



# Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 02:03 am BST

PDB ID : 4D6U  
Title : Cytochrome bc1 bound to the 4(1H)-pyridone GSK932121  
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 : 4.09 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

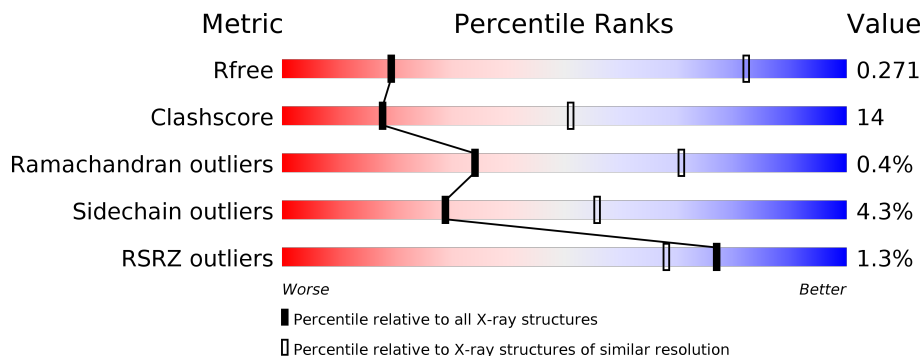
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.09 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	1193 (4.50-3.70)
Clashscore	141614	1003 (4.44-3.76)
Ramachandran outliers	138981	1005 (4.48-3.72)
Sidechain outliers	138945	1199 (4.50-3.70)
RSRZ outliers	127900	1034 (4.50-3.70)

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	 4% 72% 19% 8%
2	B	453	 4% 69% 22% 7%
3	C	379	 70% 26%
3	P	379	 68% 28%
4	D	325	 59% 13% 26%
4	Q	325	 56% 17% 26%

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Mol	Chain	Length	Quality of chain
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	N	480	
11	O	453	
12	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	G8U	C	503	-	-	X	X
14	G8U	P	503	-	-	X	X
15	PO4	D	503	-	-	-	X
15	PO4	D	504	-	-	-	X
15	PO4	F	501	-	-	-	X
15	PO4	N	501	-	-	-	X
15	PO4	S	501	-	-	-	X
16	PEE	C	505	X	-	-	-
16	PEE	D	506	X	-	-	-
16	PEE	P	505	X	-	-	-
16	PEE	Q	506	X	-	-	X
19	FES	R	501	-	-	X	-
20	GOL	R	502	-	-	-	X

## 2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 31080 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
			Total	C	N	O	S			
1	A	444	3439	2148	607	664	20	0	0	0

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

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

- Molecule 3 is a protein called CYTOCHROME B.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	73	549	341	92	114	2	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	27	Total	C	N	O	S	0	0	0
			196	121	38	36	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
			Total	C	N	O			
9	W	59	487	320	84	83	0	0	0

- Molecule 10 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	N	444	3430	2142	605	663	20	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	445	LYS	ARG	conflict	UNP P31800

- Molecule 11 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL.

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

There is a discrepancy between the modelled and reference sequences:

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

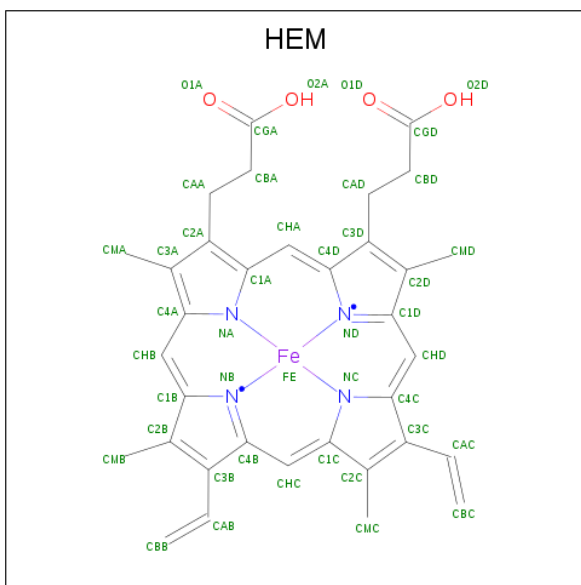
- Molecule 12 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL.

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

There is a discrepancy between the modelled and reference sequences:

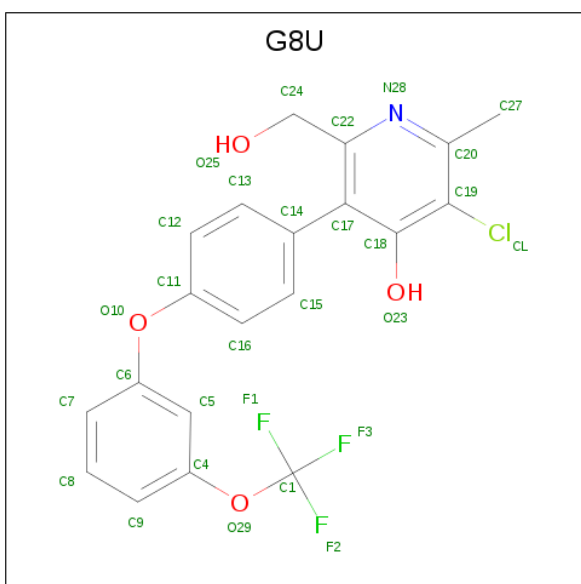
Chain	Residue	Modelled	Actual	Comment	Reference
V	64	VAL	LEU	conflict	UNP P13272

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



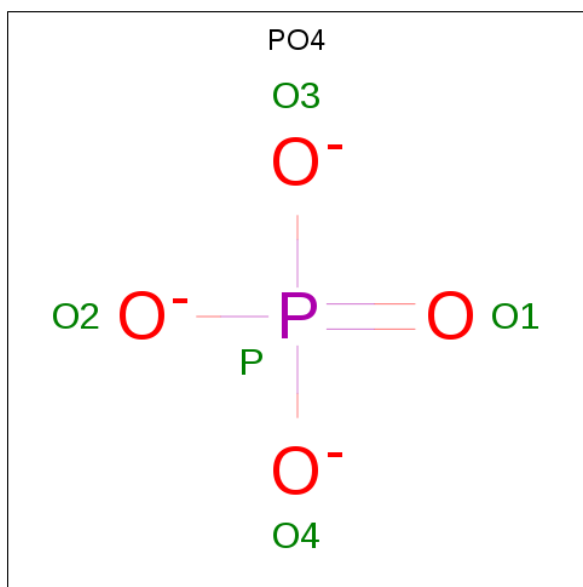
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
13	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
13	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
13	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
13	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 14 is 3-chloro-6-(hydroxymethyl)-2-methyl-5-{4-[3-(trifluoromethoxy)phenoxy]phenyl}pyridin-4-ol (three-letter code: G8U) (formula:  $C_{20}H_{15}ClF_3NO_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	Cl	F	N			O
14	C	1	29	20	1	3	1	4	0	0
14	P	1	29	20	1	3	1	4	0	0

- Molecule 15 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).

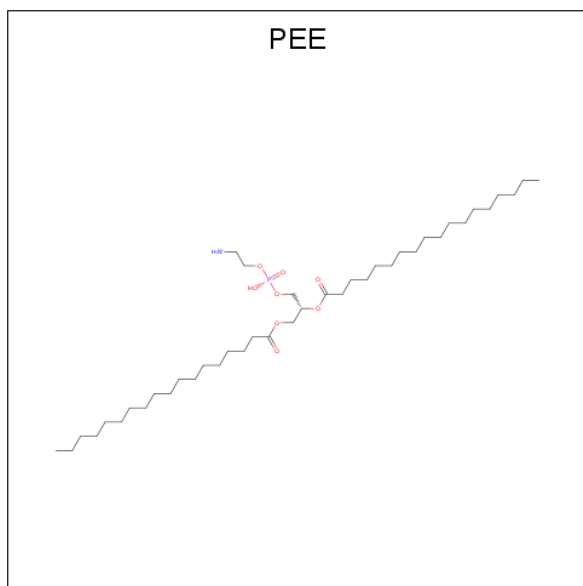


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
15	C	1	5	4	1	0	0
15	D	1	5	4	1	0	0
15	D	1	5	4	1	0	0
15	D	1	5	4	1	0	0
15	E	1	5	4	1	0	0
15	F	1	5	4	1	0	0
15	N	1	5	4	1	0	0
15	P	1	5	4	1	0	0
15	S	1	5	4	1	0	0

- Molecule 16 is 1,2-Dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE)

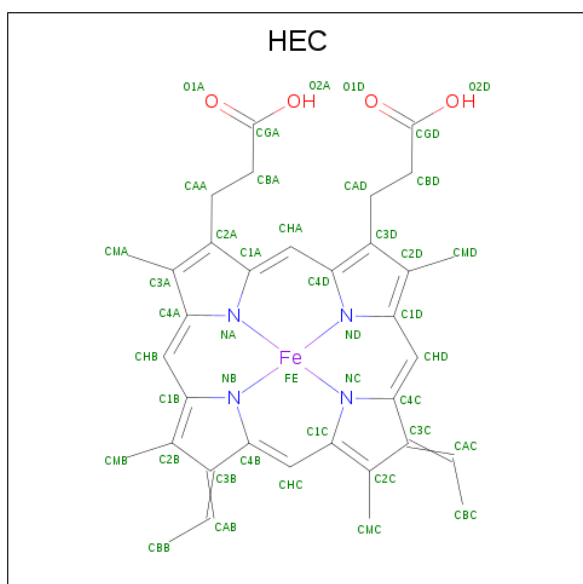


(formula:  $C_{41}H_{83}NO_8P$ ).



