	0.57
3:C:220:PHE:CZ	13:C:503:4X9:H15	2.39	0.57
1:N:3:THR:HG23	1:N:6:GLN:H	1.69	0.57
8:U:47:ARG:HB2	8:U:50:THR:HG22	1.85	0.57
3:C:103:TYR:HB2	3:C:325:PHE:HE2	1.68	0.57
3:C:220:PHE:CD1	3:C:220:PHE:C	2.78	0.57
10:O:261:SER:OG	10:O:262:ALA:N	2.38	0.57
13:P:503:4X9:H6	13:P:503:4X9:H16	1.87	0.57
3:P:349:THR:HA	3:P:352:GLN:HG2	1.86	0.56
1:A:223:TYR:HB2	1:A:228:VAL:HG21	1.87	0.56
3:P:376:LEU:HB2	6:S:20:TYR:CD2	2.40	0.56
6:F:40:ASN:OD1	6:F:41:ASP:N	2.38	0.56
4:Q:40:CYS:SG	16:Q:501:HEC:CAC	2.93	0.56
6:F:49:ARG:O	10:O:134:ARG:NH2	2.39	0.56
2:B:71:LEU:HD23	5:I:68:VAL:HG11	1.88	0.56
3:P:18:PHE:O	3:P:220:PHE:HD2	1.88	0.56
4:Q:33:TYR:HA	4:Q:37:CYS:SG	2.45	0.56
1:A:253:VAL:HB	1:A:324:PHE:HE1	1.70	0.56
4:D:178:THR:HG21	8:H:15:ASP:HA	1.87	0.56
10:O:97:SER:HA	11:V:69:SER:OG	2.06	0.56
2:B:169:ARG:NH2	2:B:238:LYS:CG	2.69	0.56
5:E:58:PHE:O	5:E:61:SER:HB3	2.06	0.56
5:I:52:ARG:HD2	5:I:53:GLU:H	1.71	0.56
3:P:145:VAL:HG21	3:P:268:ILE:CD1	2.36	0.56
6:S:40:ASN:OD1	6:S:41:ASP:N	2.38	0.56
8:H:48:SER:C	8:H:49:GLN:CG	2.75	0.56
10:O:86:THR:HA	11:V:70:LEU:HD11	1.87	0.56
10:O:71:LEU:HD23	11:V:68:VAL:HG21	1.87	0.55
3:P:103:TYR:HD1	3:P:325:PHE:HD2	1.53	0.55
3:P:70:CYS:SG	3:P:80:ARG:HD3	2.46	0.55
8:H:40:CYS:CA	8:H:43:ARG:HG2	2.36	0.55
3:C:21:LEU:HD23	3:C:220:PHE:HD2	1.72	0.55
7:G:59:TYR:C	7:G:59:TYR:HD1	2.08	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:LEU:HD13	5:I:66:ALA:HB2	1.88	0.55
1:A:27:SER:HA	1:A:199:ALA:O	2.06	0.55
4:Q:1:SER:CA	4:Q:155:GLY:HA2	2.32	0.55
8:H:35:GLU:C	8:H:39:LEU:HD12	2.27	0.55
10:O:31:ASN:ND2	10:O:225:ASN:OD1	2.39	0.55
8:H:35:GLU:O	8:H:39:LEU:HD12	2.07	0.55
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.89	0.55
16:D:501:HEC:HBD2	16:D:501:HEC:HHA	1.88	0.55
3:C:105:GLY:HA2	3:C:107:TYR:CE2	2.42	0.55
4:Q:204:MET:HG2	15:Q:506:PEE:H2	1.88	0.55
1:A:3:THR:HG23	1:A:6:GLN:H	1.71	0.54
3:C:220:PHE:C	3:C:220:PHE:HD1	2.11	0.54
10:O:90:GLU:HA	11:V:71:ASN:HD21	1.71	0.54
16:D:501:HEC:HHA	16:D:501:HEC:CBD	2.37	0.54
6:F:40:ASN:OD1	6:F:40:ASN:C	2.44	0.54
5:I:53:GLU:O	5:I:53:GLU:CG	2.56	0.54
10:O:176:LEU:HD12	11:V:64:VAL:HG23	1.90	0.54
1:N:284:TYR:CD1	11:V:73:PRO:HB3	2.38	0.54
10:O:226:ILE:HD12	10:O:227:ARG:N	2.23	0.54
3:C:8:HIS:N	3:C:9:PRO:HD3	2.23	0.54
1:A:233:PRO:O	5:E:22:THR:HA	2.07	0.54
1:N:288:ALA:HB2	1:N:300:THR:HG22	1.90	0.54
2:B:169:ARG:HD3	10:O:435:PHE:CZ	2.43	0.53
8:U:48:SER:C	8:U:49:GLN:CG	2.77	0.53
3:C:75:TYR:CE2	5:E:57:GLN:HG2	2.42	0.53
2:B:99:THR:CG2	5:I:67:SER:HG	2.22	0.53
3:C:184:ILE:CD1	3:P:187:PHE:CZ	2.91	0.53
2:B:299:VAL:HG11	2:B:336:VAL:HG13	1.90	0.53
3:C:104:TYR:CD1	3:C:208:PRO:HA	2.43	0.53
3:P:221:HIS:ND1	3:P:222:PRO:HA	2.24	0.53
4:D:211:MET:HG2	9:J:35:PHE:CE2	2.43	0.53
7:T:59:TYR:C	7:T:59:TYR:CD1	2.82	0.53
3:P:376:LEU:HD12	6:S:20:TYR:CD2	2.44	0.53
1:N:219:LEU:HG	1:N:220:SER:O	2.08	0.53
3:C:11:MET:C	3:C:11:MET:SD	2.88	0.53
13:P:503:4X9:C6	13:P:503:4X9:C16	2.84	0.53
1:A:162:PRO:HD2	1:A:234:CYS:SG	2.48	0.52
8:H:44:VAL:HG23	8:H:47:ARG:NH2	2.14	0.52
2:B:157:ALA:O	2:B:161:GLU:HG2	2.09	0.52
2:B:168:TYR:CE2	2:B:172:LEU:HD12	2.44	0.52
1:N:106:LEU:HB3	1:N:107:PRO:HD3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:299:VAL:HG11	10:O:336:VAL:HG13	1.91	0.52
4:Q:178:THR:HG21	8:U:16:PRO:HD2	1.90	0.52
3:P:375:LYS:O	6:S:17:ARG:NH1	2.37	0.52
1:N:283:THR:HB	11:V:74:ALA:HB3	1.91	0.52
6:F:107:TRP:HE1	10:O:87:ARG:HB3	1.75	0.52
3:C:11:MET:SD	3:C:11:MET:O	2.67	0.52
6:F:20:TYR:CE1	6:F:24:ALA:HB2	2.43	0.52
12:P:502:HEM:HMB1	12:P:502:HEM:HBB2	1.92	0.52
9:W:59:TYR:CD1	9:W:59:TYR:N	2.75	0.52
2:B:169:ARG:NH1	2:B:169:ARG:NH2	2.41	0.52
9:J:58:LYS:C	9:J:59:TYR:HD1	2.13	0.52
10:O:42:ALA:O	10:O:113:ARG:NH1	2.41	0.52
3:P:103:TYR:HD1	3:P:325:PHE:CD2	2.28	0.52
3:C:246:ALA:HB1	3:C:249:LEU:HB2	1.92	0.51
5:I:64:LEU:HD23	5:I:65:VAL:N	2.24	0.51
10:O:279:LEU:HA	10:O:294:SER:HB3	1.91	0.51
10:O:96:LEU:O	11:V:69:SER:HA	2.10	0.51
3:P:226:ILE:HA	3:P:229:ILE:HD12	1.92	0.51
3:P:361:LEU:O	3:P:366:MET:HG3	2.10	0.51
2:B:101:THR:HG1	2:B:103:GLU:H	1.57	0.51
3:C:277:ALA:HB1	3:C:294:LEU:HD12	1.92	0.51
4:D:141:VAL:HG23	8:H:53:ASP:OD2	2.10	0.51
2:B:435:PHE:CE2	10:O:169:ARG:HD3	2.45	0.51
10:O:49:LEU:HD23	10:O:127:THR:HG21	1.91	0.51
3:P:103:TYR:HB2	3:P:325:PHE:CE2	2.44	0.51
10:O:168:TYR:CE2	10:O:172:LEU:HD12	2.45	0.51
3:C:145:VAL:HG21	3:C:268:ILE:CD1	2.36	0.51
3:P:211:ILE:HD11	6:S:36:THR:HG22	1.93	0.51
7:T:73:ASN:HB3	7:T:75:ALA:H	1.76	0.51
2:B:226:ILE:HD12	2:B:227:ARG:N	2.25	0.51
5:I:65:VAL:HG23	5:I:77:ARG:HB2	1.91	0.51
10:O:85:ILE:HG22	11:V:70:LEU:HD11	1.90	0.51
5:I:76:VAL:O	5:I:76:VAL:HG12	2.10	0.51
1:N:27:SER:HA	1:N:199:ALA:O	2.11	0.51
2:B:435:PHE:CZ	10:O:169:ARG:HD2	2.46	0.51
3:C:181:PHE:HA	3:C:184:ILE:HG22	1.92	0.51
3:C:349:THR:HA	3:C:352:GLN:HG2	1.93	0.51
12:C:502:HEM:HBC2	12:C:502:HEM:CMC	2.38	0.51
3:P:246:ALA:HB1	3:P:249:LEU:HB2	1.92	0.51
3:P:277:ALA:HB1	3:P:294:LEU:HD12	1.93	0.51
3:C:120:LEU:HG	3:C:124:MET:CE	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:75:LEU:HD22	10:O:136:GLU:HB3	1.93	0.51
3:P:120:LEU:HG	3:P:124:MET:HE2	1.93	0.51
1:A:244:ARG:CZ	7:G:10:VAL:HB	2.41	0.50
3:C:19:ILE:HG22	3:C:20:ASP:OD1	2.11	0.50
10:O:90:GLU:HG3	11:V:71:ASN:OD1	2.09	0.50
6:S:71:ARG:O	6:S:72:GLN:HB2	2.12	0.50
4:D:137:PRO:HA	4:D:149:PHE:CD2	2.46	0.50
10:O:98:VAL:HG22	10:O:107:TYR:CD1	2.46	0.50
17:Q:505:CDL:C42	17:T:501:CDL:C78	2.90	0.50
3:C:75:TYR:CD2	5:E:57:GLN:HG2	2.47	0.50
3:P:325:PHE:C	3:P:325:PHE:CD1	2.85	0.50
12:P:502:HEM:CMB	12:P:502:HEM:HBB2	2.42	0.50
4:Q:40:CYS:SG	16:Q:501:HEC:CBC	2.98	0.50
5:R:134:ILE:HD11	5:R:185:TYR:CG	2.47	0.50
2:B:177:TYR:OH	5:I:76:VAL:CG2	2.60	0.50
1:N:223:TYR:CB	1:N:228:VAL:HG21	2.41	0.49
1:N:293:PRO:O	1:N:297:ILE:HG12	2.12	0.49
10:O:157:ALA:O	10:O:161:GLU:HG2	2.12	0.49
6:S:12:TRP:CD1	6:S:13:LEU:HD23	2.47	0.49
3:C:226:ILE:HA	3:C:229:ILE:HD12	1.94	0.49
3:P:51:LEU:HD13	12:P:501:HEM:HBD1	1.94	0.49
5:R:150:ALA:O	5:R:157:TYR:HB2	2.12	0.49
10:O:385:GLN:O	10:O:389:ALA:O	2.29	0.49
3:P:137:GLN:OE1	3:P:260:ASN:N	2.45	0.49
3:P:14:VAL:HG12	3:P:14:VAL:O	2.11	0.49
1:A:288:ALA:HB2	1:A:300:THR:HG22	1.93	0.49
3:C:70:CYS:SG	3:C:80:ARG:HD3	2.52	0.49
1:N:3:THR:OG1	1:N:4:TYR:N	2.46	0.49
2:B:83:PHE:CZ	6:S:107:TRP:HD1	2.31	0.49
2:B:308:ASP:HB2	5:I:55:LEU:CB	2.42	0.49
2:B:435:PHE:CZ	10:O:169:ARG:HD3	2.47	0.49
5:R:171:ILE:HD11	5:R:176:ALA:HB3	1.95	0.49
1:A:106:LEU:HB3	1:A:107:PRO:HD3	1.95	0.49
1:A:223:TYR:CB	1:A:228:VAL:HG21	2.42	0.49
3:C:10:LEU:HD12	3:C:10:LEU:C	2.32	0.49
4:D:231:LYS:O	6:F:71:ARG:HD3	2.13	0.49
2:B:100:SER:O	5:I:66:ALA:O	2.30	0.49
5:R:140:THR:HB	5:R:177:PRO:HD2	1.95	0.49
4:Q:211:MET:HG2	9:W:35:PHE:CE2	2.48	0.49
1:A:223:TYR:HB2	1:A:228:VAL:CG2	2.42	0.49
2:B:316:TYR:N	2:B:316:TYR:CD1	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:380:ASP:O	2:B:384:SER:HB2	2.13	0.49
10:O:169:ARG:HH21	10:O:238:LYS:HB3	1.77	0.49
3:P:105:GLY:HA2	3:P:107:TYR:CE2	2.48	0.49
1:N:443:TRP:CD1	1:N:444:LEU:HD23	2.48	0.49
1:A:294:LEU:HD13	1:A:337:VAL:HG12	1.95	0.48
1:N:386:TYR:CD2	1:N:390:ILE:HD12	2.47	0.48
2:B:169:ARG:HD2	10:O:435:PHE:CZ	2.48	0.48
2:B:129:ALA:N	2:B:130:PRO:CD	2.77	0.48
9:J:59:TYR:CD1	9:J:59:TYR:N	2.82	0.48
10:O:164:HIS:NE2	10:O:316:TYR:OH	2.40	0.48
3:P:13:ILE:O	3:P:16:ASN:ND2	2.46	0.48
12:P:502:HEM:HBC2	12:P:502:HEM:HHD	1.95	0.48
4:Q:149:PHE:CE1	4:Q:156:GLN:HB3	2.48	0.48
4:Q:36:VAL:O	16:Q:501:HEC:HMC3	2.14	0.48
7:T:25:ALA:O	7:T:27:PRO:HD3	2.14	0.48
10:O:95:LYS:HG3	11:V:72:VAL:CG2	2.44	0.48
1:A:53:ASN:HD21	1:A:165:GLN:HB3	1.79	0.48
3:C:137:GLN:OE1	3:C:260:ASN:N	2.46	0.48
3:C:312:GLN:HG3	3:C:379:TRP:CZ3	2.47	0.48
2:B:49:LEU:HD23	2:B:127:THR:HG21	1.94	0.48
3:C:103:TYR:HB2	3:C:325:PHE:CE2	2.48	0.48
2:B:97:SER:HA	5:I:69:SER:HB3	1.96	0.48
3:P:120:LEU:HG	3:P:124:MET:CE	2.43	0.48
8:U:35:GLU:C	8:U:39:LEU:HD12	2.34	0.48
10:O:95:LYS:HG3	11:V:72:VAL:HG23	1.95	0.48
10:O:229:GLY:O	10:O:230:LEU:C	2.51	0.48
10:O:96:LEU:HG	10:O:96:LEU:O	2.13	0.48
6:S:20:TYR:CD1	6:S:20:TYR:O	2.66	0.48
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.49	0.48
3:C:15:ASN:N	3:C:15:ASN:OD1	2.46	0.48
4:D:140:GLY:CA	8:H:53:ASP:HB3	2.39	0.48
3:P:131:TYR:HA	12:P:501:HEM:HAA1	1.94	0.48
3:C:103:TYR:HD1	3:C:325:PHE:HD2	1.61	0.48
1:N:245:GLU:HG3	1:N:248:LEU:HG	1.96	0.48
2:B:209:LEU:CD2	2:B:375:SER:HB2	2.43	0.48
3:C:14:VAL:HG12	3:C:14:VAL:O	2.14	0.48
3:C:29:SER:O	3:C:32:ASN:HB2	2.13	0.48
16:D:501:HEC:HMB1	16:D:501:HEC:CBB	2.44	0.48
8:H:41:ASP:O	8:H:45:SER:OG	2.19	0.48
5:I:52:ARG:HD2	5:I:53:GLU:N	2.28	0.48
3:P:104:TYR:CD1	3:P:208:PRO:HA	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:TYR:CD2	1:A:390:ILE:HD12	2.49	0.48
2:B:229:GLY:O	2:B:230:LEU:C	2.53	0.48
3:C:325:PHE:C	3:C:325:PHE:CD1	2.87	0.48
10:O:312:PHE:HD1	10:O:313:ASN:N	2.11	0.48
10:O:243:GLU:HA	10:O:424:MET:O	2.13	0.48
6:S:20:TYR:CD1	6:S:20:TYR:C	2.85	0.48
4:D:225:HIS:CE1	7:G:20:PRO:HB2	2.49	0.47
1:N:85:HIS:HB2	1:N:100:LYS:HB2	1.96	0.47
10:O:85:ILE:CG2	11:V:70:LEU:HD13	2.29	0.47
3:P:75:TYR:CE2	5:R:57:GLN:HG2	2.49	0.47
1:A:3:THR:OG1	1:A:4:TYR:N	2.47	0.47
2:B:29:LEU:CD2	2:B:30:PRO:HD2	2.43	0.47
2:B:385:GLN:O	2:B:389:ALA:O	2.32	0.47
1:A:267:ASN:O	1:A:271:GLN:HG2	2.15	0.47
3:C:211:ILE:HD11	6:F:36:THR:HG22	1.95	0.47
4:D:211:MET:HG2	9:J:35:PHE:HE2	1.79	0.47
10:O:301:LYS:HG3	10:O:301:LYS:O	2.13	0.47
10:O:316:TYR:N	10:O:316:TYR:CD1	2.80	0.47
3:P:10:LEU:HD12	3:P:10:LEU:C	2.35	0.47
4:Q:3:LEU:HD21	8:U:56:GLU:HG3	1.96	0.47
2:B:227:ARG:NE	2:B:227:ARG:HA	2.26	0.47
4:D:218:LEU:O	4:D:221:ALA:HB3	2.13	0.47
2:B:354:ASN:N	2:B:355:PRO:HD2	2.30	0.47
16:Q:501:HEC:CBB	16:Q:501:HEC:HMB1	2.45	0.47
5:R:98:VAL:O	5:R:98:VAL:CG2	2.62	0.47
8:U:35:GLU:O	8:U:39:LEU:HD12	2.15	0.47
10:O:86:THR:HA	11:V:70:LEU:HD21	1.97	0.47
3:P:14:VAL:CG1	3:P:14:VAL:O	2.63	0.47
3:P:77:TRP:CZ3	3:P:78:ILE:HG13	2.50	0.47
2:B:435:PHE:CD1	2:B:435:PHE:N	2.82	0.47
11:V:62:ARG:HB3	11:V:63:PRO:HD2	1.97	0.47
5:R:45:VAL:HG13	9:W:28:ALA:HA	1.96	0.47
15:Q:506:PEE:H11	5:R:53:ASN:OD1	2.15	0.47
7:T:59:TYR:C	7:T:59:TYR:HD1	2.17	0.47
10:O:209:LEU:CD2	10:O:375:SER:HB2	2.45	0.46
12:P:501:HEM:HHA	12:P:501:HEM:CBA	2.45	0.46
5:R:171:ILE:CD1	5:R:176:ALA:HB3	2.45	0.46
13:C:503:4X9:C12	13:C:503:4X9:C6	2.89	0.46
5:E:31:ALA:HB2	9:J:7:ALA:HB2	1.96	0.46
3:P:379:TRP:CE3	6:S:33:ARG:HD3	2.51	0.46
4:D:138:PRO:HG3	8:H:55:THR:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:358:TYR:HE1	3:P:362:ILE:HD11	1.80	0.46
8:H:40:CYS:O	8:H:43:ARG:CG	2.64	0.46
1:N:294:LEU:HD13	1:N:337:VAL:HG12	1.97	0.46
10:O:34:VAL:HG11	10:O:386:ALA:HB1	1.98	0.46
12:P:501:HEM:HBB2	12:P:501:HEM:CMB	2.42	0.46
3:C:373:GLU:HA	6:F:20:TYR:HE2	1.80	0.46
8:U:17:LEU:HD11	8:U:21:ARG:NE	2.30	0.46
1:N:442:PHE:CD1	1:N:442:PHE:C	2.89	0.46
5:R:91:TRP:HZ3	5:R:136:ILE:HD11	1.81	0.46
1:A:245:GLU:HG3	1:A:248:LEU:HG	1.97	0.46
2:B:308:ASP:HB2	5:I:55:LEU:HB2	1.97	0.46
4:D:138:PRO:HD3	4:D:149:PHE:CE2	2.50	0.46
4:D:181:GLN:OE1	8:H:77:LEU:HB3	2.16	0.46
3:P:103:TYR:CD1	3:P:325:PHE:CD2	3.04	0.46
2:B:87:ARG:HB3	6:S:107:TRP:NE1	2.30	0.46
3:C:186:PRO:HG2	12:C:501:HEM:HMC3	1.96	0.46
2:B:109:VAL:HB	2:B:119:LEU:HD12	1.98	0.46
1:A:77:LYS:HE3	2:B:291:ALA:HB1	1.97	0.46
2:B:70:ARG:HG2	5:I:68:VAL:HB	1.98	0.46
1:N:219:LEU:O	1:N:220:SER:C	2.54	0.46
10:O:169:ARG:HH21	10:O:238:LYS:CB	2.29	0.46
10:O:354:ASN:N	10:O:355:PRO:HD2	2.31	0.45
3:P:319:PRO:HD2	6:S:20:TYR:CE1	2.51	0.45
3:C:14:VAL:CG1	3:C:14:VAL:O	2.64	0.45
12:C:502:HEM:HBB2	12:C:502:HEM:CMB	2.47	0.45
4:D:40:CYS:SG	16:D:501:HEC:C3C	3.04	0.45
10:O:26:PHE:CE2	10:O:391:SER:HA	2.52	0.45
10:O:99:THR:HG23	11:V:67:SER:OG	2.15	0.45
4:Q:149:PHE:CD1	4:Q:156:GLN:HB3	2.50	0.45
3:C:233:LEU:HD22	4:D:216:LEU:HG	1.98	0.45
4:D:37:CYS:HG	16:D:501:HEC:HBB3	1.80	0.45
8:H:17:LEU:HD11	8:H:21:ARG:NE	2.31	0.45
1:N:442:PHE:C	1:N:442:PHE:HD1	2.20	0.45
10:O:213:HIS:N	10:O:214:PRO:CD	2.79	0.45
3:C:10:LEU:HD21	3:P:202:GLU:HG3	1.99	0.45
4:Q:137:PRO:HA	4:Q:149:PHE:CD2	2.52	0.45
10:O:129:ALA:N	10:O:130:PRO:CD	2.80	0.45
3:P:103:TYR:CD1	3:P:325:PHE:HD2	2.34	0.45
4:Q:3:LEU:CD2	8:U:56:GLU:HG3	2.47	0.45
4:D:216:LEU:N	4:D:217:PRO:HD2	2.31	0.45
1:N:77:LYS:HE3	10:O:291:ALA:HB1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:GLU:HG3	1:A:215:HIS:CE1	2.52	0.45
2:B:303:VAL:HG23	2:B:303:VAL:O	2.16	0.45
7:G:75:ALA:O	7:G:77:TYR:CD2	2.69	0.45
1:N:233:PRO:O	5:R:22:THR:HA	2.17	0.45
10:O:291:ALA:HA	10:O:297:GLN:NE2	2.31	0.45
6:S:68:LEU:HD11	6:S:75:LEU:HG	1.99	0.45
3:C:221:HIS:ND1	3:C:222:PRO:HA	2.32	0.45
8:H:73:LEU:HD23	8:H:73:LEU:O	2.17	0.45
5:I:70:LEU:CG	5:I:70:LEU:O	2.64	0.45
3:P:103:TYR:CE2	15:P:505:PEE:H2	2.51	0.45
1:A:140:GLU:OE2	5:I:52:ARG:O	2.35	0.45
3:P:15:ASN:OD1	3:P:15:ASN:N	2.49	0.45
2:B:87:ARG:HB3	6:S:107:TRP:HE1	1.82	0.45
6:F:26:PHE:HD1	6:F:27:ASN:N	2.15	0.44
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.52	0.44
13:P:503:4X9:H6	13:P:503:4X9:C16	2.47	0.44
5:R:175:PRO:CG	18:R:501:FES:S1	3.04	0.44
3:C:144:THR:O	3:C:148:ASN:HB2	2.17	0.44
8:H:40:CYS:CB	8:H:54:CYS:SG	3.05	0.44
5:E:45:VAL:HG13	9:J:28:ALA:HA	1.99	0.44
10:O:227:ARG:NE	10:O:227:ARG:HA	2.28	0.44
10:O:325:TYR:HD1	10:O:326:THR:N	2.14	0.44
8:U:73:LEU:O	8:U:73:LEU:HD23	2.17	0.44
1:A:149:VAL:HG23	1:A:425:PHE:CB	2.47	0.44
1:A:84:ALA:HB1	1:A:100:LYS:O	2.18	0.44
4:Q:31:GLN:O	4:Q:35:GLN:HG2	2.17	0.44
1:A:120:CYS:SG	1:A:122:LEU:HG	2.57	0.44
5:E:72:SER:HB2	3:P:168:PHE:HE2	1.81	0.44
8:U:40:CYS:O	8:U:43:ARG:HG3	2.18	0.44
2:B:164:HIS:NE2	2:B:316:TYR:OH	2.43	0.44
13:C:503:4X9:H12	13:C:503:4X9:C6	2.47	0.44
10:O:58:GLU:OE1	10:O:63:LEU:HA	2.16	0.44
10:O:85:ILE:O	11:V:70:LEU:HD21	2.17	0.44
10:O:151:ALA:HB2	11:V:76:VAL:HG21	1.98	0.44
2:B:213:HIS:N	2:B:214:PRO:CD	2.81	0.44
2:B:31:ASN:ND2	2:B:225:ASN:OD1	2.51	0.44
2:B:34:VAL:HG11	2:B:386:ALA:HB1	1.99	0.44
3:C:312:GLN:HG3	3:C:379:TRP:HZ3	1.82	0.44
10:O:124:LEU:HD22	10:O:224:LEU:HD12	2.00	0.44
10:O:70:ARG:NE	11:V:66:ALA:HB3	2.33	0.44
3:P:181:PHE:HA	3:P:184:ILE:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:29:SER:O	3:P:32:ASN:HB2	2.18	0.44
4:Q:138:PRO:HD3	4:Q:149:PHE:CE2	2.53	0.44
3:C:103:TYR:HD1	3:C:325:PHE:CD2	2.35	0.44
3:C:220:PHE:CE2	13:C:503:4X9:H15	2.52	0.44
1:N:41:ILE:HG12	1:N:195:MET:HG2	1.99	0.44
3:P:219:PRO:HB2	3:P:221:HIS:O	2.17	0.44
2:B:83:PHE:CZ	6:S:107:TRP:CD1	3.06	0.44
1:N:162:PRO:HD2	1:N:234:CYS:SG	2.58	0.44
10:O:168:TYR:N	10:O:168:TYR:CD1	2.86	0.44
10:O:208:GLY:HA3	10:O:216:LEU:HD11	2.00	0.44
2:B:98:VAL:HG22	2:B:107:TYR:CD1	2.53	0.43
3:C:99:GLY:O	3:C:100:ARG:C	2.57	0.43
3:C:50:PHE:HE2	5:E:58:PHE:HB3	1.82	0.43
1:N:84:ALA:HB1	1:N:100:LYS:O	2.18	0.43
5:R:72:SER:O	5:R:92:ARG:NE	2.50	0.43
1:A:442:PHE:CD1	1:A:442:PHE:C	2.91	0.43
2:B:47:ILE:HD11	2:B:116:VAL:HG12	1.99	0.43
12:C:501:HEM:HBC2	12:C:501:HEM:CMC	2.43	0.43
3:P:26:ASN:ND2	3:P:208:PRO:HD2	2.33	0.43
4:Q:178:THR:HG21	8:U:15:ASP:HA	2.00	0.43
2:B:291:ALA:HA	2:B:297:GLN:NE2	2.33	0.43
3:C:358:TYR:HE1	3:C:362:ILE:HD11	1.83	0.43
4:Q:48:TYR:CE2	4:Q:65:ALA:HA	2.54	0.43
1:A:369:LEU:HD12	1:A:392:LEU:HD21	2.00	0.43
2:B:299:VAL:O	2:B:299:VAL:HG12	2.18	0.43
4:D:137:PRO:HA	4:D:149:PHE:HD2	1.83	0.43
1:N:252:HIS:CE1	1:N:325:VAL:HG22	2.54	0.43
5:R:75:GLU:OE1	5:R:75:GLU:HA	2.19	0.43
10:O:47:ILE:HD11	10:O:116:VAL:HG12	1.99	0.43
2:B:243:GLU:HA	2:B:424:MET:O	2.18	0.43
1:N:267:ASN:O	1:N:271:GLN:HG2	2.18	0.43
1:A:41:ILE:HD13	1:A:190:TYR:CE1	2.54	0.43
4:D:240:PRO:O	4:D:241:LYS:HG3	2.19	0.43
5:I:68:VAL:HG12	5:I:69:SER:N	2.34	0.43
1:A:192:ALA:N	1:A:193:PRO:HD2	2.34	0.43
2:B:26:PHE:CE1	2:B:391:SER:HA	2.54	0.43
3:C:77:TRP:CZ3	3:C:78:ILE:HG13	2.54	0.43
10:O:37:SER:HA	10:O:208:GLY:O	2.19	0.43
3:P:94:LEU:O	3:P:98:VAL:HG23	2.19	0.43
1:A:246:ASP:OD2	7:G:9:ARG:HA	2.18	0.43
1:A:430:GLN:O	1:A:431:LEU:C	2.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:20:TYR:O	6:F:21:TYR:C	2.57	0.42
1:N:192:ALA:N	1:N:193:PRO:HD2	2.33	0.42
3:C:187:PHE:HZ	3:P:184:ILE:CD1	2.31	0.42
3:P:201:HIS:NE2	13:P:503:4X9:H29	2.35	0.42
6:S:18:LYS:HA	6:S:83:TYR:CD2	2.54	0.42
1:A:185:TYR:CD1	1:A:189:HIS:CD2	3.07	0.42
3:P:11:MET:C	3:P:11:MET:SD	2.97	0.42
1:N:123:GLU:HB2	1:N:126:GLN:HB2	2.00	0.42
1:N:379:ILE:HG12	1:N:389:ARG:CD	2.49	0.42
3:P:75:TYR:CD2	5:R:57:GLN:HG2	2.55	0.42
5:R:141:HIS:O	5:R:141:HIS:CG	2.72	0.42
1:A:21:ASN:HB2	1:A:221:GLY:CA	2.49	0.42
2:B:42:ALA:O	2:B:113:ARG:NH1	2.49	0.42
4:Q:216:LEU:N	4:Q:217:PRO:HD2	2.35	0.42
2:B:169:ARG:HH22	2:B:238:LYS:HG2	1.78	0.42
2:B:312:PHE:HD1	2:B:313:ASN:N	2.17	0.42
1:N:204:GLU:O	1:N:205:HIS:C	2.57	0.42
3:C:21:LEU:HD23	3:C:220:PHE:CD2	2.53	0.42
10:O:299:VAL:HG21	10:O:340:ALA:HB2	2.01	0.42
3:P:174:THR:O	3:P:177:ARG:HG2	2.20	0.42
4:Q:105:ASN:HD22	16:Q:501:HEC:HMD3	1.85	0.42
8:U:44:VAL:HA	8:U:47:ARG:CZ	2.49	0.42
3:C:26:ASN:ND2	3:C:208:PRO:HD2	2.35	0.42
3:C:310:SER:HA	3:C:374:ASN:HD21	1.85	0.42
10:O:26:PHE:HZ	10:O:390:GLY:O	2.01	0.42
10:O:83:PHE:CE1	10:O:87:ARG:HG3	2.55	0.42
3:P:17:ALA:O	3:P:18:PHE:CD1	2.72	0.42
3:P:19:ILE:HG22	3:P:20:ASP:OD1	2.19	0.42
1:A:270:LEU:HD21	1:A:414:TYR:HD2	1.85	0.42
2:B:208:GLY:HA3	2:B:216:LEU:HD11	2.01	0.42
4:D:149:PHE:CD1	4:D:156:GLN:HB3	2.55	0.42
3:P:16:ASN:N	3:P:16:ASN:HD22	2.17	0.42
4:D:143:LEU:HD11	4:D:149:PHE:HB2	2.02	0.42
4:Q:126:TYR:C	4:Q:126:TYR:CD1	2.93	0.42
4:Q:182:VAL:HG12	4:Q:183:ALA:N	2.35	0.42
3:C:140:PHE:C	3:C:140:PHE:CD1	2.93	0.42
10:O:240:HIS:ND1	10:O:241:GLY:O	2.52	0.42
5:R:44:THR:HG21	9:W:24:ILE:HD13	2.02	0.42
1:A:46:ARG:NH1	1:A:93:GLU:OE2	2.49	0.41
2:B:51:ILE:HG12	2:B:204:MET:HG2	2.02	0.41
4:Q:118:ARG:HD2	4:Q:194:ALA:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:224:ARG:HG3	7:T:26:PHE:CE1	2.55	0.41
3:C:284:ILE:HD12	3:C:293:ALA:HB2	2.01	0.41
4:D:48:TYR:CE2	4:D:65:ALA:HA	2.55	0.41
1:N:280:TYR:HB3	1:N:307:PHE:CE2	2.55	0.41
10:O:96:LEU:C	11:V:69:SER:HB3	2.41	0.41
3:P:310:SER:HA	3:P:374:ASN:HD21	1.85	0.41
2:B:299:VAL:HG21	2:B:340:ALA:HB2	2.02	0.41
3:C:13:ILE:O	3:C:16:ASN:ND2	2.52	0.41
1:N:327:ASP:OD1	1:N:328:HIS:N	2.53	0.41
1:N:40:TRP:CZ2	1:N:377:GLU:HA	2.56	0.41
10:O:435:PHE:CD1	10:O:435:PHE:N	2.88	0.41
4:Q:237:TYR:HB2	6:S:60:PHE:CD1	2.54	0.41
5:R:113:GLU:OE1	5:R:115:SER:N	2.52	0.41
3:C:17:ALA:O	3:C:18:PHE:CD1	2.74	0.41
3:C:193:ALA:O	3:C:196:HIS:HB3	2.21	0.41
1:N:149:VAL:HG23	1:N:425:PHE:CB	2.50	0.41
4:Q:131:LEU:HD11	16:Q:501:HEC:HMB2	2.02	0.41
1:A:442:PHE:HD1	1:A:442:PHE:C	2.23	0.41
4:D:198:HIS:C	4:D:198:HIS:ND1	2.73	0.41
4:D:28:ARG:HA	4:D:31:GLN:HE21	1.85	0.41
11:V:70:LEU:O	11:V:70:LEU:CG	2.66	0.41
3:C:187:PHE:CZ	3:P:184:ILE:HD11	2.56	0.41
10:O:303:VAL:O	10:O:303:VAL:HG23	2.20	0.41
10:O:417:PHE:CD1	10:O:417:PHE:C	2.94	0.41
4:Q:110:PRO:HA	4:Q:111:PRO:HD2	1.97	0.41
7:T:34:ILE:N	7:T:35:PRO:HD2	2.35	0.41
1:A:41:ILE:HG12	1:A:195:MET:HG2	2.03	0.41
1:A:37:VAL:HG23	1:A:199:ALA:HB2	2.03	0.41
4:D:140:GLY:HA3	8:H:53:ASP:CB	2.42	0.41
7:G:79:ASN:ND2	8:H:52:GLU:OE2	2.53	0.41
10:O:172:LEU:HD13	10:O:316:TYR:CD2	2.56	0.41
3:P:186:PRO:HG2	12:P:501:HEM:HMC3	2.03	0.41
4:Q:204:MET:HE3	15:Q:506:PEE:O4	2.21	0.41
1:A:294:LEU:HG	1:A:307:PHE:CZ	2.56	0.41
12:C:502:HEM:HMB1	12:C:502:HEM:HBB2	2.02	0.41
6:F:71:ARG:O	6:F:72:GLN:HB2	2.20	0.41
1:N:246:ASP:OD2	7:T:9:ARG:HA	2.20	0.41
10:O:166:ALA:HB2	10:O:244:ILE:HG13	2.03	0.41
10:O:86:THR:N	11:V:70:LEU:HD11	2.36	0.41
5:R:137:GLY:O	5:R:146:PRO:HD2	2.21	0.41
5:R:14:ARG:NH1	5:R:18:VAL:O	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:188:THR:HG23	5:R:192:MET:HB2	2.02	0.41
3:C:311:LYS:HE2	3:C:379:TRP:CD1	2.56	0.41
3:C:30:TRP:NE1	15:C:505:PEE:O4	2.53	0.41
10:O:144:LEU:HB2	10:O:183:ILE:HG23	2.02	0.41
4:D:7:PRO:HA	4:D:8:PRO:HD3	1.92	0.41
5:R:82:PRO:HD2	5:R:85:LYS:HD3	2.03	0.41
8:U:47:ARG:CD	8:U:50:THR:CG2	2.99	0.41
2:B:209:LEU:HD23	2:B:375:SER:HB2	2.02	0.40
4:D:27:ARG:NH1	9:J:59:TYR:CE2	2.90	0.40
6:F:18:LYS:HG3	6:F:83:TYR:HD2	1.86	0.40
3:P:376:LEU:CD1	6:S:20:TYR:CD2	3.03	0.40
10:O:74:SER:CB	11:V:70:LEU:HD12	2.51	0.40
4:Q:60:GLU:OE2	9:W:59:TYR:HB3	2.20	0.40
2:B:365:LYS:HG2	2:B:399:LEU:HD23	2.03	0.40
4:D:179:MET:HB3	8:H:15:ASP:OD2	2.21	0.40
5:E:16:PRO:HA	5:E:19:LEU:HD12	2.03	0.40
6:F:18:LYS:HA	6:F:83:TYR:CD2	2.57	0.40
4:Q:204:MET:HB3	4:Q:204:MET:HE3	1.86	0.40
4:Q:211:MET:HG2	9:W:35:PHE:HE2	1.84	0.40
9:W:58:LYS:C	9:W:59:TYR:CD1	2.90	0.40
4:D:19:SER:HA	9:J:47:ASN:OD1	2.21	0.40
1:N:244:ARG:CZ	7:T:10:VAL:HB	2.51	0.40
10:O:109:VAL:HB	10:O:119:LEU:HD12	2.02	0.40
10:O:309:VAL:HA	10:O:325:TYR:O	2.20	0.40
3:P:17:ALA:O	3:P:18:PHE:HD1	2.04	0.40
3:P:276:PHE:CE1	3:P:277:ALA:HB2	2.57	0.40
8:U:40:CYS:O	8:U:43:ARG:CG	2.69	0.40
9:W:4:THR:HG22	9:W:5:LEU:H	1.86	0.40
1:A:26:ALA:O	1:A:198:ALA:HA	2.21	0.40
2:B:240:HIS:ND1	2:B:241:GLY:O	2.54	0.40
3:C:138:MET:HE2	3:C:138:MET:HA	2.03	0.40
3:C:186:PRO:O	3:C:189:ILE:HB	2.21	0.40
6:F:68:LEU:HD11	6:F:75:LEU:HG	2.04	0.40
10:O:29:LEU:CD2	10:O:30:PRO:HD2	2.47	0.40
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.56	0.40
10:O:89:ILE:CG1	11:V:70:LEU:HD22	2.52	0.40
7:G:79:ASN:H	7:G:79:ASN:ND2	2.19	0.40
10:O:51:ILE:HD13	10:O:199:PHE:CE2	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:57:ASP:OD2	8:U:42:GLU:OE2[1_655]	1.73	0.47