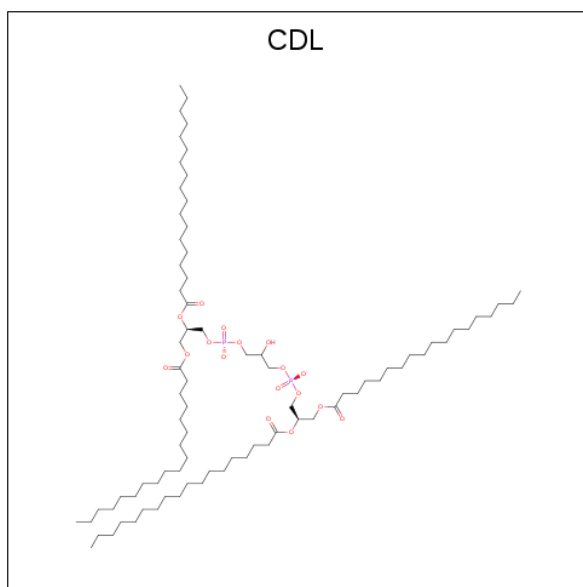
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
16	C	1	Total 49	C 39	N 1	O 8	P 1	0	0
16	D	1	Total 26	C 16	N 1	O 8	P 1	0	0
16	P	1	Total 49	C 39	N 1	O 8	P 1	0	0
16	Q	1	Total 51	C 41	N 1	O 8	P 1	0	0

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



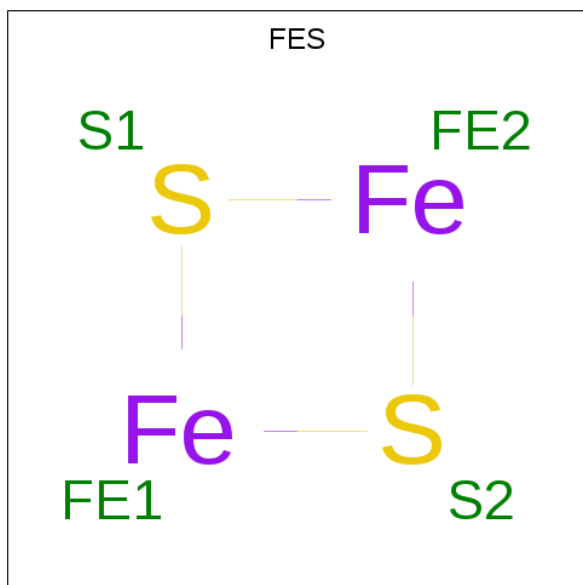
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
17	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
17	Q	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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



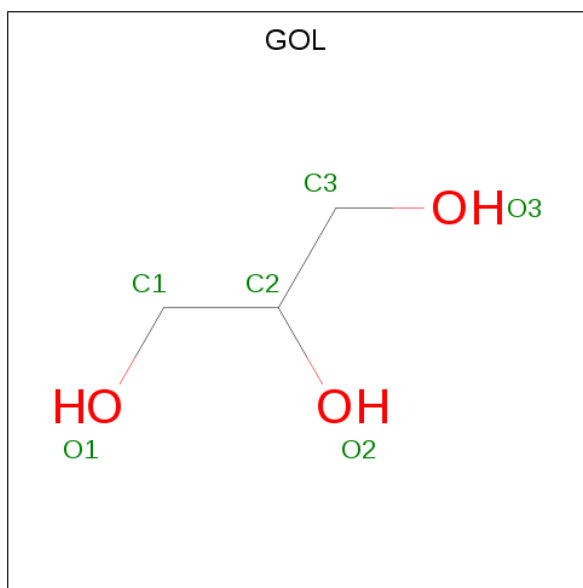
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	D	1	Total	C	O	P	0	0
			39	24	13	2		
18	G	1	Total	C	O	P	0	0
			44	25	17	2		
18	Q	1	Total	C	O	P	0	0
			39	24	13	2		
18	T	1	Total	C	O	P	0	0
			49	30	17	2		

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $Fe_2S_2$ ).



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

- Molecule 20 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).

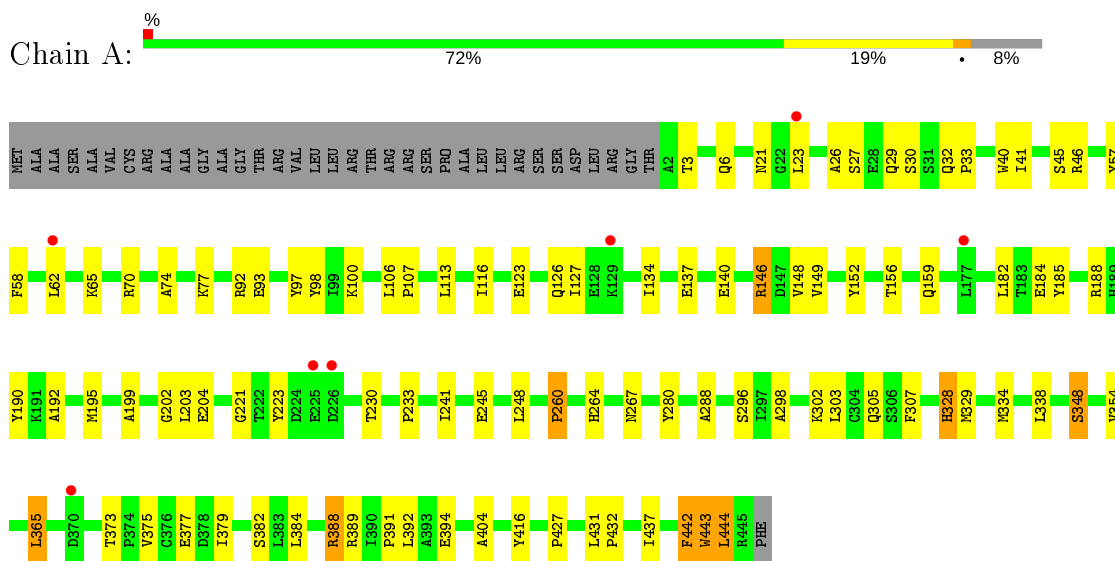


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
20	R	1	6	3	3	0	0

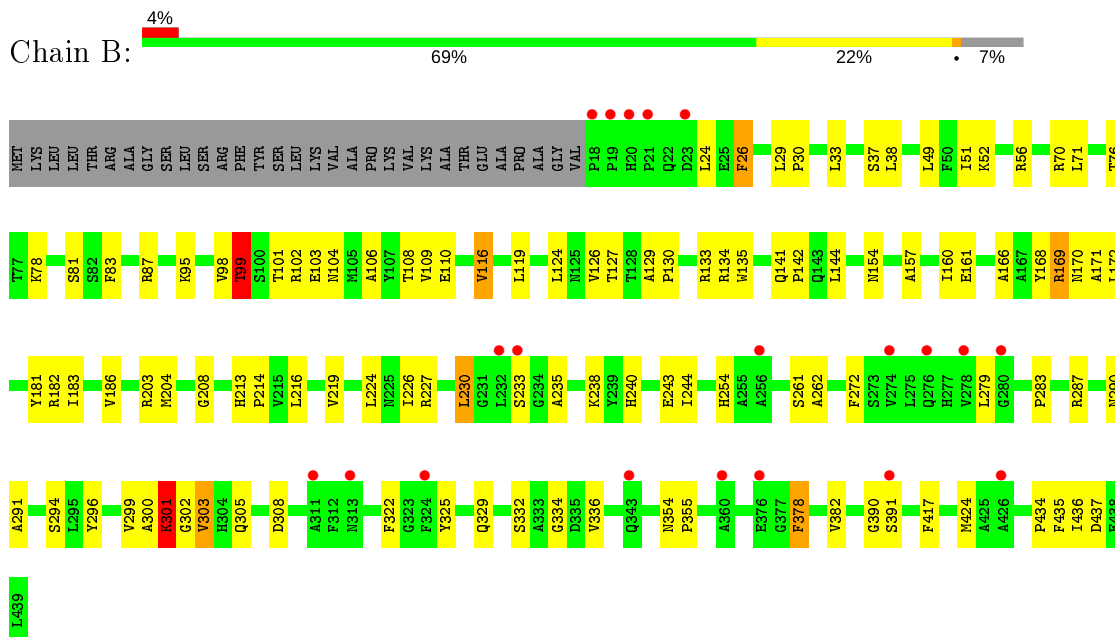
### 3 Residue-property plots [i](#)

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.

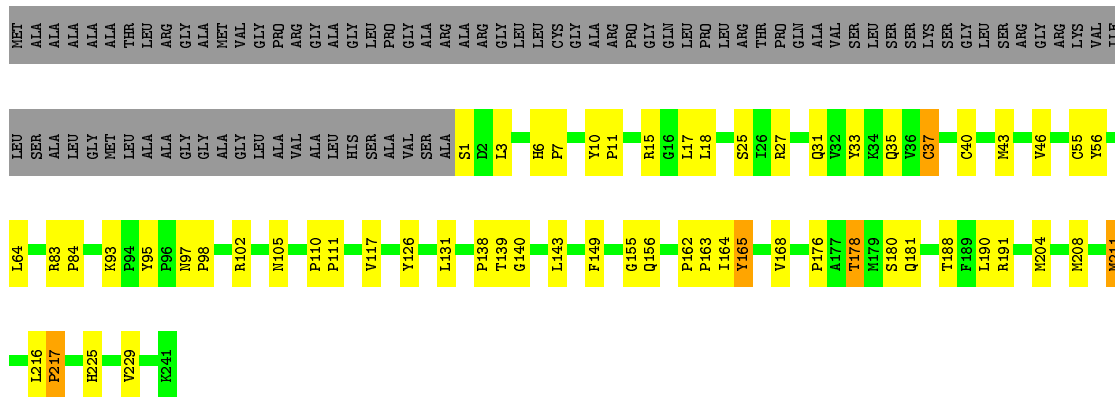
- Molecule 1: CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL



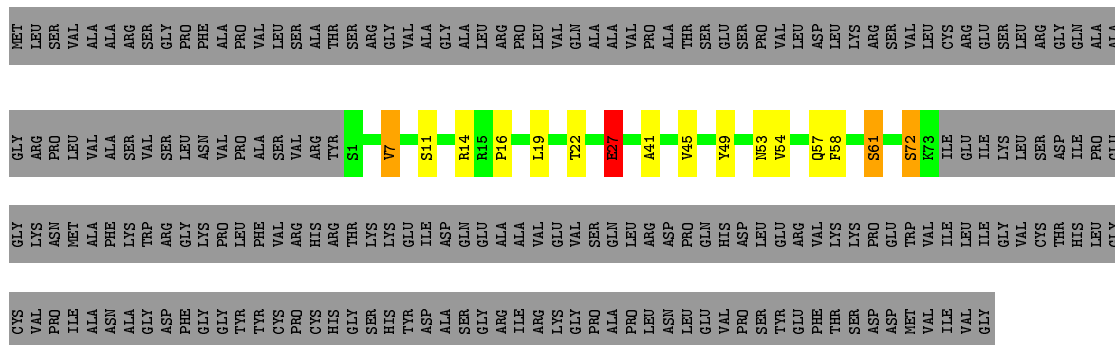
- Molecule 2: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL



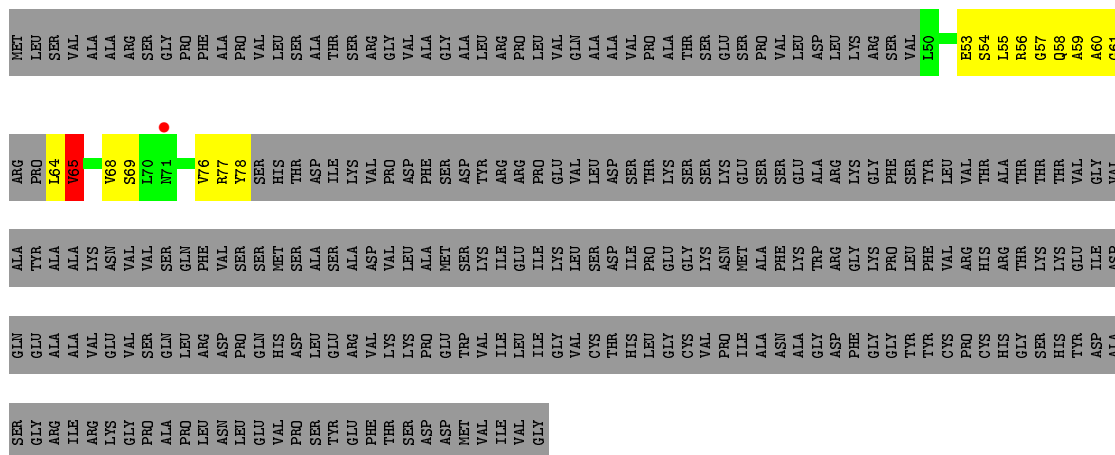




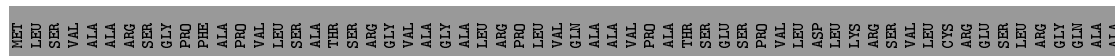
• Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

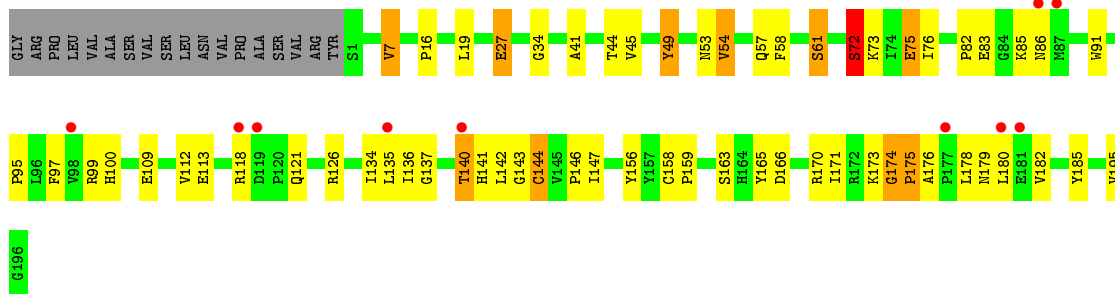


• Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

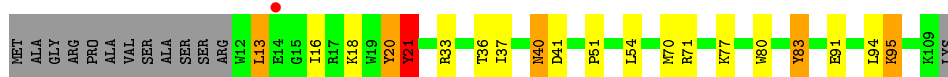


• Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL





• Molecule 6: CYTOCHROME B-C1 COMPLEX SUBUNIT 7



• Molecule 6: CYTOCHROME B-C1 COMPLEX SUBUNIT 7



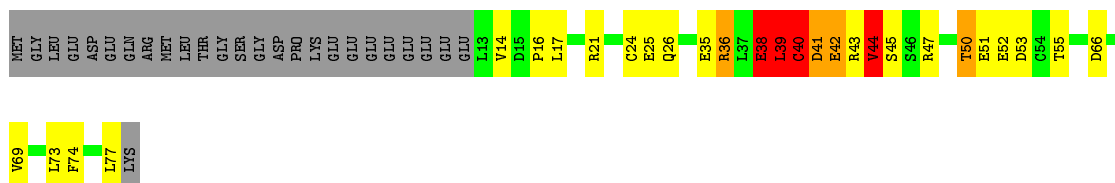
• Molecule 7: CYTOCHROME B-C1 COMPLEX SUBUNIT 8



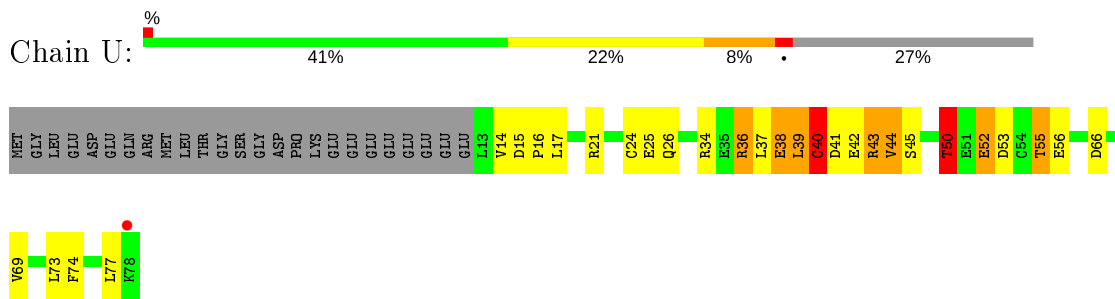
• Molecule 7: CYTOCHROME B-C1 COMPLEX SUBUNIT 8



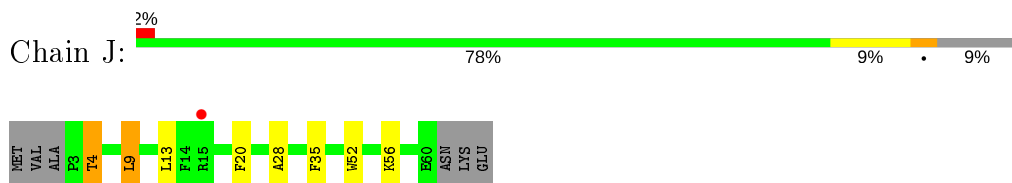
• Molecule 8: CYTOCHROME B-C1 COMPLEX SUBUNIT 6, MITOCHONDRIAL



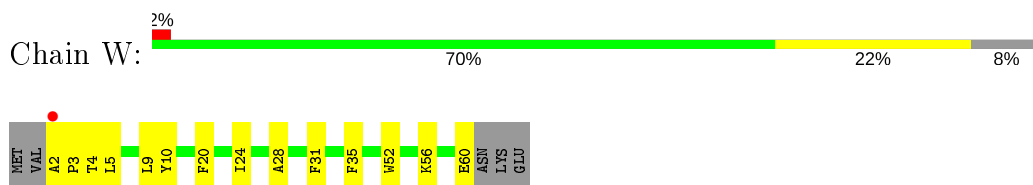
• Molecule 8: CYTOCHROME B-C1 COMPLEX SUBUNIT 6, MITOCHONDRIAL