## 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	442/480 (92%)	405 (92%)	35 (8%)	2 (0%)	29	67
1	N	442/480 (92%)	407 (92%)	33 (8%)	2 (0%)	29	67
2	B	420/453 (93%)	375 (89%)	44 (10%)	1 (0%)	47	80
3	C	372/379 (98%)	347 (93%)	23 (6%)	2 (0%)	29	67
3	P	368/379 (97%)	337 (92%)	30 (8%)	1 (0%)	41	74
4	D	238/265 (90%)	216 (91%)	21 (9%)	1 (0%)	34	71
4	Q	239/265 (90%)	218 (91%)	20 (8%)	1 (0%)	34	71
5	E	71/274 (26%)	64 (90%)	7 (10%)	0	100	100
5	I	17/274 (6%)	12 (71%)	5 (29%)	0	100	100
5	R	194/274 (71%)	174 (90%)	19 (10%)	1 (0%)	29	67
6	F	96/111 (86%)	87 (91%)	9 (9%)	0	100	100
6	S	97/111 (87%)	89 (92%)	8 (8%)	0	100	100
7	G	78/82 (95%)	67 (86%)	10 (13%)	1 (1%)	12	49
7	T	72/82 (88%)	62 (86%)	10 (14%)	0	100	100
8	H	63/91 (69%)	59 (94%)	4 (6%)	0	100	100
8	U	64/91 (70%)	61 (95%)	3 (5%)	0	100	100
9	J	56/64 (88%)	51 (91%)	5 (9%)	0	100	100
9	W	57/64 (89%)	51 (90%)	6 (10%)	0	100	100
10	O	417/453 (92%)	376 (90%)	41 (10%)	0	100	100
11	V	15/274 (6%)	12 (80%)	3 (20%)	0	100	100
All	All	3818/4946 (77%)	3470 (91%)	336 (9%)	12 (0%)	41	74

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	ASN
1	N	267	ASN
3	P	107	TYR
5	R	177	PRO
3	C	107	TYR
2	B	394	PRO
7	G	74	PRO
1	N	260	PRO
4	D	240	PRO
1	A	260	PRO
3	C	266	PRO
4	Q	240	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	368/394 (93%)	350 (95%)	18 (5%)	25	59
1	N	367/394 (93%)	347 (95%)	20 (5%)	22	57
2	B	331/355 (93%)	309 (93%)	22 (7%)	16	51
3	C	322/327 (98%)	301 (94%)	21 (6%)	17	51
3	P	318/327 (97%)	297 (93%)	21 (7%)	16	51
4	D	205/218 (94%)	196 (96%)	9 (4%)	28	63
4	Q	206/218 (94%)	196 (95%)	10 (5%)	25	59
5	E	63/228 (28%)	57 (90%)	6 (10%)	8	37
5	I	19/228 (8%)	13 (68%)	6 (32%)	0	2
5	R	168/228 (74%)	158 (94%)	10 (6%)	19	54
6	F	90/99 (91%)	82 (91%)	8 (9%)	9	40
6	S	91/99 (92%)	84 (92%)	7 (8%)	13	44
7	G	71/72 (99%)	64 (90%)	7 (10%)	8	35
7	T	66/72 (92%)	59 (89%)	7 (11%)	6	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	62/85 (73%)	54 (87%)	8 (13%)	4	24
8	U	63/85 (74%)	56 (89%)	7 (11%)	6	31
9	J	49/54 (91%)	45 (92%)	4 (8%)	11	42
9	W	49/54 (91%)	44 (90%)	5 (10%)	7	34
10	O	328/355 (92%)	304 (93%)	24 (7%)	14	46
11	V	15/228 (7%)	12 (80%)	3 (20%)	1	8
All	All	3251/4120 (79%)	3028 (93%)	223 (7%)	15	49

All (223) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LYS
1	A	58	PHE
1	A	150	PHE
1	A	156	THR
1	A	185	TYR
1	A	186	LEU
1	A	203	LEU
1	A	206	ARG
1	A	230	THR
1	A	305	GLN
1	A	324	PHE
1	A	348	SER
1	A	388	ARG
1	A	397	SER
1	A	416	TYR
1	A	442	PHE
1	A	444	LEU
1	A	445	ARG
2	B	33	LEU
2	B	96	LEU
2	B	97	SER
2	B	99	THR
2	B	101	THR
2	B	108	THR
2	B	116	VAL
2	B	150	VAL
2	B	158	HIS
2	B	170	ASN
2	B	189	VAL

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Mol	Chain	Res	Type
2	B	224	LEU
2	B	226	ILE
2	B	230	LEU
2	B	301	LYS
2	B	310	SER
2	B	312	PHE
2	B	316	TYR
2	B	324	PHE
2	B	325	TYR
2	B	417	PHE
2	B	436	ILE
3	C	10	LEU
3	C	11	MET
3	C	15	ASN
3	C	21	LEU
3	C	35	SER
3	C	63	PHE
3	C	64	SER
3	C	78	ILE
3	C	140	PHE
3	C	156	ILE
3	C	171	ASP
3	C	220	PHE
3	C	257	THR
3	C	268	ILE
3	C	276	PHE
3	C	296	PHE
3	C	310	SER
3	C	311	LYS
3	C	325	PHE
3	C	349	THR
3	C	358	TYR
4	D	3	LEU
4	D	17	LEU
4	D	19	SER
4	D	37	CYS
4	D	68	VAL
4	D	178	THR
4	D	182	VAL
4	D	216	LEU
4	D	232	SER
5	E	7	VAL

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Mol	Chain	Res	Type
5	E	27	GLU
5	E	36	SER
5	E	42	THR
5	E	54	VAL
5	E	72	SER
6	F	20	TYR
6	F	26	PHE
6	F	40	ASN
6	F	78	GLU
6	F	83	TYR
6	F	91	GLU
6	F	94	LEU
6	F	95	LYS
7	G	9	ARG
7	G	17	SER
7	G	18	LEU
7	G	41	THR
7	G	46	LEU
7	G	59	TYR
7	G	60	THR
8	H	14	VAL
8	H	43	ARG
8	H	44	VAL
8	H	47	ARG
8	H	49	GLN
8	H	50	THR
8	H	51	GLU
8	H	55	THR
5	I	50	LEU
5	I	54	SER
5	I	56	ARG
5	I	65	VAL
5	I	67	SER
5	I	70	LEU
9	J	13	LEU
9	J	20	PHE
9	J	37	GLN
9	J	59	TYR
1	N	27	SER
1	N	51	LYS
1	N	58	PHE
1	N	150	PHE

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Mol	Chain	Res	Type
1	N	156	THR
1	N	185	TYR
1	N	186	LEU
1	N	203	LEU
1	N	206	ARG
1	N	230	THR
1	N	305	GLN
1	N	324	PHE
1	N	327	ASP
1	N	348	SER
1	N	388	ARG
1	N	397	SER
1	N	416	TYR
1	N	442	PHE
1	N	444	LEU
1	N	445	ARG
10	O	33	LEU
10	O	96	LEU
10	O	97	SER
10	O	99	THR
10	O	101	THR
10	O	108	THR
10	O	116	VAL
10	O	126	VAL
10	O	150	VAL
10	O	158	HIS
10	O	170	ASN
10	O	189	VAL
10	O	224	LEU
10	O	226	ILE
10	O	230	LEU
10	O	301	LYS
10	O	310	SER
10	O	312	PHE
10	O	316	TYR
10	O	324	PHE
10	O	325	TYR
10	O	407	ASP
10	O	417	PHE
10	O	436	ILE
3	P	10	LEU
3	P	11	MET

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Mol	Chain	Res	Type
3	P	15	ASN
3	P	21	LEU
3	P	35	SER
3	P	63	PHE
3	P	64	SER
3	P	78	ILE
3	P	90	PHE
3	P	140	PHE
3	P	156	ILE
3	P	257	THR
3	P	268	ILE
3	P	276	PHE
3	P	296	PHE
3	P	310	SER
3	P	311	LYS
3	P	325	PHE
3	P	349	THR
3	P	358	TYR
3	P	379	TRP
4	Q	3	LEU
4	Q	17	LEU
4	Q	37	CYS
4	Q	40	CYS
4	Q	68	VAL
4	Q	126	TYR
4	Q	178	THR
4	Q	182	VAL
4	Q	216	LEU
4	Q	232	SER
5	R	7	VAL
5	R	27	GLU
5	R	36	SER
5	R	42	THR
5	R	54	VAL
5	R	72	SER
5	R	113	GLU
5	R	136	ILE
5	R	140	THR
5	R	160	CYS
6	S	26	PHE
6	S	40	ASN
6	S	78	GLU

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Mol	Chain	Res	Type
6	S	83	TYR
6	S	91	GLU
6	S	94	LEU
6	S	95	LYS
7	T	9	ARG
7	T	17	SER
7	T	18	LEU
7	T	41	THR
7	T	46	LEU
7	T	59	TYR
7	T	60	THR
8	U	14	VAL
8	U	43	ARG
8	U	47	ARG
8	U	49	GLN
8	U	50	THR
8	U	51	GLU
8	U	55	THR
11	V	65	VAL
11	V	67	SER
11	V	70	LEU
9	W	4	THR
9	W	13	LEU
9	W	20	PHE
9	W	37	GLN
9	W	59	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	118	GLN
1	A	189	HIS
1	A	215	HIS
1	A	271	GLN
2	B	22	GLN
2	B	104	ASN
2	B	170	ASN
2	B	290	ASN
2	B	297	GLN
2	B	343	GLN
2	B	400	GLN

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Mol	Chain	Res	Type
3	C	8	HIS
3	C	16	ASN
4	D	225	HIS
7	G	73	ASN
7	G	79	ASN
1	N	118	GLN
1	N	189	HIS
1	N	215	HIS
1	N	271	GLN
10	O	104	ASN
10	O	297	GLN
10	O	400	GLN
3	P	16	ASN
4	Q	31	GLN
6	S	79	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

29 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
17	CDL	G	501	-	43,43,99	1.55	4 (9%)	49,55,111	1.57	8 (16%)
12	HEM	C	502	3	27,50,50	1.04	2 (7%)	17,82,82	1.18	1 (5%)
19	GOL	R	502	-	5,5,5	0.33	0	5,5,5	0.45	0
12	HEM	C	501	3	27,50,50	1.18	2 (7%)	17,82,82	1.57	1 (5%)
15	PEE	Q	506	-	50,50,50	1.05	2 (4%)	53,55,55	1.23	5 (9%)
14	PO4	S	501	-	4,4,4	0.86	0	6,6,6	0.48	0
17	CDL	D	505	-	38,38,99	1.27	3 (7%)	43,47,111	1.16	4 (9%)
14	PO4	D	502	-	4,4,4	0.76	0	6,6,6	0.63	0
13	4X9	C	503	-	30,30,30	2.97	7 (23%)	43,44,44	1.43	3 (6%)
14	PO4	C	504	-	4,4,4	0.95	0	6,6,6	0.43	0
17	CDL	T	501	-	48,48,99	1.39	4 (8%)	54,60,111	1.18	4 (7%)
16	HEC	D	501	4	26,50,50	2.40	12 (46%)	18,82,82	3.15	8 (44%)
13	4X9	P	503	-	30,30,30	2.79	6 (20%)	43,44,44	1.90	8 (18%)
12	HEM	P	502	3	27,50,50	1.07	2 (7%)	17,82,82	1.48	3 (17%)
14	PO4	Q	1001	-	4,4,4	0.87	0	6,6,6	0.47	0
14	PO4	D	504	-	4,4,4	0.85	0	6,6,6	0.58	0
16	HEC	Q	501	4	26,50,50	2.41	11 (42%)	18,82,82	2.62	6 (33%)
14	PO4	D	503	-	4,4,4	0.88	0	6,6,6	0.67	0
15	PEE	C	505	-	48,48,50	1.00	2 (4%)	51,53,55	0.95	4 (7%)
14	PO4	N	501	-	4,4,4	0.72	0	6,6,6	0.98	0
17	CDL	Q	505	-	38,38,99	1.27	3 (7%)	43,47,111	1.19	5 (11%)
18	FES	R	501	5	0,4,4	0.00	-	-	-	-
15	PEE	D	506	-	25,25,50	1.49	2 (8%)	28,30,55	1.46	4 (14%)
14	PO4	F	501	-	4,4,4	0.87	0	6,6,6	0.62	0
15	PEE	P	505	-	48,48,50	1.09	2 (4%)	51,53,55	0.83	1 (1%)
12	HEM	P	501	3	27,50,50	0.91	2 (7%)	17,82,82	1.66	5 (29%)
14	PO4	N	1001	-	4,4,4	0.81	0	6,6,6	0.78	0
14	PO4	E	501	-	4,4,4	0.69	0	6,6,6	0.81	0
14	PO4	Q	1002	-	4,4,4	0.89	0	6,6,6	0.48	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	HEC	Q	501	4	-	2/6/54/54	-
17	CDL	G	501	-	-	25/52/52/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	FES	R	501	5	-	-	0/1/1/1
15	PEE	D	506	-	1/1/4/4	13/29/29/54	-
12	HEM	C	502	3	-	3/6/54/54	-
15	PEE	C	505	-	1/1/4/4	24/52/52/54	-
15	PEE	P	505	-	1/1/4/4	25/52/52/54	-
19	GOL	R	502	-	-	2/4/4/4	-
12	HEM	C	501	3	-	1/6/54/54	-
12	HEM	P	501	3	-	4/6/54/54	-
16	HEC	D	501	4	-	3/6/54/54	-
17	CDL	T	501	-	-	28/57/57/110	-
15	PEE	Q	506	-	1/1/4/4	25/54/54/54	-
13	4X9	P	503	-	-	3/13/13/13	0/3/3/3
13	4X9	C	503	-	-	5/13/13/13	0/3/3/3
17	CDL	D	505	-	-	21/43/43/110	-
17	CDL	Q	505	-	-	13/43/43/110	-
12	HEM	P	502	3	-	2/6/54/54	-

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P	503	4X9	C19-C20	8.52	1.50	1.38
13	C	503	4X9	C17-C18	8.10	1.50	1.40
13	C	503	4X9	C19-C20	7.70	1.49	1.38
13	C	503	4X9	C17-C22	7.65	1.49	1.40
16	D	501	HEC	C3C-C2C	6.89	1.47	1.40
13	P	503	4X9	C17-C18	6.76	1.48	1.40
13	P	503	4X9	C17-C22	6.73	1.48	1.40
16	Q	501	HEC	C3C-C2C	6.57	1.47	1.40
13	C	503	4X9	C18-C19	5.96	1.49	1.39
17	G	501	CDL	OA6-CA5	5.25	1.47	1.35
16	Q	501	HEC	C3B-C2B	5.22	1.46	1.40
16	D	501	HEC	C3B-C2B	5.06	1.46	1.40
15	D	506	PEE	O3-C30	5.00	1.48	1.33
17	T	501	CDL	OB6-CB5	4.95	1.48	1.34
17	G	501	CDL	OB6-CB5	4.89	1.48	1.34
17	Q	505	CDL	OA6-CA5	4.87	1.48	1.34
17	G	501	CDL	OB8-CB7	4.85	1.47	1.33
15	P	505	PEE	O2-C10	4.84	1.48	1.34
15	Q	506	PEE	O2-C10	4.78	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P	503	4X9	O28-C18	-4.78	1.25	1.37
17	D	505	CDL	OA6-CA5	4.76	1.47	1.34
17	T	501	CDL	OB8-CB7	4.73	1.47	1.33
15	P	505	PEE	O3-C30	4.70	1.47	1.33
17	T	501	CDL	OA6-CA5	4.68	1.45	1.35
15	C	505	PEE	O2-C10	4.66	1.47	1.34
13	C	503	4X9	O28-C18	-4.56	1.26	1.37
17	Q	505	CDL	OA8-CA7	4.54	1.46	1.33
15	D	506	PEE	O2-C10	4.53	1.47	1.34
12	C	501	HEM	C3B-C2B	-4.51	1.34	1.40
13	P	503	4X9	C18-C19	4.50	1.46	1.39
17	D	505	CDL	OA8-CA7	4.49	1.46	1.33
15	Q	506	PEE	O3-C30	4.28	1.45	1.33
15	C	505	PEE	O3-C30	4.12	1.45	1.33
16	D	501	HEC	C3B-C4B	3.39	1.49	1.43
16	Q	501	HEC	C2A-C3A	3.30	1.47	1.37
16	D	501	HEC	C2A-C3A	3.27	1.47	1.37
13	P	503	4X9	C19-CL	3.23	1.79	1.72
16	Q	501	HEC	C3D-C2D	3.19	1.47	1.37
16	Q	501	HEC	C4A-C3A	3.11	1.49	1.42
17	G	501	CDL	OA8-CA7	3.01	1.48	1.33
16	Q	501	HEC	C1A-C2A	3.00	1.49	1.42
16	Q	501	HEC	C3B-C4B	2.97	1.48	1.43
16	D	501	HEC	C3D-C2D	2.96	1.46	1.37
13	C	503	4X9	C19-CL	2.88	1.79	1.72
12	P	502	HEM	C3B-C2B	-2.76	1.36	1.40
12	P	502	HEM	C4D-C3D	2.75	1.48	1.42
16	D	501	HEC	C1C-CHC	2.73	1.48	1.41
16	D	501	HEC	C4A-C3A	2.67	1.48	1.42
16	D	501	HEC	C3C-C4C	2.64	1.47	1.43
16	Q	501	HEC	C1B-CHB	2.62	1.48	1.41
12	P	501	HEM	C4D-C3D	2.58	1.48	1.42
17	Q	505	CDL	PB2-OB5	2.58	1.64	1.54
16	Q	501	HEC	C1C-CHC	2.48	1.47	1.41
12	C	501	HEM	C4D-C3D	2.47	1.48	1.42
17	T	501	CDL	OA8-CA7	2.47	1.45	1.33
17	D	505	CDL	PB2-OB5	2.45	1.64	1.54
16	Q	501	HEC	C3C-C4C	2.42	1.47	1.43
16	Q	501	HEC	C1D-CHD	2.35	1.47	1.41
13	C	503	4X9	O3-C1	2.33	1.44	1.31
16	D	501	HEC	C1B-CHB	2.30	1.47	1.41
16	D	501	HEC	C1D-CHD	2.29	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	502	HEM	C3B-C2B	-2.18	1.37	1.40
12	P	501	HEM	C3B-C2B	-2.06	1.37	1.40
16	D	501	HEC	C4D-CHA	2.06	1.46	1.41
12	C	502	HEM	C3C-C2C	-2.05	1.37	1.40
16	D	501	HEC	C1A-C2A	2.01	1.47	1.42