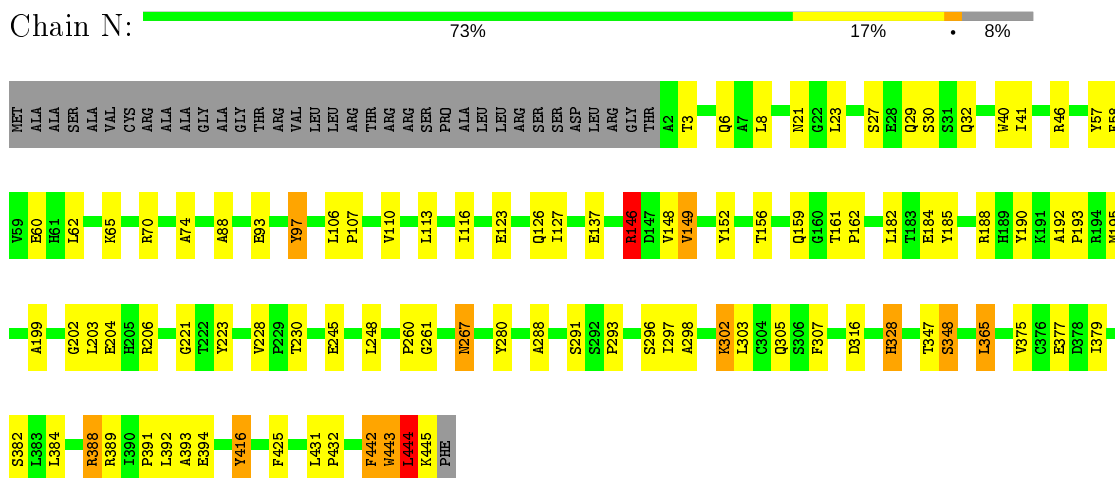
• Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT 9



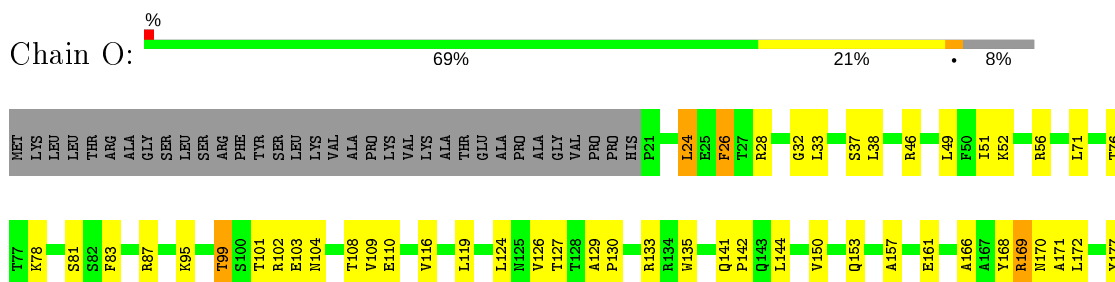
• Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT 9



• Molecule 10: CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL



• Molecule 11: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.49Å 129.49Å 719.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 4.09 49.65 – 4.09	Depositor EDS
% Data completeness (in resolution range)	80.6 (50.00-4.09) 80.7 (49.65-4.09)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.57 (at 4.14Å)	Xtrriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.223 , 0.271 0.222 , 0.271	Depositor DCC
$R_{free}$ test set	2147 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	123.3	Xtrriage
Anisotropy	0.395	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 135.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.086 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	31080	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	163.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CDL, PO4, G8U, FES, HEC, PEE, HEM

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	0.53	6/3511 (0.2%)	0.74	9/4766 (0.2%)
2	B	0.75	18/3224 (0.6%)	0.78	10/4375 (0.2%)
3	C	0.59	7/3065 (0.2%)	0.64	2/4196 (0.0%)
3	P	0.57	5/3031 (0.2%)	0.64	3/4150 (0.1%)
4	D	0.68	6/1971 (0.3%)	0.62	1/2676 (0.0%)
4	Q	0.62	5/1977 (0.3%)	0.62	3/2684 (0.1%)
5	E	1.41	7/557 (1.3%)	0.70	1/752 (0.1%)
5	I	0.64	0/196	0.96	1/263 (0.4%)
5	R	0.72	8/1552 (0.5%)	0.74	5/2100 (0.2%)
6	F	0.95	8/879 (0.9%)	0.69	1/1180 (0.1%)
6	S	0.91	8/888 (0.9%)	0.73	2/1191 (0.2%)
7	G	0.84	6/699 (0.9%)	1.26	4/946 (0.4%)
7	T	0.78	5/645 (0.8%)	0.70	0/873
8	H	1.04	4/534 (0.7%)	1.20	6/718 (0.8%)
8	U	1.00	5/543 (0.9%)	1.27	10/729 (1.4%)
9	J	0.55	1/495 (0.2%)	0.55	0/667
9	W	0.51	0/500	0.59	0/675
10	N	0.62	8/3501 (0.2%)	0.72	8/4752 (0.2%)
11	O	0.69	15/3197 (0.5%)	0.69	5/4336 (0.1%)
12	V	0.70	0/129	1.04	2/177 (1.1%)
All	All	0.70	122/31094 (0.4%)	0.74	73/42206 (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
2	B	1	1
5	R	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	H	0	1
10	N	0	1
12	V	0	1
All	All	1	6

All (122) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	N	444	LEU	C-N	-20.33	0.87	1.34
5	E	27	GLU	CD-OE1	20.21	1.47	1.25
5	E	27	GLU	CD-OE2	15.40	1.42	1.25
2	B	169	ARG	CZ-NH1	15.31	1.52	1.33
4	D	93	LYS	CE-NZ	14.76	1.85	1.49
8	H	38	GLU	CD-OE1	14.61	1.41	1.25
8	U	38	GLU	CD-OE1	12.42	1.39	1.25
6	F	20	TYR	CE2-CZ	-11.29	1.23	1.38
4	D	95	TYR	CE1-CZ	-11.09	1.24	1.38
5	E	49	TYR	CE1-CZ	-11.04	1.24	1.38
2	B	296	TYR	CE1-CZ	-10.86	1.24	1.38
5	R	27	GLU	CG-CD	-10.81	1.35	1.51
11	O	296	TYR	CE1-CZ	-10.34	1.25	1.38
4	Q	95	TYR	CE1-CZ	-10.25	1.25	1.38
11	O	169	ARG	CZ-NH1	10.22	1.46	1.33
7	G	74	PRO	N-CD	10.18	1.62	1.47
8	H	55	THR	CB-CG2	-10.13	1.19	1.52
6	S	20	TYR	CE1-CZ	-10.12	1.25	1.38
5	R	49	TYR	CE1-CZ	-9.70	1.25	1.38
6	F	21	TYR	CE1-CZ	-9.54	1.26	1.38
4	D	95	TYR	CG-CD1	-8.98	1.27	1.39
4	Q	95	TYR	CG-CD1	-8.93	1.27	1.39
5	R	27	GLU	CD-OE1	8.93	1.35	1.25
5	E	27	GLU	CG-CD	-8.85	1.38	1.51
6	F	20	TYR	CG-CD2	-8.75	1.27	1.39
8	U	55	THR	CB-CG2	-8.74	1.23	1.52
6	F	20	TYR	CG-CD1	-8.73	1.27	1.39
4	D	95	TYR	CG-CD2	-8.73	1.27	1.39
8	U	50	THR	CB-CG2	-8.69	1.23	1.52
6	S	20	TYR	CG-CD2	-8.68	1.27	1.39
4	Q	95	TYR	CG-CD2	-8.68	1.27	1.39
5	E	49	TYR	CG-CD2	-8.63	1.27	1.39
6	S	20	TYR	CG-CD1	-8.60	1.27	1.39
6	S	21	TYR	CE1-CZ	-8.56	1.27	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	49	TYR	CG-CD2	-8.50	1.28	1.39
1	A	388	ARG	CZ-NH1	-8.37	1.22	1.33
4	Q	95	TYR	CE2-CZ	-8.33	1.27	1.38
11	O	296	TYR	CG-CD2	-8.32	1.28	1.39
11	O	296	TYR	CG-CD1	-8.24	1.28	1.39
2	B	296	TYR	CG-CD1	-8.19	1.28	1.39
2	B	301	LYS	CE-NZ	8.09	1.69	1.49
2	B	296	TYR	CG-CD2	-8.00	1.28	1.39
7	T	30	PHE	CG-CD1	-7.89	1.26	1.38
4	D	95	TYR	CE2-CZ	-7.86	1.28	1.38
11	O	322	PHE	CG-CD2	-7.86	1.26	1.38
6	S	20	TYR	CE2-CZ	-7.79	1.28	1.38
7	G	30	PHE	CG-CD1	-7.74	1.27	1.38
6	F	20	TYR	CE1-CZ	-7.65	1.28	1.38
5	R	49	TYR	CG-CD1	-7.62	1.29	1.39
11	O	296	TYR	CE2-CZ	-7.58	1.28	1.38
3	C	359	PHE	CG-CD1	-7.54	1.27	1.38
3	C	91	PHE	CG-CD2	-7.52	1.27	1.38
2	B	26	PHE	CG-CD1	-7.50	1.27	1.38
2	B	108	THR	CB-CG2	-7.49	1.27	1.52
3	P	359	PHE	CG-CD2	-7.42	1.27	1.38
6	F	21	TYR	CG-CD1	-7.41	1.29	1.39
2	B	296	TYR	CE2-CZ	-7.38	1.28	1.38
5	R	49	TYR	CE2-CZ	-7.37	1.28	1.38
3	P	91	PHE	CG-CD1	-7.34	1.27	1.38
2	B	322	PHE	CG-CD2	-7.34	1.27	1.38
4	Q	93	LYS	CB-CG	-7.33	1.32	1.52
11	O	26	PHE	CG-CD1	-7.29	1.27	1.38
1	A	146	ARG	CZ-NH1	-7.29	1.23	1.33
10	N	348	SER	CB-OG	7.29	1.51	1.42
3	C	359	PHE	CG-CD2	-7.29	1.27	1.38
7	G	30	PHE	CG-CD2	-7.19	1.27	1.38
7	T	30	PHE	CG-CD2	-7.18	1.27	1.38
6	S	21	TYR	CG-CD1	-7.11	1.29	1.39
3	P	91	PHE	CG-CD2	-7.11	1.28	1.38
3	C	91	PHE	CG-CD1	-7.10	1.28	1.38
1	A	97	TYR	CE1-CZ	-7.06	1.29	1.38
5	E	49	TYR	CG-CD1	-7.02	1.30	1.39
10	N	97	TYR	CE1-CZ	-7.02	1.29	1.38
3	P	359	PHE	CG-CD1	-6.96	1.28	1.38
8	H	38	GLU	CD-OE2	6.91	1.33	1.25
6	F	21	TYR	CG-CD2	-6.88	1.30	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	O	108	THR	CB-CG2	-6.87	1.29	1.52
11	O	272	PHE	CG-CD1	-6.86	1.28	1.38
7	T	41	THR	CB-OG1	6.83	1.56	1.43
3	C	10	LEU	CG-CD2	-6.81	1.26	1.51
4	D	93	LYS	CB-CG	-6.73	1.34	1.52
2	B	272	PHE	CG-CD1	-6.72	1.28	1.38
2	B	99	THR	CB-OG1	6.68	1.56	1.43
11	O	378	PHE	CG-CD2	-6.67	1.28	1.38
2	B	169	ARG	NE-CZ	6.60	1.41	1.33
7	T	17	SER	CB-OG	6.57	1.50	1.42
9	J	4	THR	CB-OG1	6.50	1.56	1.43
6	F	21	TYR	CE2-CZ	-6.49	1.30	1.38
10	N	388	ARG	CZ-NH1	-6.33	1.24	1.33
5	E	49	TYR	CE2-CZ	-6.31	1.30	1.38
2	B	322	PHE	CG-CD1	-6.26	1.29	1.38
11	O	322	PHE	CG-CD1	-6.24	1.29	1.38
8	U	39	LEU	CG-CD2	6.14	1.74	1.51
6	S	21	TYR	CG-CD2	-6.06	1.31	1.39
7	G	41	THR	CB-OG1	6.00	1.55	1.43
2	B	378	PHE	CG-CD2	-5.99	1.29	1.38
10	N	97	TYR	CG-CD1	-5.96	1.31	1.39
5	R	27	GLU	CD-OE2	5.91	1.32	1.25
6	S	21	TYR	CE2-CZ	-5.81	1.30	1.38
7	G	17	SER	CB-OG	5.73	1.49	1.42
11	O	99	THR	CB-OG1	5.66	1.54	1.43
2	B	378	PHE	CG-CD1	-5.66	1.30	1.38
2	B	272	PHE	CG-CD2	-5.62	1.30	1.38
2	B	26	PHE	CG-CD2	-5.55	1.30	1.38
11	O	26	PHE	CG-CD2	-5.51	1.30	1.38
10	N	146	ARG	CZ-NH1	-5.38	1.26	1.33
1	A	302	LYS	CG-CD	-5.37	1.34	1.52
8	H	42	GLU	CD-OE2	5.37	1.31	1.25
10	N	302	LYS	CB-CG	-5.30	1.38	1.52
3	P	194	MET	SD-CE	5.26	2.07	1.77
11	O	378	PHE	CG-CD1	-5.25	1.30	1.38
11	O	272	PHE	CG-CD2	-5.21	1.30	1.38
3	C	91	PHE	CE2-CZ	-5.20	1.27	1.37
1	A	97	TYR	CG-CD2	-5.20	1.32	1.39
3	C	194	MET	SD-CE	5.16	2.06	1.77
1	A	348	SER	CB-OG	5.16	1.49	1.42
7	G	30	PHE	CE2-CZ	-5.16	1.27	1.37
7	T	30	PHE	CE2-CZ	-5.14	1.27	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	175	PRO	N-CD	5.13	1.55	1.47
2	B	99	THR	CB-CG2	-5.12	1.35	1.52
10	N	97	TYR	CG-CD2	-5.03	1.32	1.39
8	U	42	GLU	CG-CD	5.01	1.59	1.51