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	P	503	4X9	C18-C19-C20	-7.02	118.33	122.79
16	Q	501	HEC	C1D-C2D-C3D	-6.86	102.23	107.00
16	D	501	HEC	C1D-C2D-C3D	-6.10	102.75	107.00
16	D	501	HEC	CBA-CAA-C2A	5.95	123.43	112.48
16	D	501	HEC	CMC-C2C-C3C	5.18	131.91	125.82
15	D	506	PEE	O2-C10-C11	5.07	122.42	111.50
13	P	503	4X9	C20-C19-CL	5.04	128.27	121.14
16	D	501	HEC	CAA-CBA-CGA	-4.85	104.54	112.67
13	C	503	4X9	C18-C19-C20	-4.82	119.73	122.79
17	G	501	CDL	OA6-CA5-C11	4.81	119.95	111.09
15	Q	506	PEE	C2-O2-C10	4.63	129.18	117.79
17	G	501	CDL	OB6-CB5-C51	4.51	123.37	110.80
16	Q	501	HEC	CMB-C2B-C3B	4.46	131.07	125.82
17	T	501	CDL	OA6-CA5-C11	4.22	118.85	111.09
12	C	501	HEM	CBA-CAA-C2A	-4.22	104.71	112.49
13	P	503	4X9	C18-C19-CL	-4.18	113.39	118.08
16	D	501	HEC	CMB-C2B-C3B	4.08	130.62	125.82
17	D	505	CDL	OA6-CA5-C11	3.98	120.08	111.50
17	G	501	CDL	OB8-CB7-C71	3.95	124.29	111.91
16	Q	501	HEC	CMC-C2C-C3C	3.80	130.29	125.82
15	Q	506	PEE	O2-C10-C11	3.80	119.68	111.50
17	Q	505	CDL	OA6-CA5-C11	3.76	119.61	111.50
17	T	501	CDL	OB6-CB5-C51	3.74	119.55	111.50
13	C	503	4X9	C18-C17-C22	-3.60	116.06	119.57
16	D	501	HEC	CAD-CBD-CGD	-3.43	106.91	112.67
17	D	505	CDL	OA8-CA7-C31	3.42	122.63	111.91
16	Q	501	HEC	CAD-CBD-CGD	-3.40	106.97	112.67
15	P	505	PEE	O2-C10-C11	3.35	118.73	111.50
13	C	503	4X9	C22-N30-C20	3.21	124.37	119.64
12	P	502	HEM	CBA-CAA-C2A	-3.21	106.57	112.49
15	D	506	PEE	O3-C30-C31	3.14	121.75	111.91
12	P	501	HEM	C1D-C2D-C3D	-3.13	104.81	107.00
13	P	503	4X9	C29-C22-C17	-3.07	117.85	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	P	503	4X9	C29-C22-N30	3.03	121.18	116.49
17	G	501	CDL	CA6-OA8-CA7	2.97	124.55	117.10
15	C	505	PEE	O2-C10-C11	2.96	117.88	111.50
15	C	505	PEE	O3-C30-C31	2.94	121.15	111.91
15	Q	506	PEE	O3-C3-C2	2.93	116.95	108.43
17	T	501	CDL	OB8-CB7-C71	2.87	120.92	111.91
12	P	501	HEM	CAA-CBA-CGA	2.86	117.46	112.67
17	Q	505	CDL	OA8-CA7-C31	2.80	120.70	111.91
16	Q	501	HEC	CAA-CBA-CGA	-2.80	107.97	112.67
17	G	501	CDL	OB8-CB6-CB4	2.79	116.56	108.43
17	D	505	CDL	OA8-CA7-OA9	-2.73	116.71	123.59
15	Q	506	PEE	O3-C30-C31	2.69	120.34	111.91
15	D	506	PEE	O2-C10-O4	-2.67	117.25	123.70
13	P	503	4X9	C22-N30-C20	2.66	123.56	119.64
12	P	501	HEM	CAD-CBD-CGD	-2.63	108.27	112.67
17	T	501	CDL	OA6-CA5-OA7	-2.62	117.76	122.96
17	G	501	CDL	OB6-CB5-OB7	-2.59	117.44	123.70
15	C	505	PEE	O3-C30-O5	-2.56	117.12	123.59
17	Q	505	CDL	OB4-PB2-OB3	2.55	120.68	110.68
17	Q	505	CDL	OA8-CA7-OA9	-2.55	117.16	123.59
17	G	501	CDL	OB8-CB7-OB9	-2.46	117.40	123.59
16	D	501	HEC	C4C-C3C-C2C	-2.31	103.86	106.35
17	G	501	CDL	OA8-CA7-C31	2.30	122.39	112.38
12	P	501	HEM	C4A-C3A-C2A	2.28	108.58	107.00
17	Q	505	CDL	PB2-OB2-CB2	2.24	124.48	118.30
12	P	501	HEM	CMA-C3A-C4A	-2.16	125.14	128.46
12	C	502	HEM	CBD-CAD-C3D	2.15	116.44	112.48
17	D	505	CDL	OB4-PB2-OB3	2.12	119.00	110.68
12	P	502	HEM	CMA-C3A-C4A	-2.12	125.20	128.46
13	P	503	4X9	C26-C20-C19	-2.12	121.79	123.01
16	Q	501	HEC	CBA-CAA-C2A	2.12	116.38	112.48
12	P	502	HEM	C3C-C4C-NC	-2.11	106.97	110.94
15	Q	506	PEE	O3-C30-O5	-2.10	118.29	123.59
13	P	503	4X9	O28-C18-C17	2.09	124.34	119.56
15	D	506	PEE	O3-C30-O5	-2.09	118.33	123.59
16	D	501	HEC	CMA-C3A-C2A	2.06	128.82	124.94
15	C	505	PEE	C3-C2-C1	-2.00	107.06	111.79

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
15	Q	506	PEE	C2

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Mol	Chain	Res	Type	Atom
15	C	505	PEE	C2
15	D	506	PEE	C2
15	P	505	PEE	C2

All (199) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	G	501	CDL	O1-C1-CB2-OB2
17	G	501	CDL	CA2-C1-CB2-OB2
17	G	501	CDL	CA3-OA5-PA1-OA4
17	G	501	CDL	CB4-CB3-OB5-PB2
17	G	501	CDL	C51-CB5-OB6-CB4
12	C	502	HEM	C2D-C3D-CAD-CBD
12	C	502	HEM	C4D-C3D-CAD-CBD
19	R	502	GOL	C1-C2-C3-O3
15	Q	506	PEE	C1-O3P-P-O2P
17	D	505	CDL	CB2-OB2-PB2-OB4
17	D	505	CDL	CB2-OB2-PB2-OB5
17	T	501	CDL	O1-C1-CB2-OB2
17	T	501	CDL	CA3-OA5-PA1-OA3
17	T	501	CDL	CB2-OB2-PB2-OB3
17	T	501	CDL	CB2-OB2-PB2-OB5
17	T	501	CDL	CB3-OB5-PB2-OB2
17	T	501	CDL	CB3-OB5-PB2-OB3
17	T	501	CDL	CB3-OB5-PB2-OB4
16	D	501	HEC	C1A-C2A-CAA-CBA
16	D	501	HEC	C2D-C3D-CAD-CBD
16	D	501	HEC	C4D-C3D-CAD-CBD
12	P	502	HEM	C2D-C3D-CAD-CBD
12	P	502	HEM	C4D-C3D-CAD-CBD
16	Q	501	HEC	C1A-C2A-CAA-CBA
16	Q	501	HEC	C3A-C2A-CAA-CBA
17	Q	505	CDL	CB2-OB2-PB2-OB3
17	Q	505	CDL	CB2-OB2-PB2-OB4
17	Q	505	CDL	CB2-OB2-PB2-OB5
15	D	506	PEE	O4P-C4-C5-N
15	D	506	PEE	C5-C4-O4P-P
15	D	506	PEE	C1-O3P-P-O2P
15	P	505	PEE	O4P-C4-C5-N
12	P	501	HEM	C1A-C2A-CAA-CBA
12	P	501	HEM	C3A-C2A-CAA-CBA
17	T	501	CDL	C11-CA5-OA6-CA4

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Mol	Chain	Res	Type	Atoms
17	Q	505	CDL	OA9-CA7-OA8-CA6
17	T	501	CDL	OA7-CA5-OA6-CA4
17	G	501	CDL	OB7-CB5-OB6-CB4
17	Q	505	CDL	C31-CA7-OA8-CA6
17	G	501	CDL	C11-CA5-OA6-CA4
17	G	501	CDL	O1-C1-CA2-OA2
17	T	501	CDL	OA9-CA7-OA8-CA6
17	T	501	CDL	C31-CA7-OA8-CA6
13	C	503	4X9	F23-C1-O3-C4
17	G	501	CDL	CB2-C1-CA2-OA2
17	D	505	CDL	CA2-C1-CB2-OB2
15	D	506	PEE	C31-C30-O3-C3
15	D	506	PEE	O5-C30-O3-C3
17	G	501	CDL	OA6-CA4-CA6-OA8
17	D	505	CDL	C31-CA7-OA8-CA6
15	P	505	PEE	C10-C11-C12-C13
15	Q	506	PEE	C10-C11-C12-C13
17	Q	505	CDL	CA7-C31-C32-C33
17	T	501	CDL	CB4-CB3-OB5-PB2
15	P	505	PEE	C30-C31-C32-C33
15	P	505	PEE	C11-C10-O2-C2
17	G	501	CDL	OA7-CA5-OA6-CA4
17	D	505	CDL	O1-C1-CB2-OB2
15	P	505	PEE	C16-C17-C18-C19
17	G	501	CDL	CA3-OA5-PA1-OA2
17	T	501	CDL	CA2-OA2-PA1-OA5
15	D	506	PEE	C1-O3P-P-O4P
15	D	506	PEE	C4-O4P-P-O3P
15	P	505	PEE	C1-O3P-P-O4P
17	T	501	CDL	CA2-C1-CB2-OB2
15	P	505	PEE	O4-C10-O2-C2
15	Q	506	PEE	C17-C18-C19-C20
15	C	505	PEE	C21-C22-C23-C24
15	Q	506	PEE	C31-C32-C33-C34
15	C	505	PEE	C18-C19-C20-C21
17	D	505	CDL	OA9-CA7-OA8-CA6
15	C	505	PEE	C15-C16-C17-C18
15	C	505	PEE	C30-C31-C32-C33
13	C	503	4X9	F24-C1-O3-C4
15	Q	506	PEE	C22-C23-C24-C25
15	Q	506	PEE	C32-C33-C34-C35
15	C	505	PEE	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
15	P	505	PEE	C13-C14-C15-C16
12	C	502	HEM	C3D-CAD-CBD-CGD
15	Q	506	PEE	C11-C12-C13-C14
15	Q	506	PEE	C21-C22-C23-C24
15	C	505	PEE	C19-C20-C21-C22
17	Q	505	CDL	C38-C39-C40-C41
15	P	505	PEE	C34-C35-C36-C37
17	T	501	CDL	C73-C74-C75-C76
15	C	505	PEE	C42-C43-C44-C45
15	P	505	PEE	C42-C43-C44-C45
15	Q	506	PEE	O4P-C4-C5-N
15	P	505	PEE	C32-C33-C34-C35
15	Q	506	PEE	C34-C35-C36-C37
15	Q	506	PEE	C39-C40-C41-C42
15	P	505	PEE	C37-C38-C39-C40
17	T	501	CDL	C52-C53-C54-C55
13	C	503	4X9	F25-C1-O3-C4
17	D	505	CDL	C38-C39-C40-C41
15	P	505	PEE	C1-C2-C3-O3
15	P	505	PEE	C18-C19-C20-C21
17	T	501	CDL	C72-C73-C74-C75
15	Q	506	PEE	C19-C20-C21-C22
15	C	505	PEE	C40-C41-C42-C43
17	Q	505	CDL	C34-C35-C36-C37
17	G	501	CDL	C31-CA7-OA8-CA6
17	D	505	CDL	CA4-CA3-OA5-PA1
15	D	506	PEE	C11-C10-O2-C2
17	D	505	CDL	C37-C38-C39-C40
15	C	505	PEE	O4-C10-O2-C2
17	T	501	CDL	CB7-C71-C72-C73
15	C	505	PEE	C10-C11-C12-C13
17	G	501	CDL	C71-CB7-OB8-CB6
17	D	505	CDL	C11-CA5-OA6-CA4
15	C	505	PEE	C11-C10-O2-C2
15	P	505	PEE	O2-C2-C3-O3
17	Q	505	CDL	C36-C37-C38-C39
15	D	506	PEE	O4-C10-O2-C2
17	G	501	CDL	OB5-CB3-CB4-CB6
15	P	505	PEE	C12-C13-C14-C15
15	Q	506	PEE	C16-C17-C18-C19
17	G	501	CDL	OB9-CB7-OB8-CB6
15	P	505	PEE	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
15	Q	506	PEE	C42-C43-C44-C45
15	P	505	PEE	C38-C39-C40-C41
15	C	505	PEE	C31-C30-O3-C3
15	P	505	PEE	C1-C2-O2-C10
17	D	505	CDL	CB2-OB2-PB2-OB3
17	D	505	CDL	OA5-CA3-CA4-OA6
15	D	506	PEE	O3P-C1-C2-O2
17	D	505	CDL	OA7-CA5-OA6-CA4
15	C	505	PEE	C22-C23-C24-C25
17	D	505	CDL	C36-C37-C38-C39
12	C	501	HEM	C3D-CAD-CBD-CGD
12	P	501	HEM	C3D-CAD-CBD-CGD
15	Q	506	PEE	O3P-C1-C2-C3
17	D	505	CDL	OA5-CA3-CA4-CA6
15	D	506	PEE	O3P-C1-C2-C3
15	P	505	PEE	C19-C20-C21-C22
17	T	501	CDL	C51-C52-C53-C54
15	P	505	PEE	C33-C34-C35-C36
15	P	505	PEE	C21-C22-C23-C24
17	Q	505	CDL	C33-C34-C35-C36
15	Q	506	PEE	C36-C37-C38-C39
17	G	501	CDL	CA3-CA4-CA6-OA8
15	Q	506	PEE	C1-O3P-P-O4P
15	C	505	PEE	C1-O3P-P-O4P
19	R	502	GOL	O2-C2-C3-O3
17	G	501	CDL	OB5-CB3-CB4-OB6
15	C	505	PEE	O5-C30-O3-C3
17	T	501	CDL	C75-C76-C77-C78
17	G	501	CDL	OA9-CA7-OA8-CA6
15	C	505	PEE	O3P-C1-C2-C3
15	P	505	PEE	C36-C37-C38-C39
15	C	505	PEE	C12-C13-C14-C15
15	Q	506	PEE	C1-C2-O2-C10
13	P	503	4X9	F24-C1-O3-C4
17	D	505	CDL	C33-C34-C35-C36
17	T	501	CDL	C71-CB7-OB8-CB6
17	G	501	CDL	C72-C73-C74-C75
15	C	505	PEE	C38-C39-C40-C41
15	Q	506	PEE	C1-O3P-P-O1P
17	T	501	CDL	CA2-OA2-PA1-OA4
15	D	506	PEE	C4-O4P-P-O1P
15	P	505	PEE	C1-O3P-P-O1P

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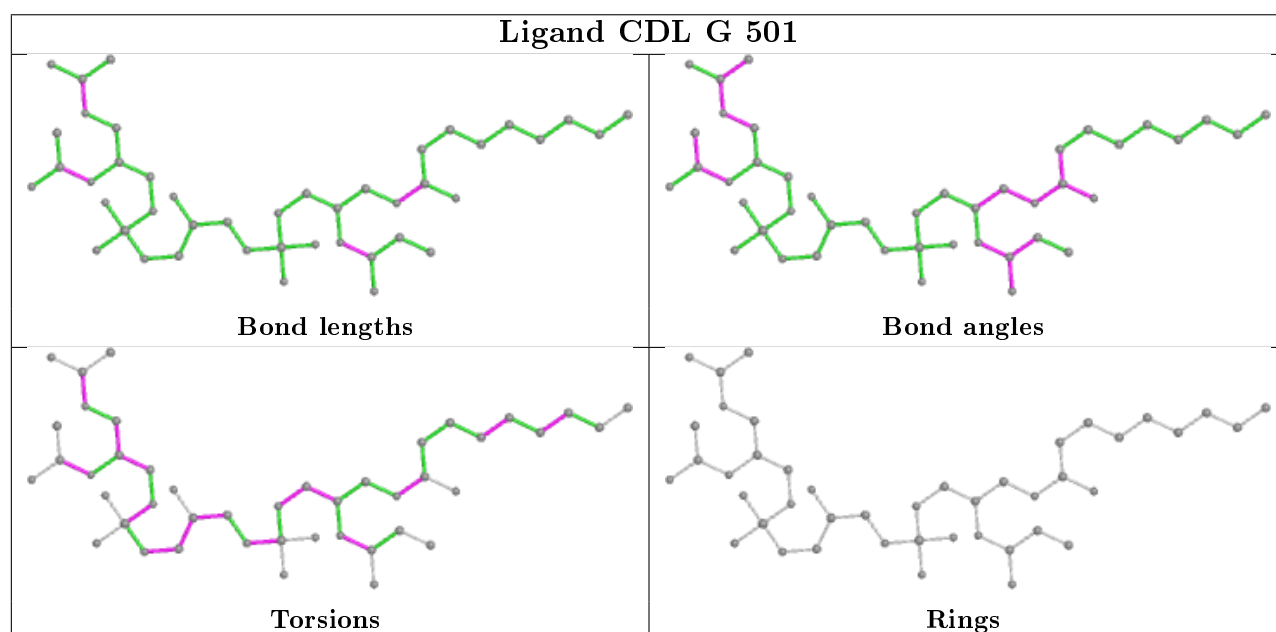
Mol	Chain	Res	Type	Atoms
15	P	505	PEE	C5-C4-O4P-P
17	G	501	CDL	OA5-CA3-CA4-OA6
15	C	505	PEE	O3P-C1-C2-O2
15	Q	506	PEE	C40-C41-C42-C43
17	T	501	CDL	OB9-CB7-OB8-CB6
15	C	505	PEE	C1-C2-O2-C10
17	T	501	CDL	OA5-CA3-CA4-CA6
17	T	501	CDL	OA5-CA3-CA4-OA6
15	Q	506	PEE	C41-C42-C43-C44
17	G	501	CDL	CB2-OB2-PB2-OB5
15	C	505	PEE	C4-O4P-P-O3P
17	Q	505	CDL	CA3-OA5-PA1-OA2
17	D	505	CDL	C34-C35-C36-C37
15	Q	506	PEE	C1-C2-C3-O3
17	Q	505	CDL	C37-C38-C39-C40
15	C	505	PEE	O4P-C4-C5-N
17	T	501	CDL	C71-C72-C73-C74
13	C	503	4X9	C5-C4-O3-C1
17	D	505	CDL	CA3-CA4-CA6-OA8
17	G	501	CDL	C1-CA2-OA2-PA1
13	C	503	4X9	C9-C4-O3-C1
15	Q	506	PEE	C13-C14-C15-C16
17	G	501	CDL	OA5-CA3-CA4-CA6
15	Q	506	PEE	O2-C2-C3-O3
17	T	501	CDL	C53-C54-C55-C56
15	D	506	PEE	C32-C33-C34-C35
17	G	501	CDL	C74-C75-C76-C77
13	P	503	4X9	F25-C1-O3-C4
17	D	505	CDL	C35-C36-C37-C38
15	C	505	PEE	C13-C14-C15-C16
12	P	501	HEM	C2A-CAA-CBA-CGA
17	D	505	CDL	C12-C11-CA5-OA6
15	C	505	PEE	C1-O3P-P-O1P
17	Q	505	CDL	CA3-OA5-PA1-OA3
13	P	503	4X9	F23-C1-O3-C4
15	Q	506	PEE	C18-C19-C20-C21
17	T	501	CDL	C74-C75-C76-C77
17	D	505	CDL	C12-C11-CA5-OA7

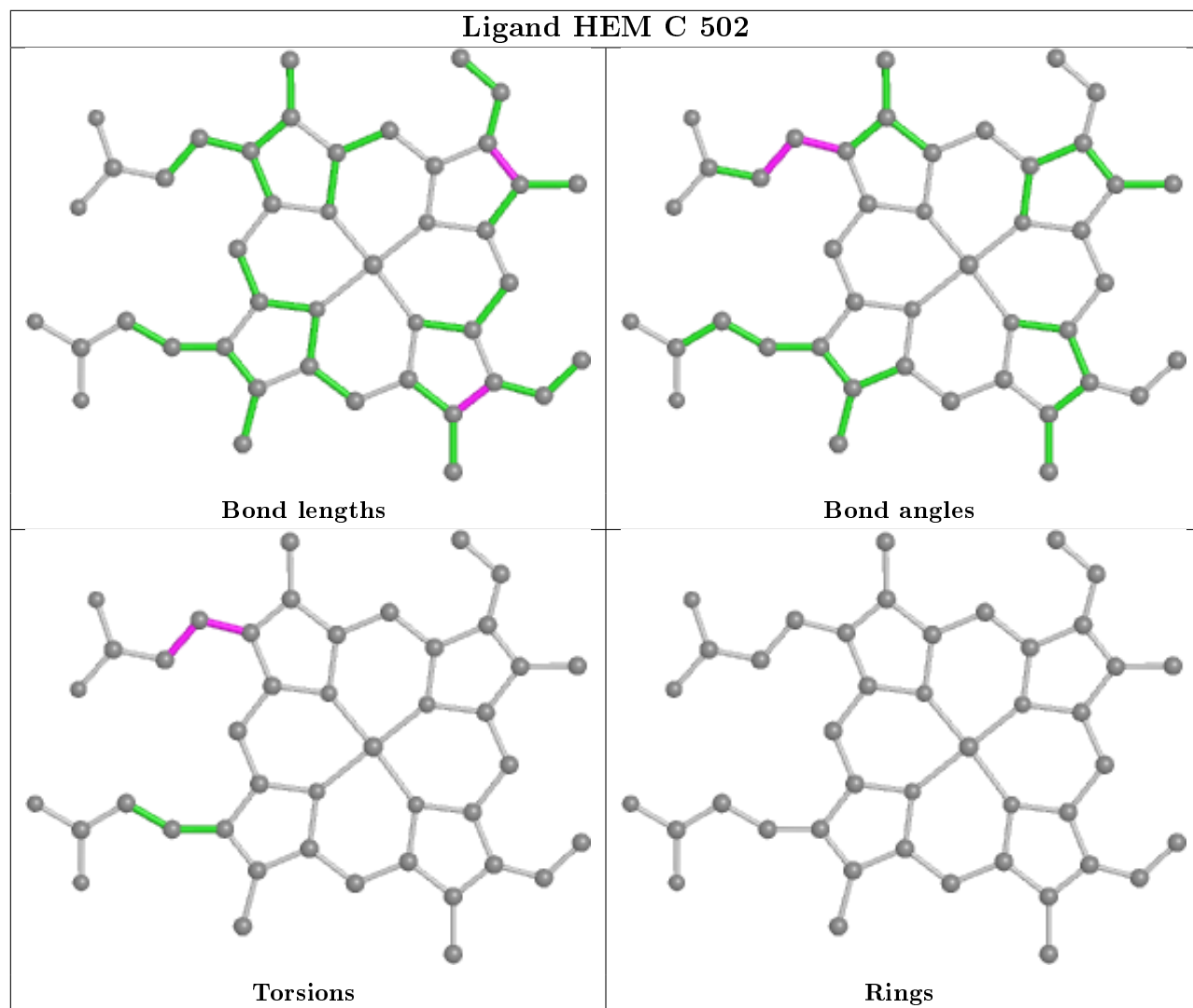
There are no ring outliers.

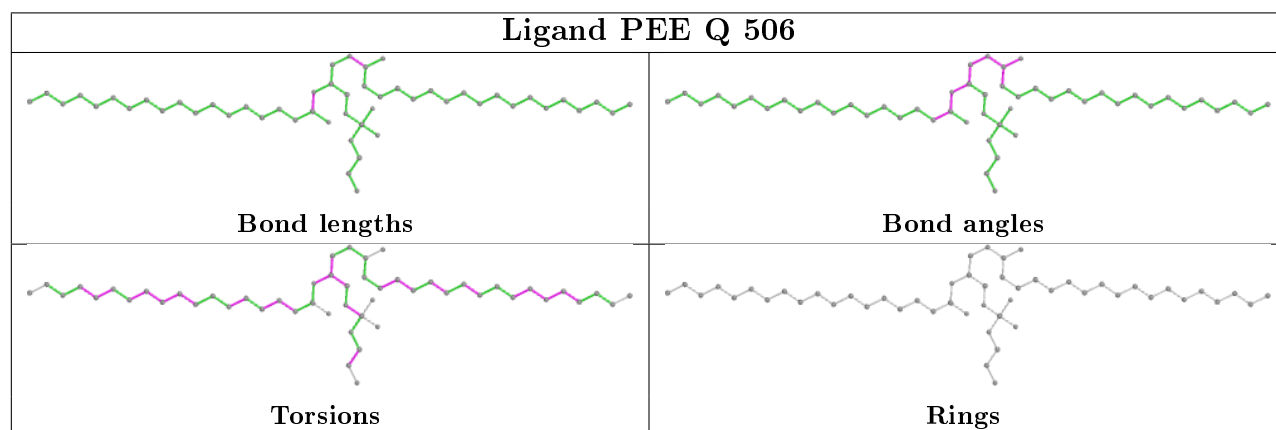
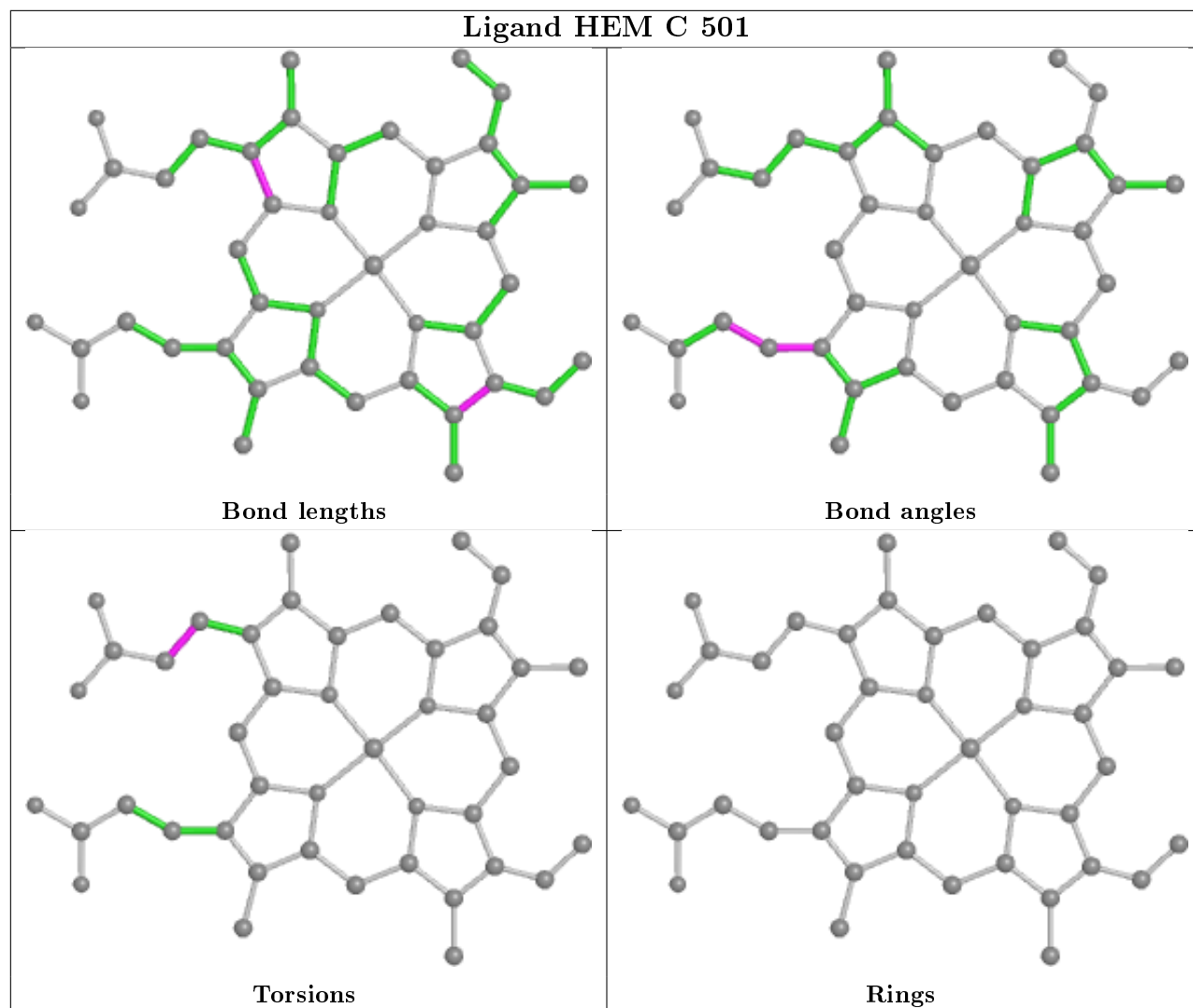
14 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	C	502	HEM	6	0
12	C	501	HEM	4	0
15	Q	506	PEE	3	0
13	C	503	4X9	6	0
17	T	501	CDL	1	0
16	D	501	HEC	12	0
13	P	503	4X9	5	0
12	P	502	HEM	3	0
16	Q	501	HEC	10	0
15	C	505	PEE	1	0
17	Q	505	CDL	1	0
18	R	501	FES	3	0
15	P	505	PEE	1	0
12	P	501	HEM	7	0

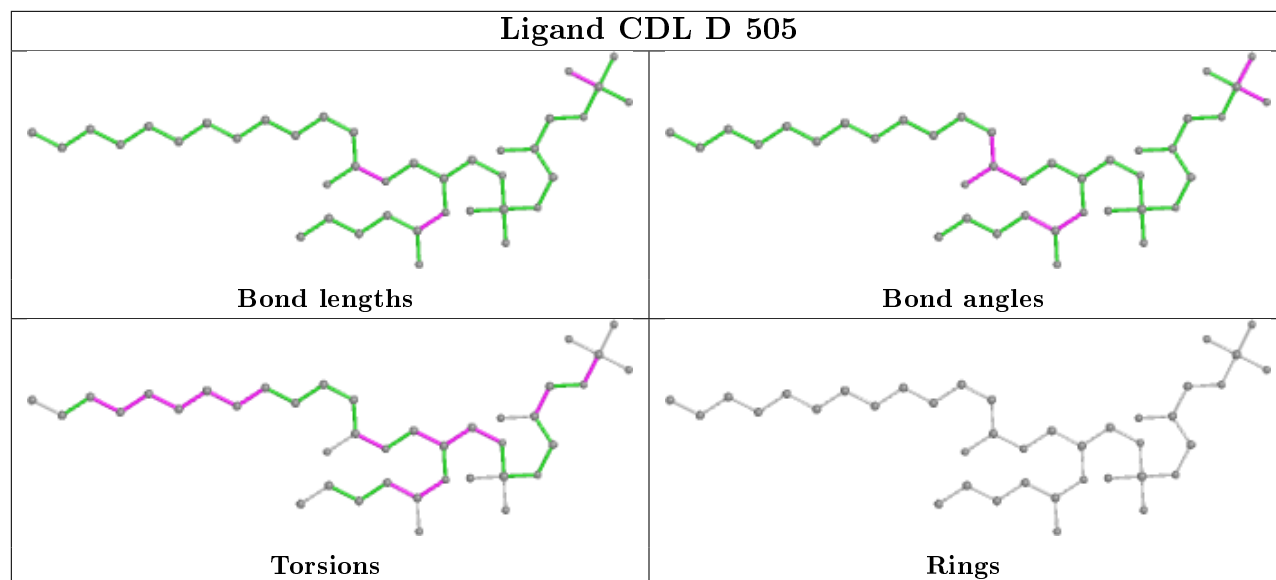
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