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	75	ALA	CB-CA-C	-21.60	77.69	110.10
7	G	76	ALA	N-CA-CB	-17.49	85.61	110.10
1	A	146	ARG	NE-CZ-NH1	17.36	128.98	120.30
2	B	300	ALA	CB-CA-C	-15.03	87.56	110.10
2	B	224	LEU	CB-CG-CD1	-13.39	88.23	111.00
2	B	301	LYS	CD-CE-NZ	-13.35	80.99	111.70
1	A	146	ARG	NH1-CZ-NH2	-13.14	104.94	119.40
7	G	75	ALA	N-CA-C	12.91	145.86	111.00
10	N	146	ARG	NE-CZ-NH1	12.66	126.63	120.30
8	H	50	THR	OG1-CB-CG2	-12.49	81.27	110.00
8	U	42	GLU	OE1-CD-OE2	11.24	136.79	123.30
8	U	50	THR	CA-CB-CG2	-10.81	97.27	112.40
11	O	224	LEU	CB-CG-CD1	-10.78	92.68	111.00
11	O	116	VAL	CG1-CB-CG2	-10.54	94.03	110.90
8	H	50	THR	CA-CB-OG1	10.53	131.12	109.00
8	U	52	GLU	N-CA-CB	10.14	128.85	110.60
1	A	302	LYS	CB-CG-CD	-10.00	85.60	111.60
10	N	302	LYS	CG-CD-CE	-9.94	82.09	111.90
2	B	116	VAL	CG1-CB-CG2	-9.93	95.02	110.90
8	H	40	CYS	CA-CB-SG	8.81	129.86	114.00
8	U	39	LEU	CB-CG-CD2	-8.78	96.08	111.00
8	U	50	THR	OG1-CB-CG2	-8.60	90.21	110.00
1	A	365	LEU	CA-CB-CG	8.53	134.92	115.30
6	S	95	LYS	CD-CE-NZ	8.05	130.21	111.70
10	N	365	LEU	CA-CB-CG	7.96	133.62	115.30
11	O	224	LEU	CB-CG-CD2	7.96	124.52	111.00
2	B	301	LYS	N-CA-CB	7.87	124.76	110.60
8	H	50	THR	CA-CB-CG2	-7.82	101.45	112.40
10	N	388	ARG	NE-CZ-NH2	7.71	124.16	120.30
8	U	39	LEU	CB-CG-CD1	7.54	123.83	111.00
5	E	27	GLU	CB-CG-CD	-7.22	94.71	114.20
2	B	301	LYS	CG-CD-CE	-7.14	90.48	111.90
11	O	169	ARG	NE-CZ-NH2	-7.11	116.75	120.30
8	U	52	GLU	N-CA-C	-6.96	92.21	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	302	GLY	N-CA-C	-6.95	95.73	113.10
1	A	365	LEU	CB-CG-CD2	-6.86	99.33	111.00
6	F	95	LYS	CD-CE-NZ	6.80	127.34	111.70
6	S	99	ARG	NE-CZ-NH2	-6.79	116.90	120.30
2	B	169	ARG	NE-CZ-NH1	6.74	123.67	120.30
7	G	74	PRO	CA-N-CD	-6.71	102.10	111.50
5	R	27	GLU	CB-CG-CD	-6.55	96.51	114.20
8	H	39	LEU	CB-CG-CD1	6.41	121.89	111.00
11	O	169	ARG	NE-CZ-NH1	6.38	123.49	120.30
4	Q	93	LYS	N-CA-CB	-6.37	99.14	110.60
10	N	388	ARG	NH1-CZ-NH2	-6.25	112.53	119.40
8	U	40	CYS	CA-CB-SG	6.23	125.21	114.00
4	D	93	LYS	CB-CA-C	-6.18	98.05	110.40
5	R	144	CYS	N-CA-CB	6.16	121.68	110.60
8	U	42	GLU	CG-CD-OE1	-6.15	106.01	118.30
12	V	62	ARG	CB-CG-CD	6.12	127.52	111.60
8	U	44	VAL	CG1-CB-CG2	-6.11	101.13	110.90
1	A	388	ARG	NE-CZ-NH1	6.07	123.33	120.30
3	P	10	LEU	CD1-CG-CD2	-6.02	92.44	110.50
3	C	194	MET	CG-SD-CE	-5.91	90.75	100.20
2	B	303	VAL	CB-CA-C	-5.90	100.20	111.40
5	R	72	SER	N-CA-C	5.86	126.83	111.00
3	P	10	LEU	CA-CB-CG	5.78	128.59	115.30
10	N	146	ARG	NE-CZ-NH2	-5.77	117.42	120.30
10	N	388	ARG	NE-CZ-NH1	5.71	123.15	120.30
3	P	10	LEU	CB-CA-C	-5.66	99.44	110.20
4	Q	93	LYS	CG-CD-CE	-5.61	95.06	111.90
10	N	206	ARG	NE-CZ-NH2	-5.55	117.53	120.30
2	B	301	LYS	N-CA-C	5.46	125.76	111.00
5	R	75	GLU	N-CA-C	-5.45	96.29	111.00
12	V	62	ARG	CA-CB-CG	-5.42	101.48	113.40
8	H	44	VAL	CG1-CB-CG2	-5.32	102.39	110.90
1	A	388	ARG	NE-CZ-NH2	5.24	122.92	120.30
3	C	90	PHE	CB-CG-CD2	-5.16	117.19	120.80
1	A	388	ARG	NH1-CZ-NH2	-5.14	113.75	119.40
4	Q	93	LYS	CD-CE-NZ	5.12	123.48	111.70
5	R	174	GLY	C-N-CD	5.11	139.12	128.40
5	I	65	VAL	CB-CA-C	-5.07	101.77	111.40
1	A	302	LYS	CB-CA-C	-5.07	100.26	110.40