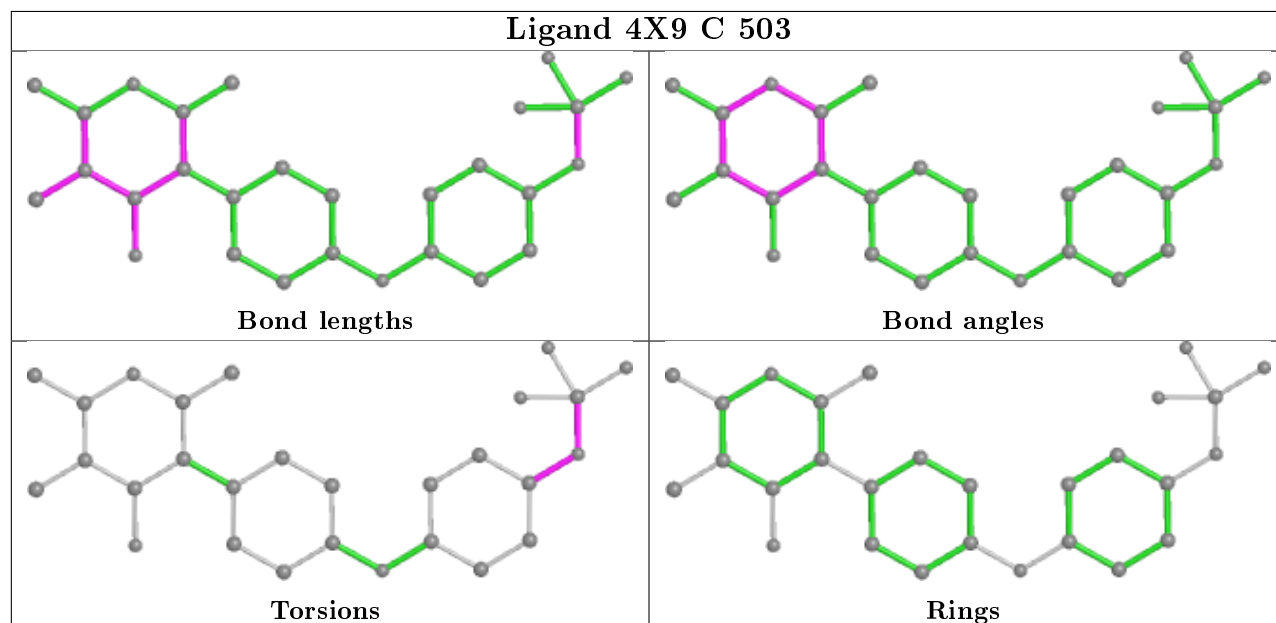




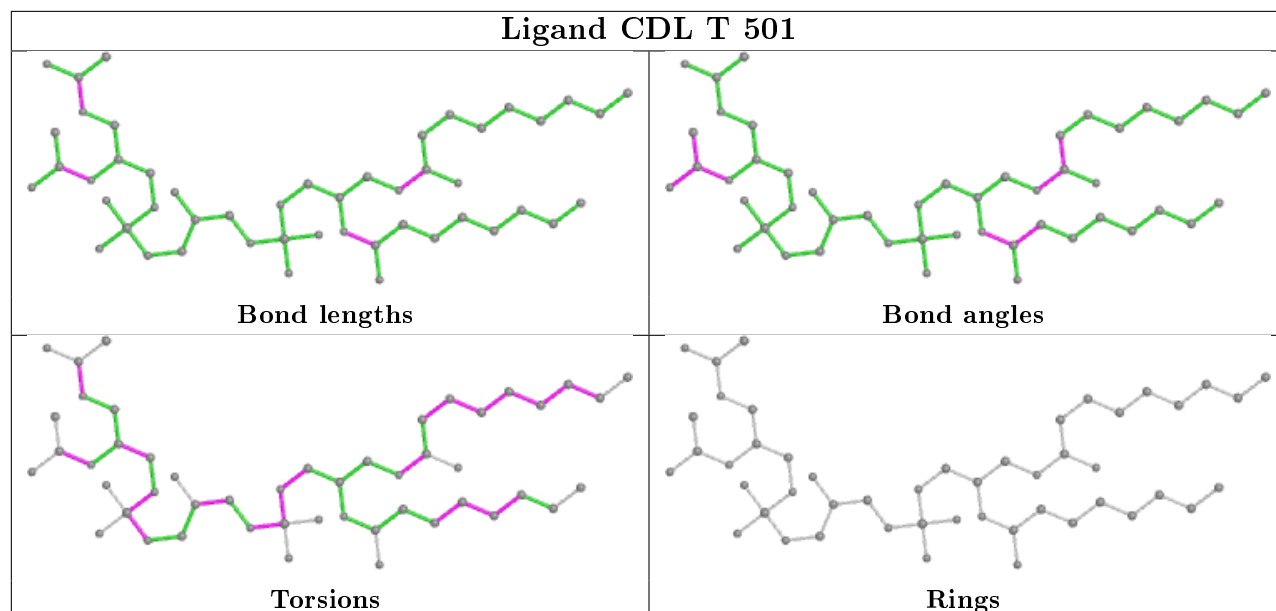
## Ligand CDL D 505



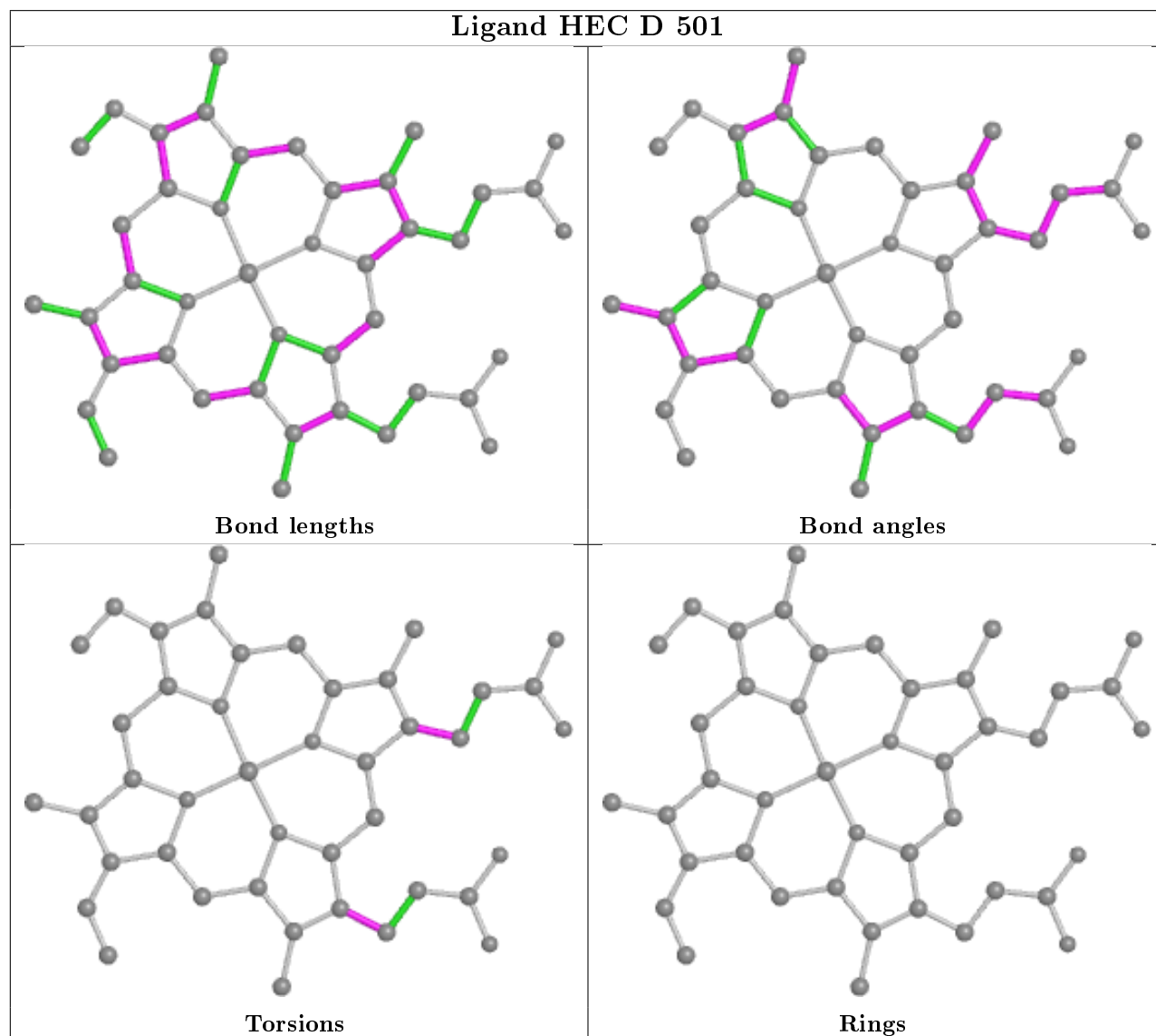
## Ligand 4X9 C 503



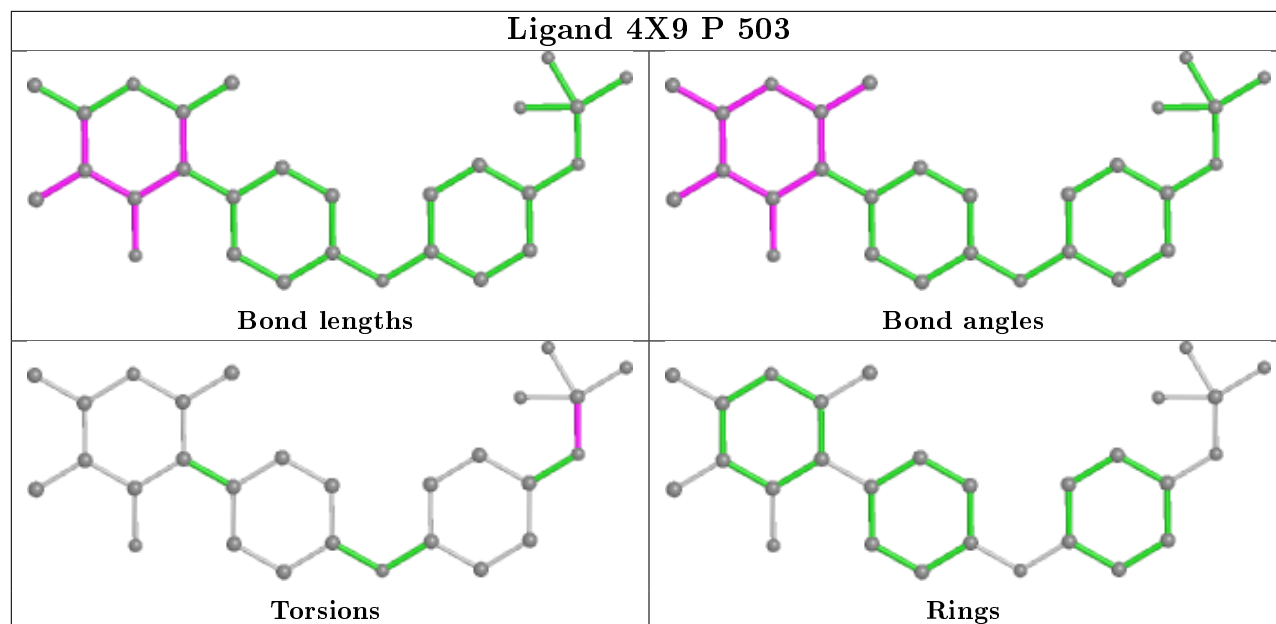
## Ligand CDL T 501



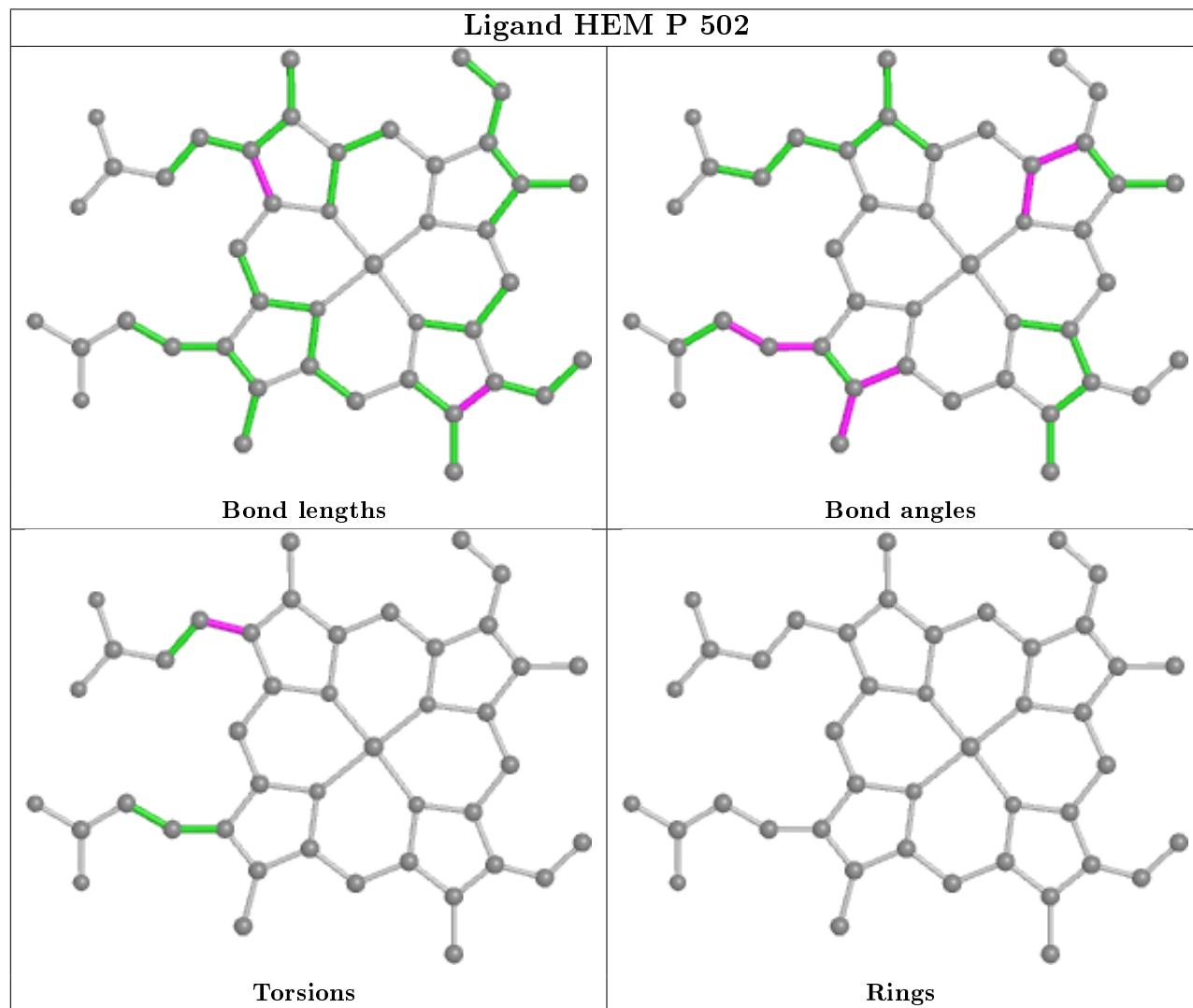
## Ligand HEC D 501



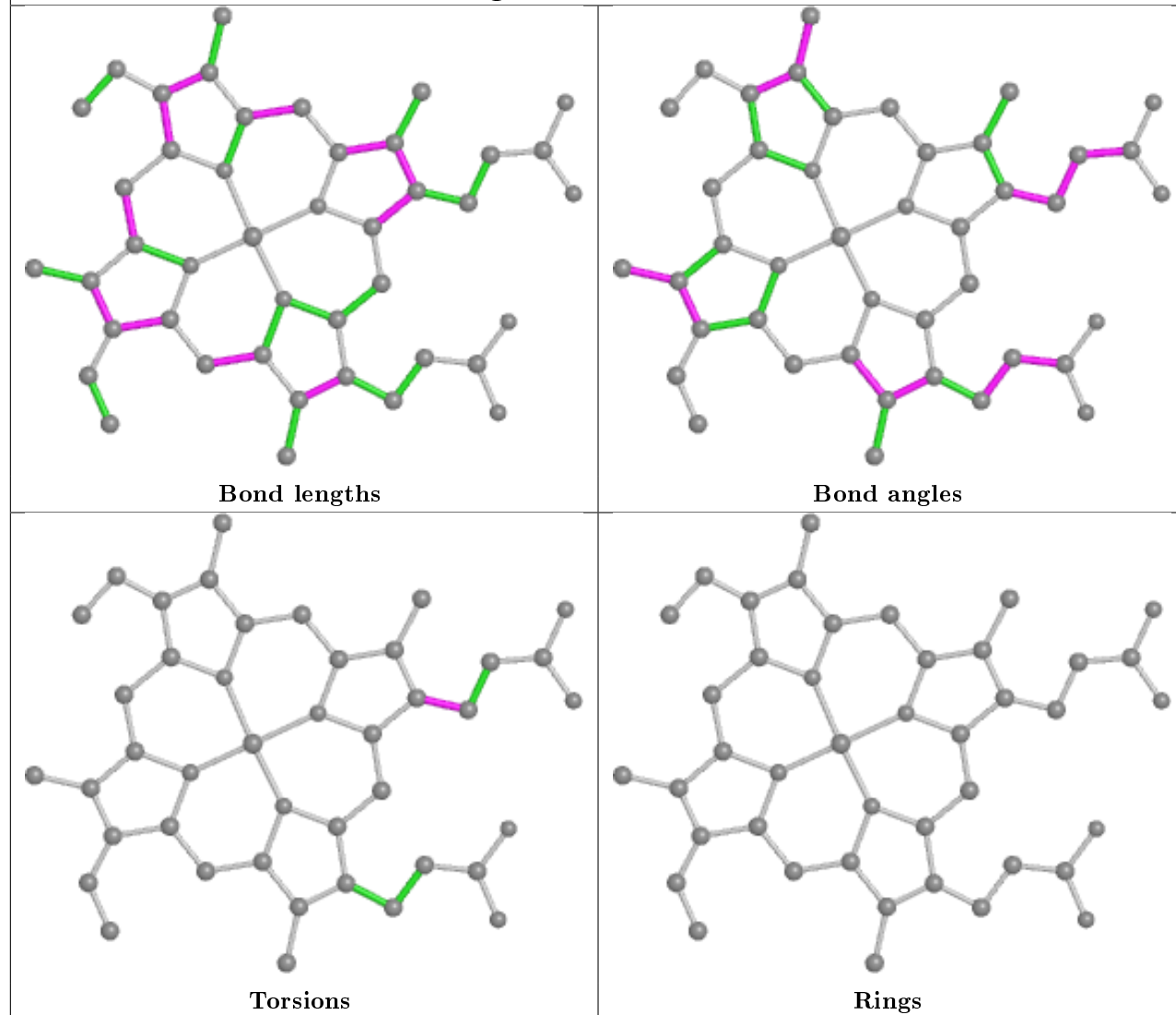
## Ligand 4X9 P 503



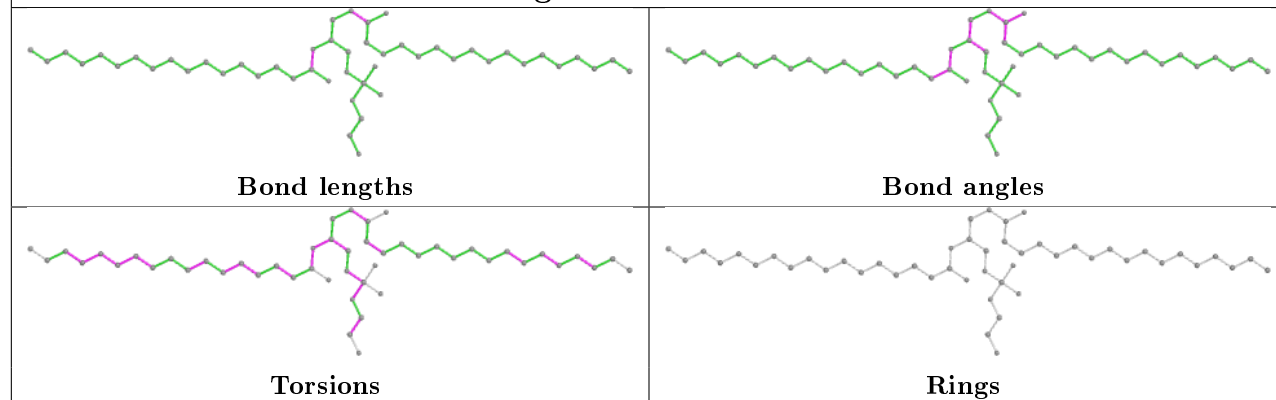
## Ligand HEM P 502



## Ligand HEC Q 501

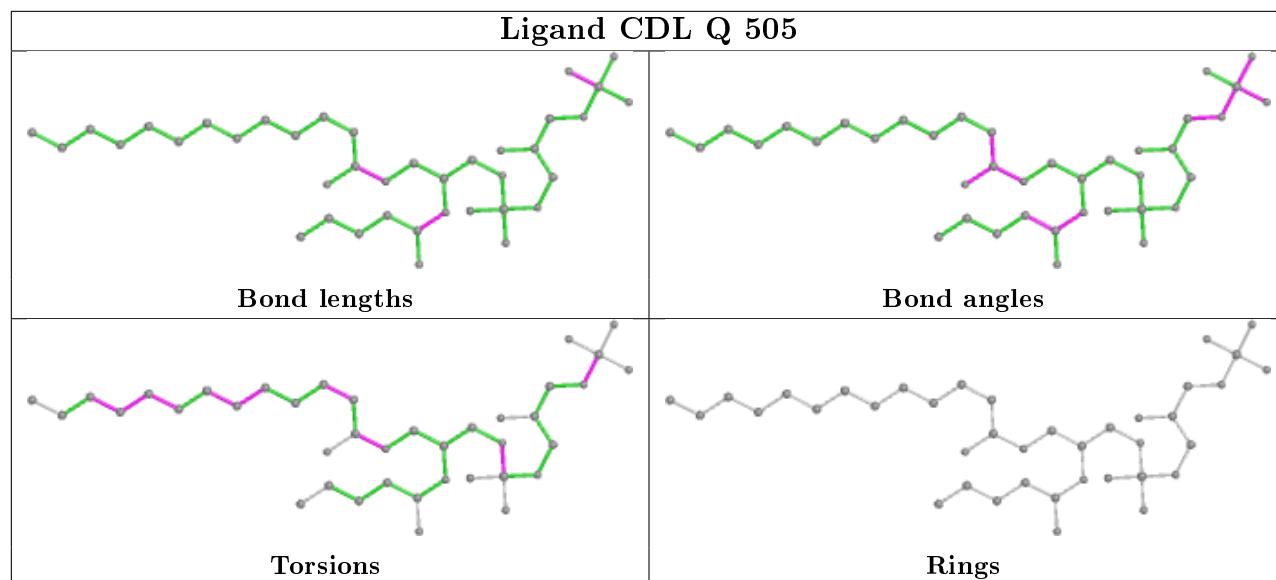


## Ligand PEE C 505

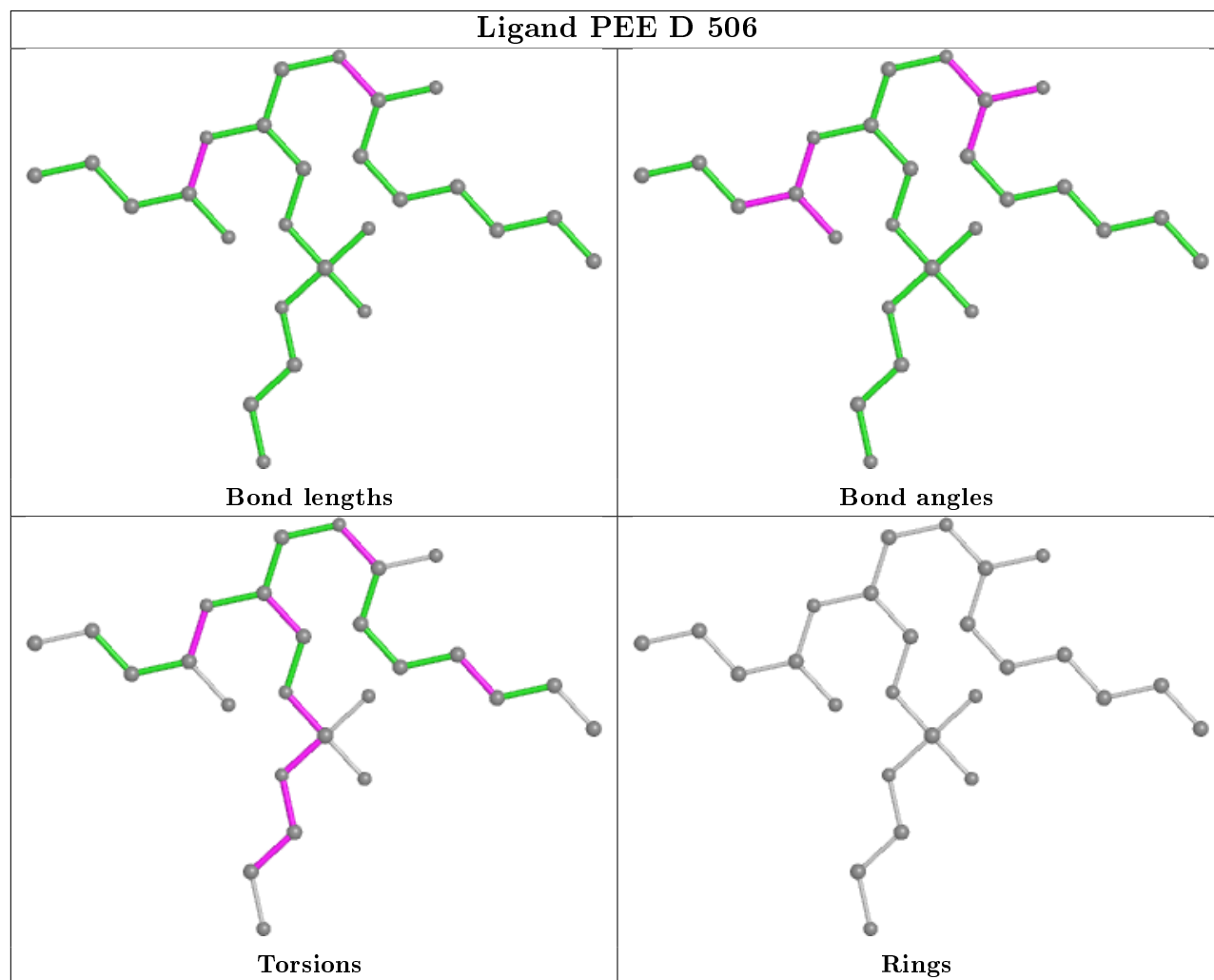


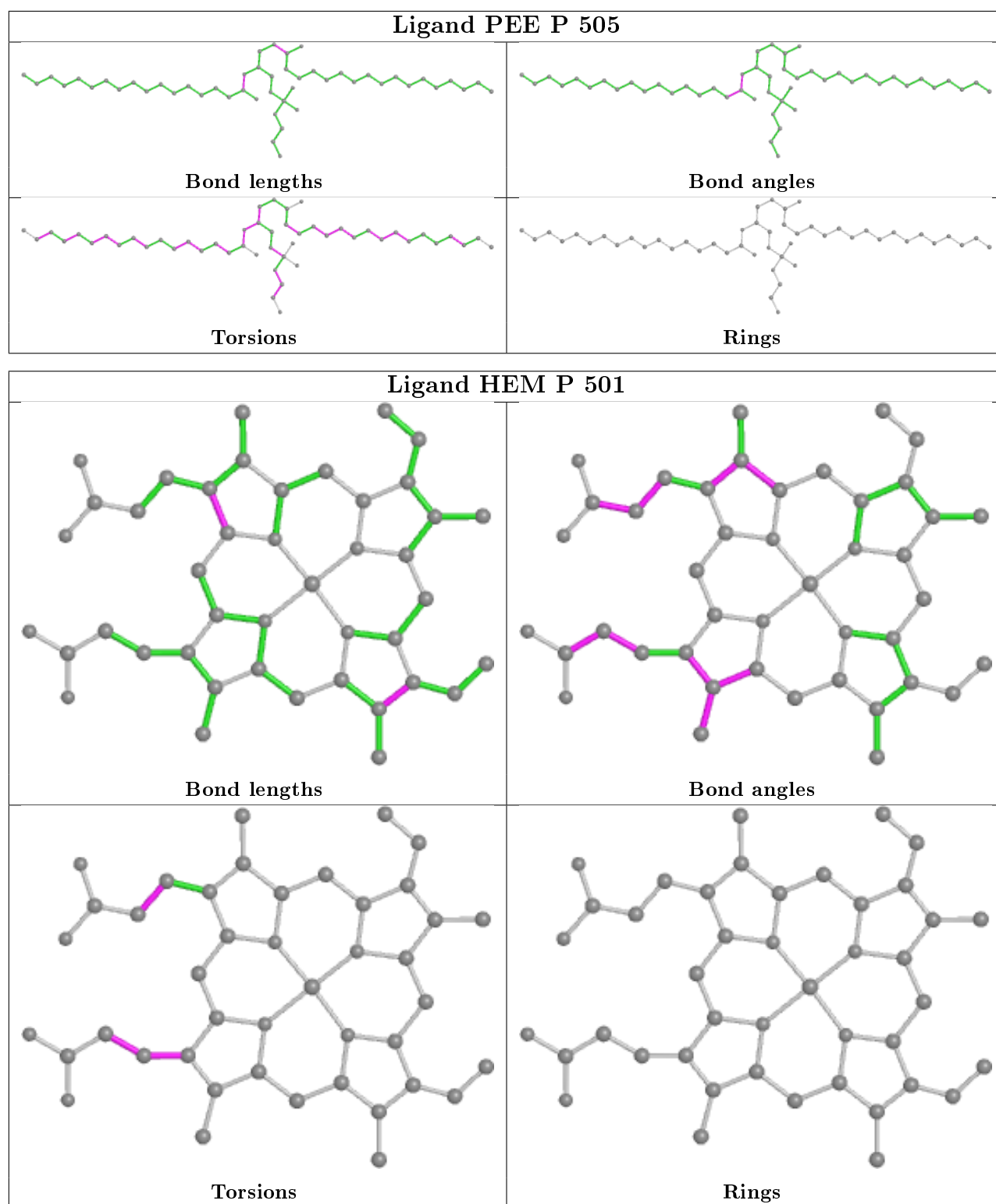


## Ligand CDL Q 505



## Ligand PEE D 506





## 5.7 Other polymers ⓘ

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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	444/480 (92%)	-0.14	9 (2%) 65 48	92, 150, 191, 255	0
1	N	444/480 (92%)	-0.33	7 (1%) 72 55	87, 132, 176, 243	0
2	B	422/453 (93%)	0.14	29 (6%) 16 9	108, 157, 200, 247	0
3	C	374/379 (98%)	-0.50	0 100 100	77, 103, 137, 225	0
3	P	370/379 (97%)	-0.44	1 (0%) 94 88	79, 112, 148, 183	0
4	D	240/265 (90%)	-0.31	2 (0%) 86 73	92, 121, 153, 178	0
4	Q	241/265 (90%)	-0.10	6 (2%) 57 39	86, 131, 168, 211	0
5	E	73/274 (26%)	-0.36	1 (1%) 75 59	93, 130, 158, 170	0
5	I	21/274 (7%)	0.63	1 (4%) 30 18	146, 192, 220, 228	0
5	R	196/274 (71%)	-0.15	2 (1%) 82 69	91, 150, 193, 230	0
6	F	98/111 (88%)	-0.44	2 (2%) 65 48	91, 124, 157, 171	0
6	S	99/111 (89%)	-0.44	0 100 100	85, 122, 168, 182	0
7	G	80/82 (97%)	-0.29	1 (1%) 77 61	88, 119, 189, 293	0
7	T	74/82 (90%)	-0.40	2 (2%) 54 36	83, 124, 181, 201	0
8	H	65/91 (71%)	-0.47	0 100 100	103, 136, 171, 223	0
8	U	66/91 (72%)	0.09	5 (7%) 13 7	132, 163, 213, 245	0
9	J	58/64 (90%)	-0.06	0 100 100	103, 137, 165, 175	0
9	W	59/64 (92%)	-0.19	1 (1%) 70 53	102, 121, 153, 162	0
10	O	419/453 (92%)	-0.21	7 (1%) 70 53	97, 146, 193, 250	0
11	V	17/274 (6%)	1.19	3 (17%) 1 0	176, 209, 228, 268	0
All	All	3860/4946 (78%)	-0.23	79 (2%) 65 48	77, 133, 189, 293	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	226	ASP	5.9
11	V	62	ARG	4.8
2	B	232	LEU	4.7
1	N	225	GLU	4.2
2	B	21	PRO	4.0
10	O	232	LEU	4.0
2	B	36	ALA	4.0
8	U	44	VAL	3.8
8	U	50	THR	3.8
2	B	23	ASP	3.7
11	V	63	PRO	3.6
1	N	243	HIS	3.6
8	U	51	GLU	3.4
10	O	231	GLY	3.4
2	B	19	PRO	3.4
10	O	233	SER	3.4
5	E	73	LYS	3.3
10	O	234	GLY	3.3
2	B	274	VAL	3.3
4	Q	1	SER	3.1
1	A	225	GLU	3.1
1	N	226	ASP	3.1
2	B	272	PHE	3.0
2	B	208	GLY	3.0
4	D	241	LYS	3.0
5	I	77	ARG	3.0
6	F	109	LYS	3.0
2	B	439	LEU	2.9
4	Q	143	LEU	2.9
9	W	2	ALA	2.9
2	B	276	GLN	2.8
2	B	322	PHE	2.8
2	B	233	SER	2.8
2	B	220	ALA	2.7
4	Q	146	GLY	2.7
2	B	417	PHE	2.7
8	U	78	LYS	2.7
2	B	352	LEU	2.7
1	A	127	ILE	2.7
2	B	275	LEU	2.6
1	A	177	LEU	2.6
2	B	407	ASP	2.5
2	B	38	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	182	LEU	2.5
2	B	344	VAL	2.4
11	V	70	LEU	2.4
6	F	106	GLU	2.4
2	B	229	GLY	2.3
10	O	41	TYR	2.3
3	P	168	PHE	2.3
2	B	231	GLY	2.3
4	Q	142	SER	2.3
1	A	83	GLY	2.3
1	A	303	LEU	2.3
7	T	74	PRO	2.3
10	O	122	PHE	2.3
2	B	20	HIS	2.2
5	R	77	LYS	2.2
2	B	311	ALA	2.2
1	A	126	GLN	2.2
7	T	14	ILE	2.2
1	N	394	GLU	2.2
1	N	424	GLY	2.2
2	B	227	ARG	2.2
1	N	425	PHE	2.2
4	Q	167	GLU	2.2
7	G	76	ALA	2.1
2	B	410	VAL	2.1
4	Q	149	PHE	2.1
5	R	98	VAL	2.1
2	B	347	ILE	2.1
1	A	84	ALA	2.1
2	B	313	ASN	2.1
4	D	180	SER	2.1
10	O	229	GLY	2.1
8	U	52	GLU	2.1
2	B	217	LYS	2.1
2	B	43	PRO	2.0
1	N	393	ALA	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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.

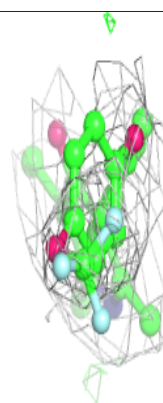
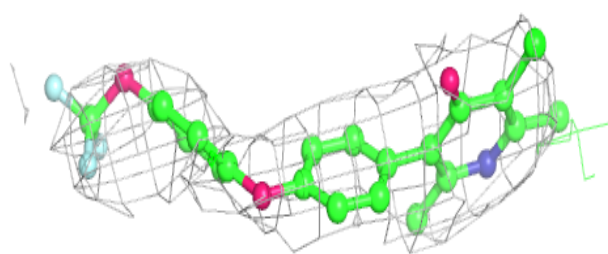
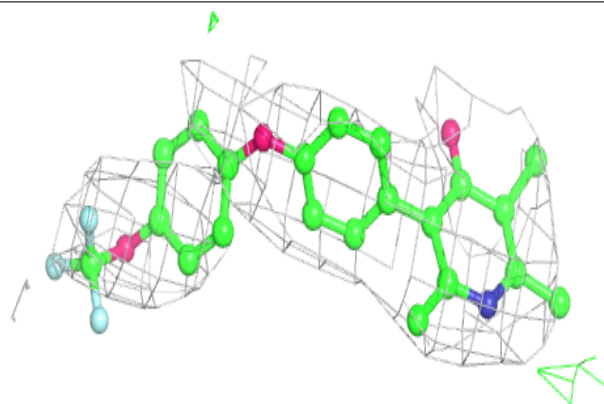
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
14	PO4	S	501	5/5	0.39	0.52	225,226,243,252	0
14	PO4	F	501	5/5	0.51	0.58	242,243,245,246	0
14	PO4	D	504	5/5	0.57	0.23	179,190,194,195	0
14	PO4	Q	1001	5/5	0.66	0.20	194,205,216,232	0
14	PO4	N	501	5/5	0.67	0.45	112,126,127,137	0
14	PO4	D	502	5/5	0.71	0.27	176,192,199,203	0
19	GOL	R	502	6/6	0.72	1.89	169,181,193,193	0
14	PO4	Q	1002	5/5	0.72	0.20	210,211,220,230	0
14	PO4	E	501	5/5	0.74	0.32	124,134,144,145	0
14	PO4	D	503	5/5	0.82	0.61	168,169,177,181	0
14	PO4	C	504	5/5	0.82	0.39	121,121,134,149	0
13	4X9	P	503	28/28	0.88	0.32	109,147,226,261	0
15	PEE	Q	506	51/51	0.90	0.40	100,134,171,187	0
13	4X9	C	503	28/28	0.90	0.39	116,143,206,215	0
15	PEE	C	505	49/51	0.91	0.49	94,116,135,137	0
17	CDL	D	505	39/100	0.91	0.27	85,124,146,148	0
17	CDL	G	501	44/100	0.92	0.28	95,115,153,168	0
17	CDL	T	501	49/100	0.92	0.31	93,129,160,167	0
15	PEE	P	505	49/51	0.93	0.33	100,122,154,156	0
14	PO4	N	1001	5/5	0.93	0.42	120,127,135,137	0
17	CDL	Q	505	39/100	0.93	0.28	100,126,146,148	0
15	PEE	D	506	26/51	0.93	0.26	107,127,169,176	0
18	FES	R	501	4/4	0.97	0.14	125,158,164,170	0
12	HEM	C	502	43/43	0.98	0.26	71,85,99,106	0
12	HEM	P	502	43/43	0.98	0.23	74,89,104,106	0
12	HEM	P	501	43/43	0.98	0.30	86,101,116,124	0
12	HEM	C	501	43/43	0.98	0.27	89,99,107,115	0
16	HEC	D	501	43/43	0.98	0.24	80,111,127,138	0
16	HEC	Q	501	43/43	0.98	0.28	106,117,136,143	0

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.

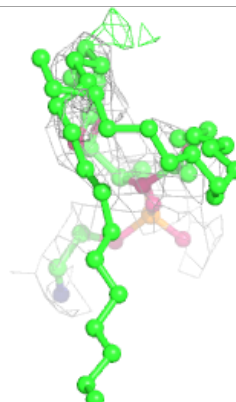
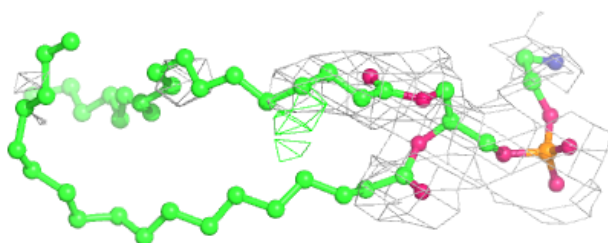
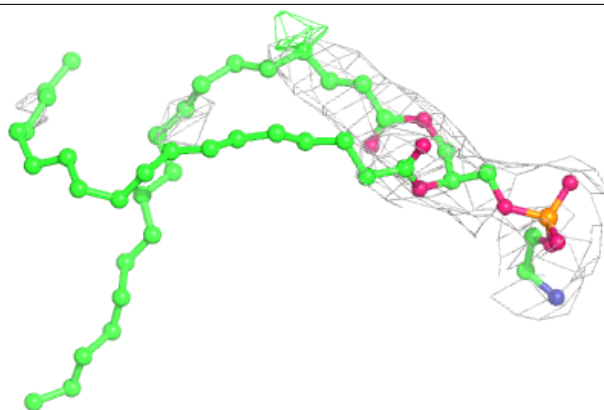
**Electron density around 4X9 P 503:**

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



**Electron density around PEE Q 506:**

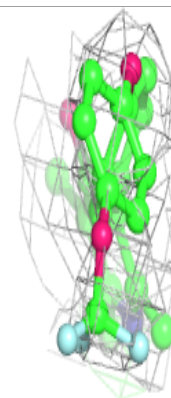
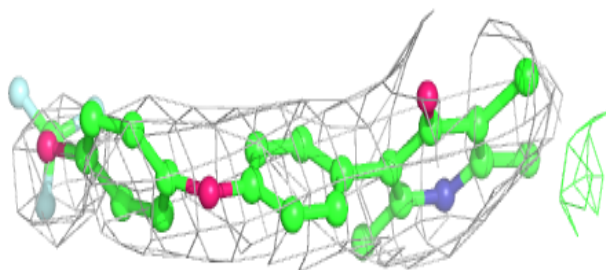
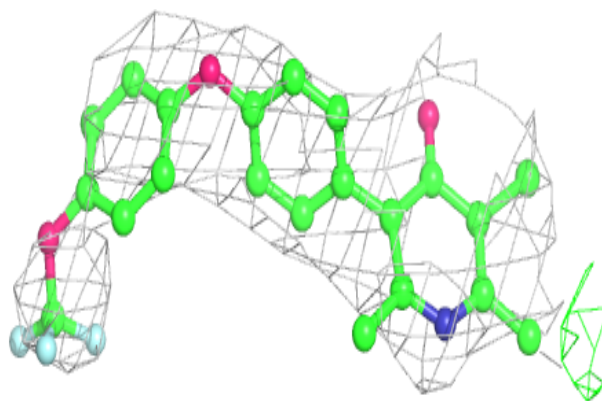
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



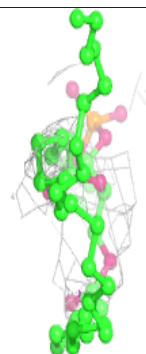
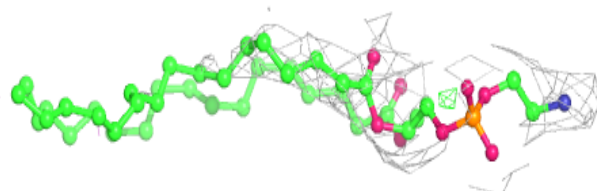
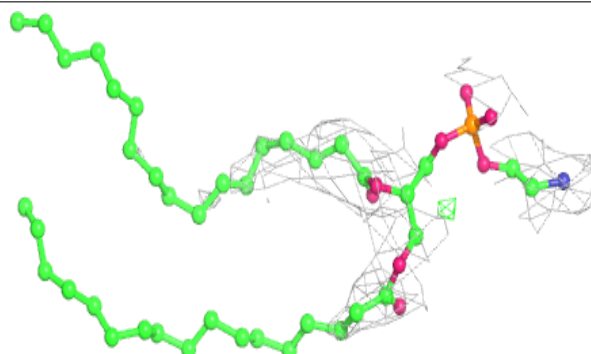


**Electron density around 4X9 C 503:**

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

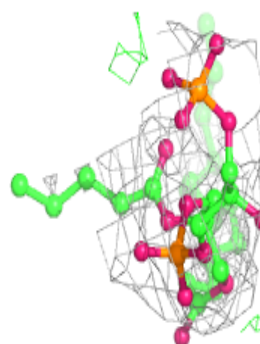
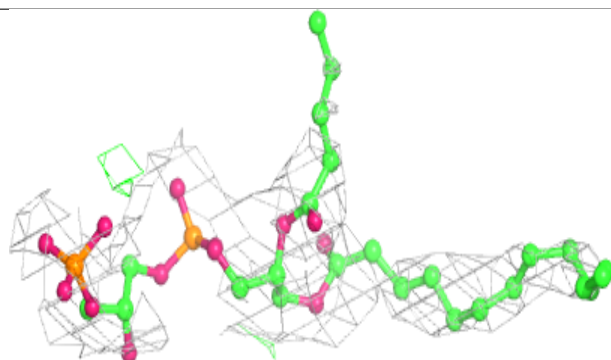
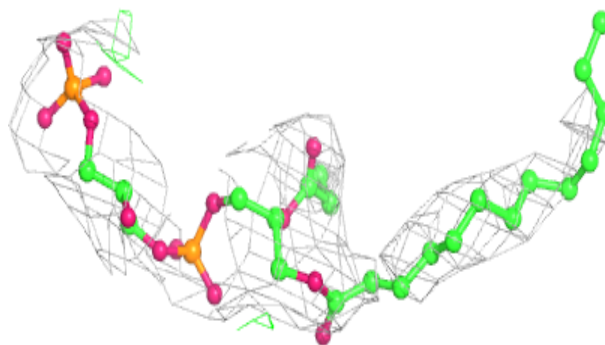
**Electron density around PEE C 505:**

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

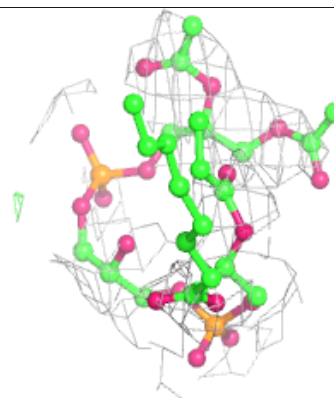
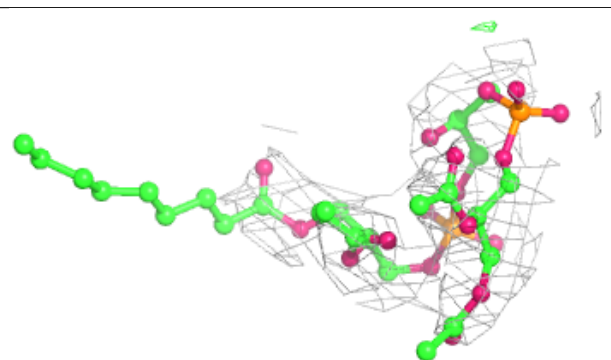
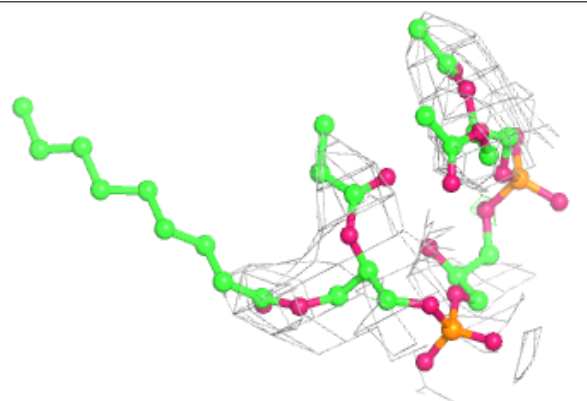