All (1) chirality outliers are listed below:



Mol	Chain	Res	Type	Atom
2	B	301	LYS	CA

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	ARG	Sidechain
2	B	301	LYS	Peptide
8	H	42	GLU	Sidechain
10	N	444	LEU	Mainchain
5	R	27	GLU	Sidechain
12	V	63	PRO	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3439	0	3337	78	0
2	B	3164	0	3144	83	0
3	C	2968	0	3028	122	0
3	P	2936	0	2996	103	0
4	D	1912	0	1862	45	0
4	Q	1918	0	1870	51	0
5	E	549	0	547	18	0
5	I	196	0	204	32	0
5	R	1518	0	1504	57	0
6	F	860	0	849	24	0
6	S	869	0	862	21	0
7	G	677	0	673	55	0
7	T	624	0	630	18	0
8	H	529	0	511	34	0
8	U	538	0	524	29	0
9	J	482	0	483	5	0
9	W	487	0	487	12	0
10	N	3430	0	3329	76	0
11	O	3140	0	3121	72	0
12	V	127	0	135	9	0
13	C	86	0	60	8	0
13	P	86	0	60	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	C	29	0	13	13	0
14	P	29	0	13	9	0
15	C	5	0	0	0	0
15	D	15	0	0	0	0
15	E	5	0	0	0	0
15	F	5	0	0	0	0
15	N	5	0	0	0	0
15	P	5	0	0	0	0
15	S	5	0	0	0	0
16	C	49	0	72	0	0
16	D	26	0	26	1	0
16	P	49	0	72	4	0
16	Q	51	0	82	3	0
17	D	43	0	32	8	0
17	Q	43	0	32	8	0
18	D	39	0	39	0	0
18	G	44	0	32	0	0
18	Q	39	0	39	0	0
18	T	49	0	42	5	0
19	R	4	0	0	3	0
20	R	6	0	8	0	0
All	All	31080	0	30718	841	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (841) 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:U:39:LEU:CG	8:U:39:LEU:CD2	1.74	1.56
2:B:301:LYS:NZ	2:B:301:LYS:CE	1.69	1.51
3:C:194:MET:SD	3:C:194:MET:CE	2.06	1.43
3:P:194:MET:SD	3:P:194:MET:CE	2.07	1.42
4:D:93:LYS:NZ	4:D:93:LYS:CE	1.85	1.39
7:G:71:ARG:CZ	7:G:72:LYS:NZ	1.87	1.38
7:G:71:ARG:NE	7:G:72:LYS:HZ1	1.22	1.37
7:G:71:ARG:CZ	7:G:72:LYS:HZ1	1.39	1.35
11:O:169:ARG:NH2	11:O:240:HIS:CD2	2.01	1.27
10:N:444:LEU:CA	10:N:445:LYS:N	2.08	1.17
7:G:71:ARG:NE	7:G:72:LYS:NZ	1.86	1.15
10:N:444:LEU:O	10:N:445:LYS:N	1.81	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:301:LYS:NZ	2:B:301:LYS:CD	2.10	1.14
7:G:74:PRO:HD2	7:G:78:GLU:OE2	1.47	1.14
10:N:444:LEU:C	10:N:445:LYS:CA	2.15	1.13
14:P:503:G8U:H5	14:P:503:G8U:H16	1.22	1.12
1:A:442:PHE:O	1:A:443:TRP:O	1.65	1.09
7:G:71:ARG:HB3	7:G:72:LYS:HE2	1.13	1.08
14:C:503:G8U:C5	14:C:503:G8U:H12	1.82	1.07
7:G:75:ALA:O	8:H:43:ARG:HD2	1.57	1.04
5:R:141:HIS:CD2	5:R:175:PRO:HG2	1.94	1.03
14:C:503:G8U:H5	14:C:503:G8U:H12	1.07	1.03
3:C:377:LEU:HD11	6:F:20:TYR:HE2	1.24	1.02
12:V:62:ARG:HB2	12:V:78:TYR:CD1	1.94	1.01
1:A:58:PHE:HE2	1:A:182:LEU:HD13	1.25	1.00
7:G:71:ARG:HB3	7:G:72:LYS:CE	1.91	1.00
3:C:379:TRP:CZ2	6:F:33:ARG:HD3	1.97	0.98
2:B:168:TYR:HD2	2:B:172:LEU:HB2	1.27	0.98
7:G:71:ARG:NH2	7:G:72:LYS:NZ	2.10	0.98
14:P:503:G8U:H16	14:P:503:G8U:C5	1.90	0.96
8:U:39:LEU:CD2	8:U:39:LEU:CB	2.44	0.95
11:O:168:TYR:HD2	11:O:172:LEU:HB2	1.30	0.94
1:A:58:PHE:CE2	1:A:182:LEU:HD13	2.01	0.94
11:O:169:ARG:HH22	11:O:240:HIS:CD2	1.78	0.94
2:B:303:VAL:O	2:B:303:VAL:HG23	1.65	0.93
3:C:373:GLU:O	3:C:377:LEU:HD12	1.68	0.93
14:C:503:G8U:H5	14:C:503:G8U:C12	1.91	0.93
1:A:58:PHE:CE2	1:A:182:LEU:CD1	2.52	0.92
7:G:72:LYS:HE2	7:G:72:LYS:H	1.31	0.92
8:H:50:THR:O	8:H:51:GLU:HG2	1.69	0.92
7:G:76:ALA:O	7:G:77:TYR:CG	2.23	0.92
10:N:444:LEU:C	10:N:445:LYS:N	0.87	0.92
11:O:170:ASN:HD21	11:O:238:LYS:H	1.15	0.91
7:G:71:ARG:HE	7:G:72:LYS:HZ1	1.14	0.91
3:C:106:SER:HB3	13:C:502:HEM:HBD2	1.51	0.90
7:G:71:ARG:NH2	7:G:72:LYS:HZ1	1.68	0.90
4:Q:1:SER:HA	4:Q:155:GLY:HA2	1.52	0.90
1:A:58:PHE:HE2	1:A:182:LEU:CD1	1.85	0.89
8:U:50:THR:HG22	8:U:50:THR:O	1.73	0.89
1:A:57:TYR:OH	1:A:137:GLU:OE1	1.89	0.89
11:O:78:LYS:HB2	11:O:129:ALA:HB1	1.55	0.89
2:B:78:LYS:HB2	2:B:129:ALA:HB1	1.53	0.88
10:N:58:PHE:CE2	10:N:62:LEU:HD11	2.08	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:39:LEU:CD2	8:U:39:LEU:CD1	2.52	0.88
2:B:169:ARG:HE	2:B:240:HIS:HB2	1.35	0.88
3:P:90:PHE:HE2	3:P:123:VAL:CG1	1.86	0.88
3:P:90:PHE:CE2	3:P:123:VAL:HG11	2.09	0.87
1:A:58:PHE:CZ	1:A:62:LEU:HD11	2.10	0.86
13:P:501:HEM:HBC2	13:P:501:HEM:HMC1	1.57	0.86
2:B:170:ASN:HD21	2:B:238:LYS:H	1.21	0.86
3:C:18:PHE:CZ	14:C:503:G8U:C11	2.60	0.85
7:G:73:ASN:HB3	7:G:74:PRO:CD	2.07	0.85
3:P:90:PHE:HE2	3:P:123:VAL:HG11	1.38	0.85
11:O:224:LEU:O	11:O:224:LEU:HD12	1.77	0.85
10:N:57:TYR:OH	10:N:137:GLU:OE1	1.95	0.85
3:C:45:ILE:HA	13:C:501:HEM:HMC3	1.59	0.84
10:N:443:TRP:CE3	10:N:443:TRP:HA	2.12	0.84
7:G:74:PRO:CD	7:G:78:GLU:OE2	2.25	0.84
7:G:71:ARG:CZ	7:G:72:LYS:HZ3	1.91	0.83
11:O:224:LEU:C	11:O:224:LEU:HD12	1.99	0.83
1:A:58:PHE:CE2	1:A:62:LEU:HD11	2.14	0.82
3:C:377:LEU:HD11	6:F:20:TYR:CE2	2.13	0.82
10:N:443:TRP:HE3	10:N:443:TRP:HA	1.45	0.81
1:A:444:LEU:O	1:A:444:LEU:HD23	1.81	0.81
7:G:72:LYS:H	7:G:72:LYS:CE	1.94	0.80
7:G:73:ASN:HB3	7:G:74:PRO:HD3	1.62	0.80
10:N:58:PHE:CE2	10:N:182:LEU:CD1	2.66	0.79
3:C:377:LEU:CD1	6:F:20:TYR:HE2	1.94	0.79
8:H:44:VAL:HG23	8:H:52:GLU:HB3	1.65	0.79
4:D:178:THR:HG21	8:H:16:PRO:HD2	1.65	0.79
3:P:185:LEU:HA	3:P:188:ILE:HD12	1.62	0.79
5:I:60:ALA:CB	5:I:78:TYR:HA	2.14	0.79
2:B:301:LYS:NZ	2:B:301:LYS:HD2	1.95	0.78
7:G:71:ARG:CB	7:G:72:LYS:HE2	2.07	0.78
10:N:58:PHE:CZ	10:N:62:LEU:HD11	2.19	0.78
7:G:72:LYS:HE2	7:G:72:LYS:N	2.00	0.77
5:I:61:GLY:O	5:I:78:TYR:HB3	1.83	0.77
3:C:75:TYR:CE2	5:E:57:GLN:HG2	2.19	0.77
1:A:140:GLU:OE2	5:I:53:GLU:HB3	1.84	0.77
3:P:77:TRP:CH2	3:P:78:ILE:HD11	2.20	0.76
2:B:169:ARG:NE	2:B:240:HIS:HB2	2.00	0.76
11:O:101:THR:HB	11:O:104:ASN:H	1.51	0.76
5:I:60:ALA:HB1	5:I:78:TYR:HD1	1.50	0.76
7:G:71:ARG:NH2	7:G:72:LYS:HZ2	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:58:PHE:HE2	10:N:182:LEU:HD13	1.51	0.75
2:B:168:TYR:CD2	2:B:172:LEU:HB2	2.18	0.74
10:N:58:PHE:HE2	10:N:182:LEU:CD1	1.99	0.74
5:I:60:ALA:HB1	5:I:78:TYR:CD1	2.21	0.74
10:N:58:PHE:CE2	10:N:182:LEU:HD13	2.22	0.74
11:O:71:LEU:HD23	12:V:68:VAL:HG21	1.68	0.74
2:B:101:THR:HB	2:B:104:ASN:H	1.52	0.74
1:A:58:PHE:HZ	1:A:127:ILE:HG12	1.52	0.74
1:A:58:PHE:CE2	1:A:62:LEU:CD1	2.71	0.73
1:A:58:PHE:CE2	1:A:182:LEU:HD11	2.23	0.73
11:O:169:ARG:NH2	11:O:240:HIS:HD2	1.82	0.73
5:R:171:ILE:HG12	5:R:176:ALA:O	1.87	0.73
3:C:226:ILE:HA	3:C:229:ILE:HD12	1.71	0.72
8:H:38:GLU:HA	8:H:41:ASP:HB2	1.69	0.72
3:C:379:TRP:CH2	6:F:33:ARG:HD3	2.23	0.72
10:N:58:PHE:CE2	10:N:62:LEU:CD1	2.72	0.72
11:O:169:ARG:CZ	11:O:240:HIS:CD2	2.70	0.72
12:V:62:ARG:CB	12:V:78:TYR:CD1	2.72	0.72
2:B:303:VAL:O	2:B:303:VAL:CG2	2.37	0.72
5:R:141:HIS:HD2	5:R:175:PRO:HG2	1.51	0.71
4:D:33:TYR:HA	4:D:37:CYS:SG	2.30	0.71
4:Q:37:CYS:SG	17:Q:501:HEC:CAB	2.78	0.71
3:P:197:LEU:HD22	3:P:201:HIS:HE1	1.56	0.71
5:I:60:ALA:HB1	5:I:78:TYR:HA	1.72	0.71
3:P:226:ILE:HA	3:P:229:ILE:HD12	1.73	0.70
3:C:379:TRP:CE2	6:F:33:ARG:HD3	2.26	0.70
4:Q:139:THR:OG1	8:U:41:ASP:OD1	2.09	0.70
4:D:40:CYS:SG	17:D:501:HEC:HBC3	2.31	0.70
3:C:168:PHE:HE2	5:R:72:SER:HB2	1.56	0.70
14:P:503:G8U:C16	14:P:503:G8U:H5	2.07	0.69
4:Q:31:GLN:O	4:Q:35:GLN:HG2	1.91	0.69
10:N:146:ARG:HH11	10:N:146:ARG:HG2	1.58	0.69
10:N:58:PHE:CE2	10:N:182:LEU:HD11	2.26	0.69
3:C:168:PHE:CE2	5:R:72:SER:HB2	2.27	0.69
9:W:56:LYS:HE3	9:W:60:GLU:OE1	1.93	0.69
3:P:348:ILE:O	3:P:352:GLN:HG2	1.92	0.69
3:C:379:TRP:CZ2	6:F:33:ARG:CD	2.74	0.69
7:G:74:PRO:HD2	7:G:78:GLU:CD	2.12	0.69
7:G:77:TYR:O	7:G:80:ASP:O	2.09	0.69
10:N:21:ASN:HB2	10:N:221:GLY:HA3	1.75	0.68
1:A:21:ASN:HB2	1:A:221:GLY:HA3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:185:LEU:HA	3:C:188:ILE:HD12	1.75	0.68
2:B:71:LEU:HD23	5:I:68:VAL:HG11	1.75	0.68
11:O:168:TYR:CD2	11:O:172:LEU:HB2	2.22	0.68
7:G:72:LYS:CD	7:G:72:LYS:H	2.06	0.68
8:H:40:CYS:HB2	8:H:43:ARG:NH2	2.09	0.68
5:R:171:ILE:HG22	5:R:179:ASN:OD1	1.94	0.68
8:H:36:ARG:HA	8:H:39:LEU:HB2	1.74	0.68
3:C:145:VAL:HG21	3:C:268:ILE:HD12	1.76	0.67
3:P:379:TRP:CE3	6:S:33:ARG:HD3	2.29	0.67
3:C:150:LEU:HB2	3:C:161:VAL:HG23	1.76	0.67
4:D:31:GLN:O	4:D:35:GLN:HG2	1.94	0.67
10:N:328:HIS:O	10:N:328:HIS:CD2	2.48	0.67
3:P:90:PHE:CE2	3:P:123:VAL:CG1	2.73	0.67
3:C:8:HIS:N	3:C:9:PRO:HD3	2.10	0.66
10:N:328:HIS:HD2	10:N:328:HIS:O	1.78	0.66
3:P:193:ALA:HB1	14:P:503:G8U:F2	1.84	0.66
11:O:170:ASN:ND2	11:O:238:LYS:H	1.93	0.66
11:O:169:ARG:CZ	11:O:240:HIS:CG	2.78	0.66
12:V:76:VAL:HG13	12:V:76:VAL:O	1.94	0.66
2:B:435:PHE:CD2	11:O:169:ARG:NH1	2.64	0.66
3:C:187:PHE:CZ	3:P:184:ILE:CD1	2.79	0.66
7:G:71:ARG:NE	7:G:72:LYS:HZ3	1.87	0.65
4:D:149:PHE:CE1	4:D:156:GLN:HB3	2.31	0.65
6:F:18:LYS:HG3	6:F:83:TYR:HD2	1.61	0.65
1:A:57:TYR:HE2	1:A:134:ILE:HG23	1.61	0.65
7:G:75:ALA:CB	8:H:43:ARG:NH1	2.59	0.65
3:P:191:ALA:HA	3:P:194:MET:HE3	1.78	0.65
7:G:75:ALA:HB2	8:H:43:ARG:NH1	2.11	0.65
3:P:17:ALA:O	3:P:18:PHE:HD1	1.79	0.65
1:A:245:GLU:HG3	1:A:248:LEU:HG	1.79	0.65
10:N:328:HIS:NE2	7:T:5:GLY:O	2.29	0.65
5:I:76:VAL:HG13	5:I:76:VAL:O	1.97	0.65
3:P:11:MET:O	3:P:14:VAL:HB	1.97	0.64
14:P:503:G8U:F1	14:P:503:G8U:H9	1.87	0.64
3:C:18:PHE:CZ	14:C:503:G8U:O10	2.49	0.64
3:P:103:TYR:HD1	3:P:325:PHE:CD2	2.16	0.64
4:Q:33:TYR:HA	4:Q:37:CYS:SG	2.37	0.64
10:N:298:ALA:O	10:N:302:LYS:HA	1.98	0.64
8:U:39:LEU:CD2	8:U:39:LEU:HB3	2.28	0.64
3:C:17:ALA:O	3:C:18:PHE:HD1	1.82	0.63
3:P:77:TRP:CH2	3:P:78:ILE:CD1	2.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:194:MET:CG	3:C:194:MET:CE	2.77	0.63
10:N:379:ILE:HG12	10:N:389:ARG:HD2	1.79	0.63
3:P:75:TYR:CE2	5:R:57:GLN:HG2	2.33	0.63
6:F:40:ASN:OD1	6:F:41:ASP:N	2.32	0.63
4:D:165:TYR:HE1	4:D:168:VAL:HG23	1.64	0.63
3:P:103:TYR:HB2	3:P:325:PHE:CE2	2.33	0.63
3:C:200:LEU:CD2	3:C:201:HIS:HD2	2.12	0.63
3:C:77:TRP:CH2	3:C:78:ILE:HD11	2.34	0.63
3:P:145:VAL:HG21	3:P:268:ILE:HD12	1.80	0.63
8:H:40:CYS:HB2	8:H:43:ARG:CZ	2.29	0.62
5:R:82:PRO:HD2	5:R:85:LYS:HD3	1.81	0.62
3:C:104:TYR:CD1	3:C:208:PRO:HA	2.34	0.62