**Electron density around CDL D 505:**

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

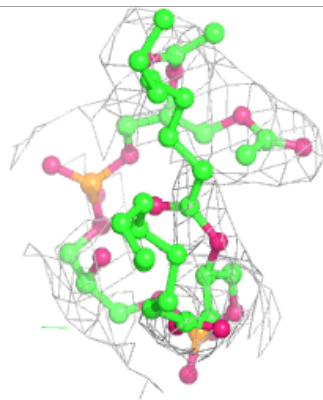
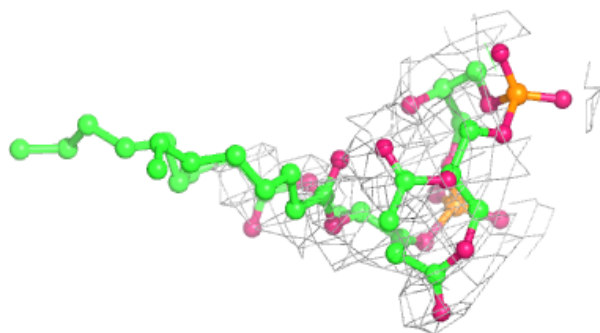
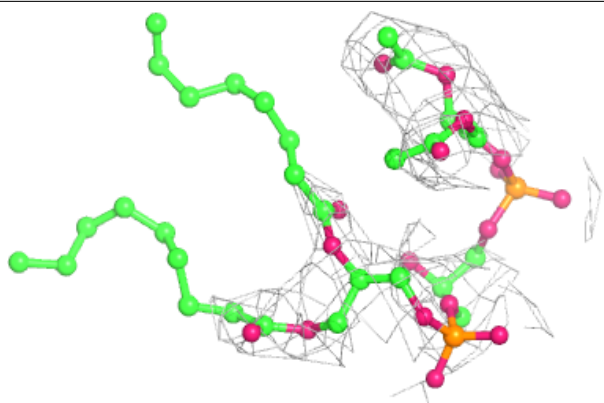
**Electron density around CDL G 501:**

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

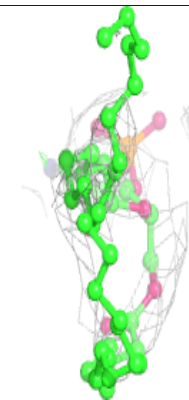
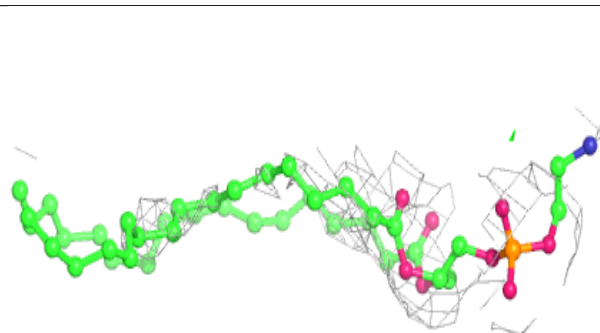
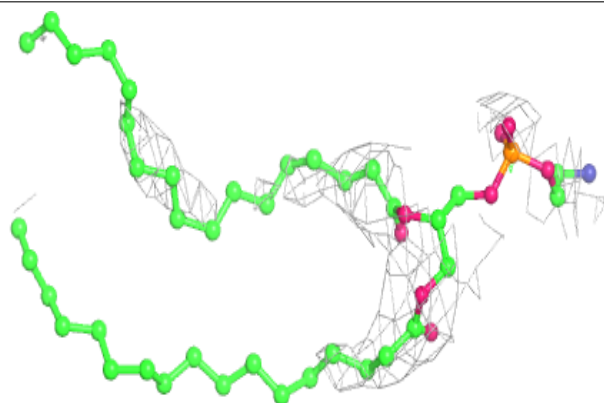


**Electron density around CDL T 501:**

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

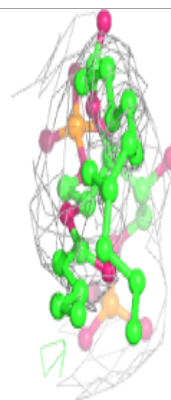
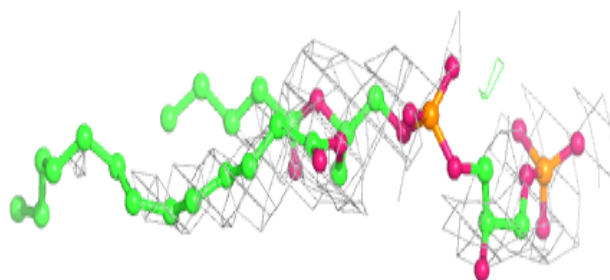
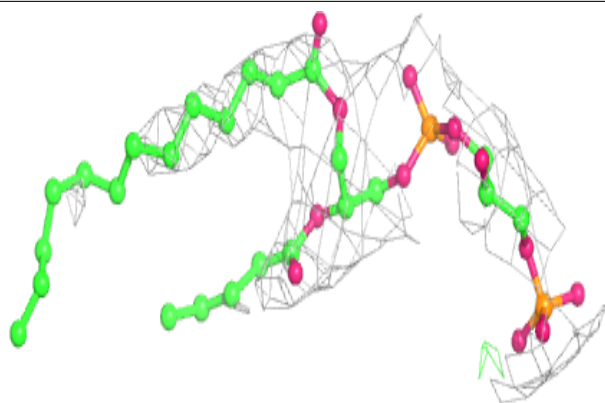
**Electron density around PEE P 505:**

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

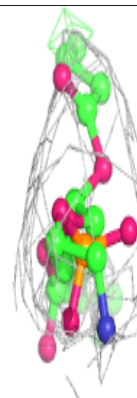
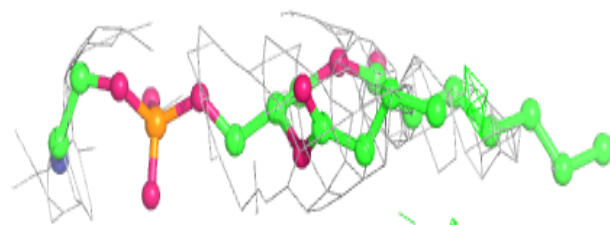
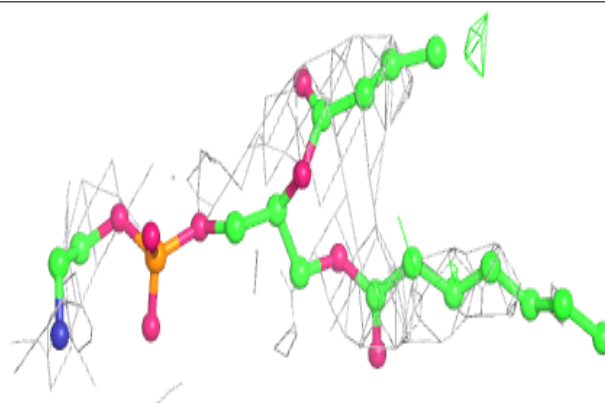


**Electron density around CDL Q 505:**

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

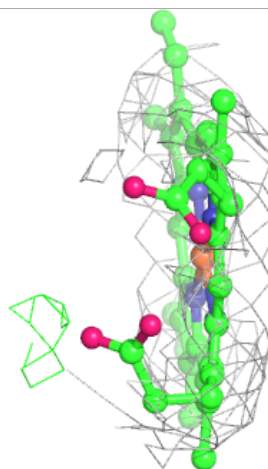
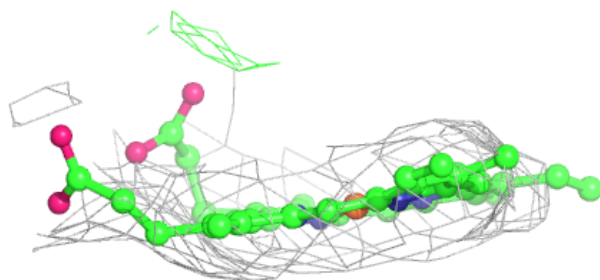
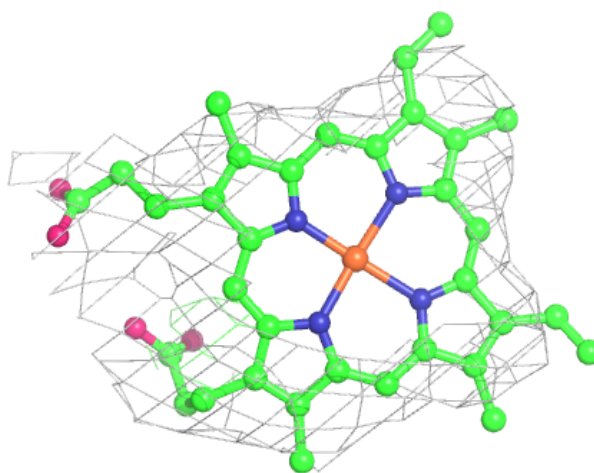
**Electron density around PEE D 506:**

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



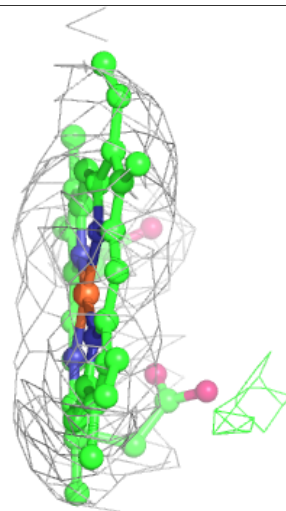
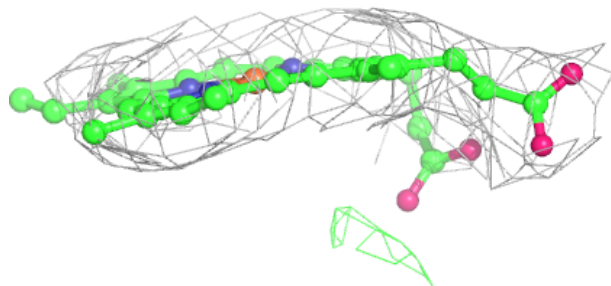
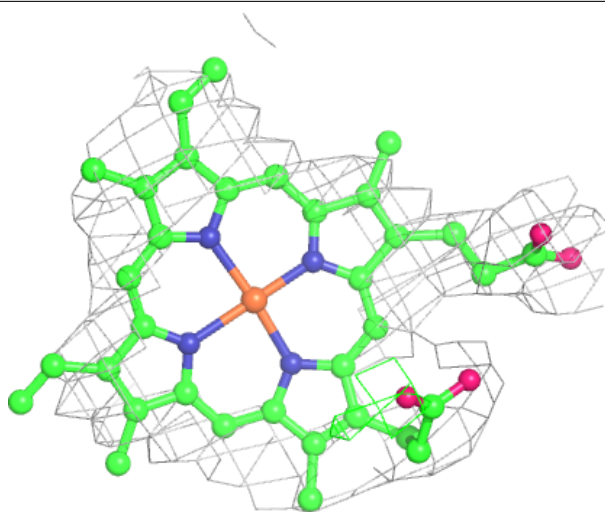
**Electron density around HEM C 502:**

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



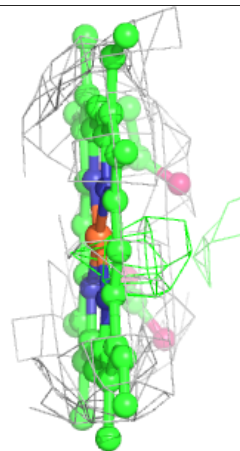
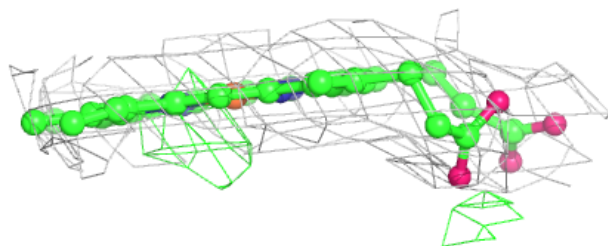
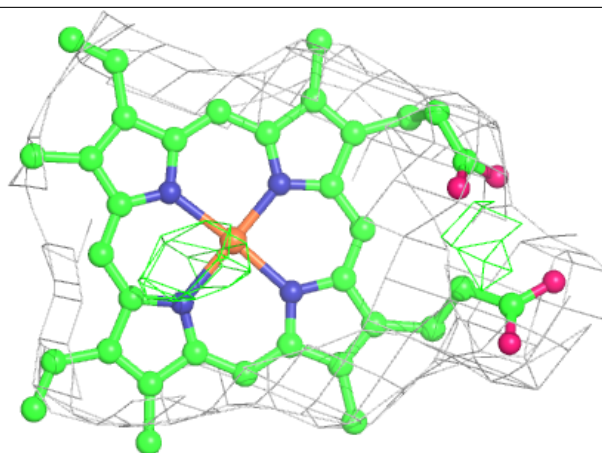
**Electron density around HEM P 502:**

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



**Electron density around HEM P 501:**

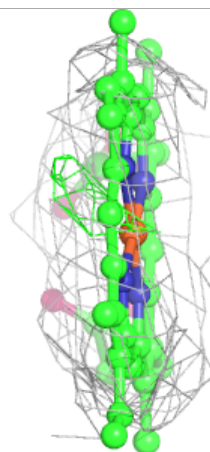
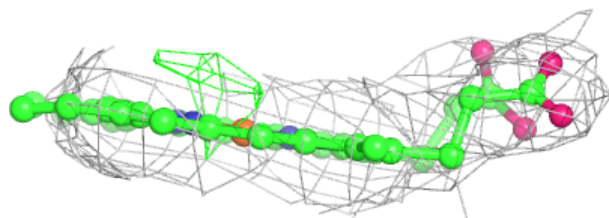
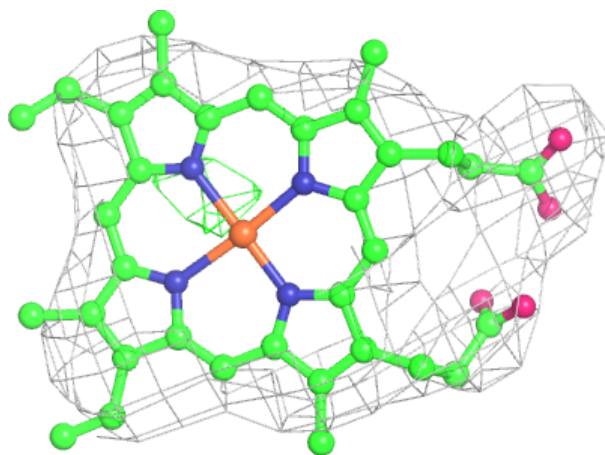
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEM C 501:**

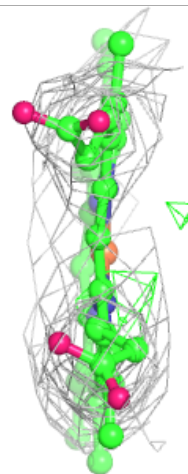
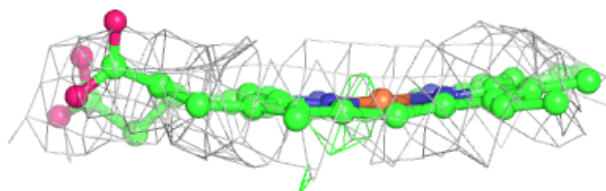
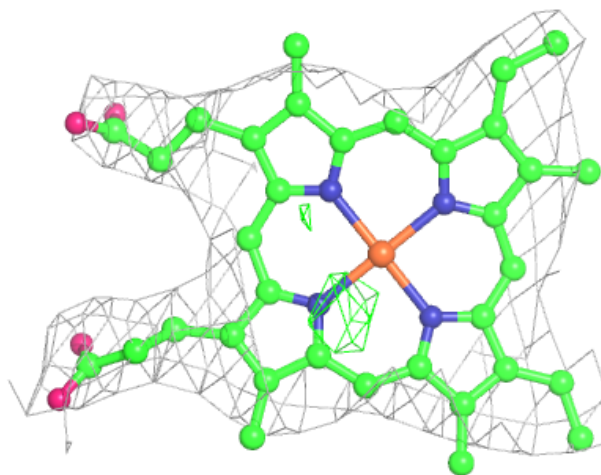
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

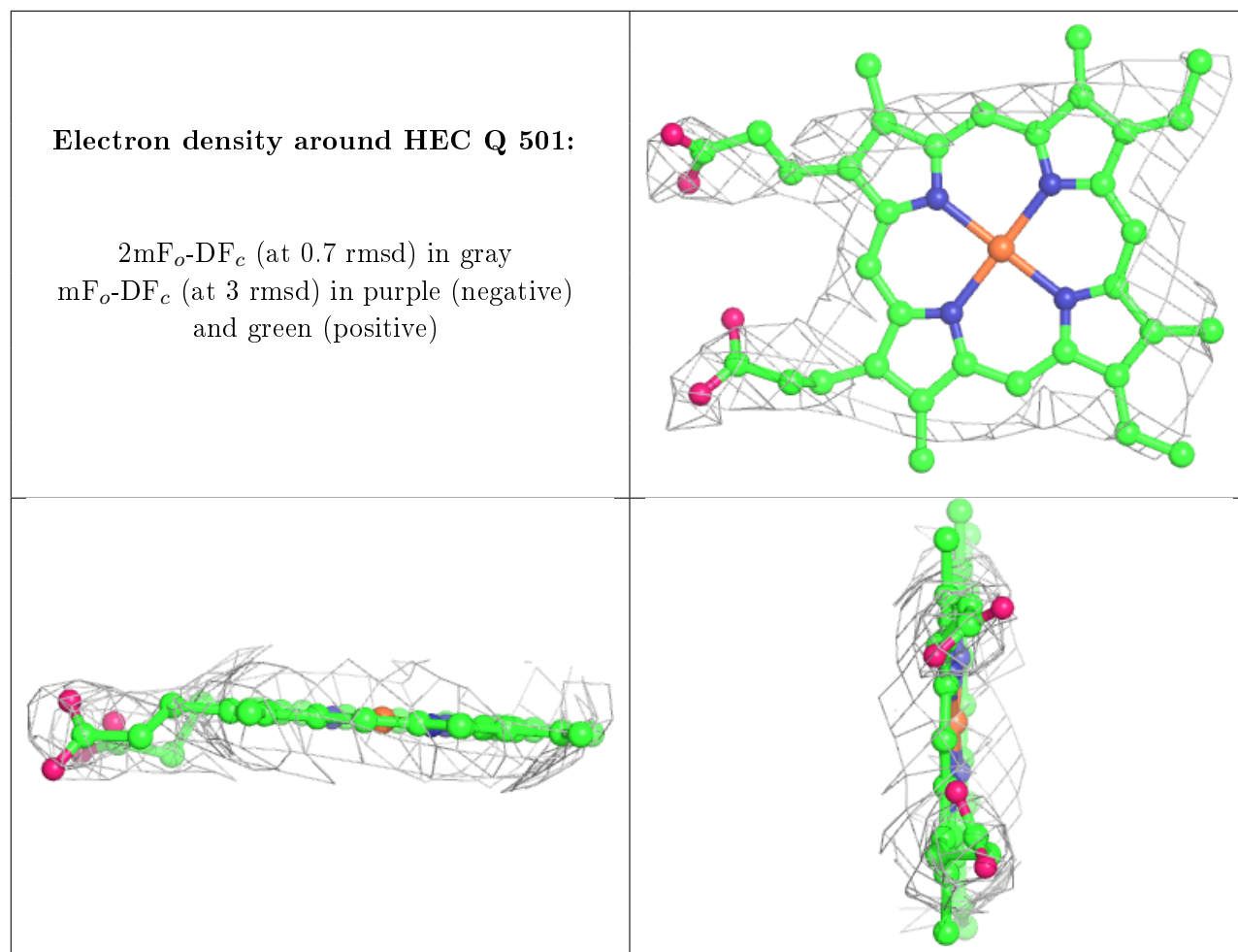




**Electron density around HEC D 501:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.