5:R:142:LEU:O	5:R:143:GLY:C	2.38	0.62
8:U:36:ARG:HA	8:U:39:LEU:HB2	1.81	0.62
2:B:157:ALA:O	2:B:161:GLU:HG2	1.99	0.62
10:N:245:GLU:HG3	10:N:248:LEU:HG	1.80	0.62
4:D:116:ILE:HG12	17:D:501:HEC:HMA3	1.82	0.62
7:G:76:ALA:O	7:G:77:TYR:CD2	2.52	0.62
11:O:170:ASN:OD1	11:O:171:ALA:N	2.32	0.62
5:E:58:PHE:O	5:E:61:SER:HB3	1.99	0.62
3:P:18:PHE:CZ	14:P:503:G8U:C11	2.83	0.62
1:A:58:PHE:CZ	1:A:127:ILE:HG12	2.34	0.62
2:B:98:VAL:O	5:I:68:VAL:O	2.18	0.62
5:R:45:VAL:HG13	9:W:28:ALA:HA	1.81	0.62
10:N:261:GLY:O	10:N:267:ASN:ND2	2.33	0.61
5:R:140:THR:OG1	5:R:176:ALA:HB1	2.00	0.61
3:C:234:LEU:HD23	4:D:216:LEU:HD11	1.82	0.61
11:O:279:LEU:HA	11:O:294:SER:HB3	1.82	0.61
3:P:361:LEU:O	3:P:366:MET:HG3	2.01	0.61
8:H:44:VAL:CG2	8:H:52:GLU:HB3	2.30	0.61
2:B:279:LEU:HA	2:B:294:SER:HB3	1.82	0.61
3:C:11:MET:O	3:C:14:VAL:HB	2.01	0.61
10:N:58:PHE:CZ	10:N:127:ILE:HG23	2.35	0.61
2:B:208:GLY:HA3	2:B:216:LEU:HD11	1.81	0.61
5:E:53:ASN:O	5:E:57:GLN:HG3	2.00	0.61
2:B:299:VAL:HG11	2:B:336:VAL:HG13	1.83	0.61
7:G:71:ARG:CZ	7:G:72:LYS:HZ2	2.06	0.61
3:C:186:PRO:HG3	13:C:501:HEM:HBB2	1.83	0.61
3:P:191:ALA:HA	3:P:194:MET:CE	2.30	0.61
5:I:55:LEU:HD23	5:I:58:GLN:HG2	1.82	0.60
11:O:303:VAL:O	11:O:303:VAL:HG23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:194:MET:CE	3:P:194:MET:CG	2.79	0.60
3:C:277:ALA:HB1	3:C:294:LEU:CD1	2.31	0.60
10:N:3:THR:HG23	10:N:6:GLN:H	1.66	0.60
4:Q:37:CYS:HB3	17:Q:501:HEC:CHC	2.32	0.60
3:C:205:SER:OG	14:C:503:G8U:H271	2.01	0.60
3:P:234:LEU:HD23	4:Q:216:LEU:HD11	1.84	0.60
5:I:54:SER:HA	5:I:56:ARG:NH1	2.16	0.60
3:C:103:TYR:HD1	3:C:325:PHE:CD2	2.20	0.60
5:I:60:ALA:HB3	5:I:78:TYR:HA	1.84	0.60
3:C:348:ILE:O	3:C:352:GLN:HG2	2.01	0.60
3:C:361:LEU:O	3:C:366:MET:HG3	2.01	0.60
3:P:150:LEU:HB2	3:P:161:VAL:HG23	1.82	0.60
2:B:301:LYS:CD	2:B:301:LYS:HZ3	2.13	0.59
3:C:8:HIS:H	3:C:9:PRO:HD3	1.67	0.59
4:Q:149:PHE:CE1	4:Q:156:GLN:HB3	2.37	0.59
2:B:169:ARG:NH2	2:B:240:HIS:HD2	1.98	0.59
14:C:503:G8U:C12	14:C:503:G8U:C5	2.53	0.59
1:A:57:TYR:CE2	1:A:134:ILE:HG23	2.37	0.59
1:A:288:ALA:O	1:A:296:SER:HB2	2.03	0.59
7:T:37:VAL:O	7:T:41:THR:OG1	2.17	0.59
1:A:328:HIS:CD2	1:A:329:MET:HG2	2.38	0.59
10:N:58:PHE:HZ	10:N:127:ILE:HG12	1.67	0.59
10:N:443:TRP:O	10:N:444:LEU:HB2	2.02	0.59
6:S:40:ASN:OD1	6:S:41:ASP:N	2.34	0.59
3:C:378:LYS:O	3:C:378:LYS:HG3	2.01	0.59
3:P:77:TRP:CZ3	3:P:78:ILE:HD13	2.38	0.59
2:B:141:GLN:HB2	2:B:142:PRO:HD3	1.84	0.59
3:C:200:LEU:HD22	3:C:201:HIS:CD2	2.38	0.58
5:E:16:PRO:HA	5:E:19:LEU:HD12	1.85	0.58
3:P:18:PHE:O	3:P:220:PHE:CD2	2.55	0.58
5:R:173:LYS:CG	5:R:174:GLY:H	2.16	0.58
1:A:58:PHE:CD2	1:A:182:LEU:HD22	2.38	0.58
1:A:443:TRP:CD1	1:A:444:LEU:CD2	2.86	0.58
2:B:154:ASN:HD22	5:I:76:VAL:HG11	1.68	0.58
13:P:501:HEM:HHA	13:P:501:HEM:CBA	2.32	0.58
1:A:443:TRP:NE1	1:A:444:LEU:HD22	2.18	0.58
10:N:106:LEU:HB3	10:N:107:PRO:HD3	1.84	0.58
3:C:200:LEU:HD23	3:C:201:HIS:HD2	1.69	0.58
11:O:141:GLN:HB2	11:O:142:PRO:HD3	1.86	0.58
4:Q:131:LEU:HD11	17:Q:501:HEC:HMB2	1.86	0.58
1:A:379:ILE:HG12	1:A:389:ARG:HD2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:187:PHE:CZ	3:P:184:ILE:HD12	2.38	0.58
8:H:17:LEU:HD11	8:H:21:ARG:NE	2.19	0.58
5:I:65:VAL:HG23	5:I:78:TYR:HB2	1.86	0.58
7:T:34:ILE:N	7:T:35:PRO:HD2	2.19	0.58
11:O:157:ALA:O	11:O:161:GLU:HG2	2.04	0.58
3:P:28:SER:HB2	18:T:501:CDL:HB21	1.85	0.58
7:G:75:ALA:O	8:H:43:ARG:CD	2.43	0.58
3:P:246:ALA:HB1	3:P:249:LEU:HB2	1.86	0.58
2:B:24:LEU:HD12	2:B:38:LEU:HB2	1.85	0.57
5:R:58:PHE:O	5:R:61:SER:HB3	2.04	0.57
3:C:246:ALA:HB1	3:C:249:LEU:HB2	1.85	0.57
4:D:143:LEU:HD11	4:D:149:PHE:HB2	1.85	0.57
3:P:277:ALA:HB1	3:P:294:LEU:CD1	2.33	0.57
14:P:503:G8U:C16	14:P:503:G8U:C5	2.62	0.57
2:B:169:ARG:HE	2:B:240:HIS:CB	2.12	0.57
4:D:149:PHE:HE1	4:D:156:GLN:HB3	1.70	0.57
4:D:139:THR:OG1	8:H:41:ASP:OD1	2.22	0.57
11:O:208:GLY:HA3	11:O:216:LEU:HD11	1.86	0.57
3:C:379:TRP:CH2	6:F:33:ARG:CD	2.87	0.57
11:O:272:PHE:CE1	11:O:413:ALA:HB1	2.40	0.57
2:B:99:THR:HB	2:B:106:ALA:HB3	1.86	0.57
3:C:377:LEU:CD1	6:F:20:TYR:CE2	2.81	0.57
1:A:382:SER:HB3	1:A:389:ARG:HA	1.87	0.57
11:O:177:TYR:OH	12:V:76:VAL:HG23	2.05	0.57
2:B:170:ASN:OD1	2:B:171:ALA:N	2.37	0.56
3:C:200:LEU:CD2	3:C:201:HIS:CD2	2.88	0.56
11:O:24:LEU:HD12	11:O:38:LEU:HB2	1.87	0.56
13:P:501:HEM:HBA1	13:P:501:HEM:HHA	1.87	0.56
3:C:29:SER:O	3:C:32:ASN:HB2	2.05	0.56
1:A:159:GLN:HB3	5:E:7:VAL:HG21	1.87	0.56
10:N:382:SER:HB3	10:N:389:ARG:HA	1.87	0.56
4:Q:10:TYR:HB3	8:U:74:PHE:CE1	2.40	0.56
1:A:106:LEU:HB3	1:A:107:PRO:HD3	1.87	0.56
11:O:243:GLU:HA	11:O:424:MET:O	2.04	0.56
4:Q:143:LEU:HD11	4:Q:149:PHE:HB2	1.87	0.56
1:A:3:THR:HG23	1:A:6:GLN:H	1.71	0.56
7:G:59:TYR:CD1	7:G:59:TYR:C	2.77	0.56
10:N:123:GLU:HB2	10:N:126:GLN:HB2	1.88	0.56
3:P:193:ALA:CB	14:P:503:G8U:F2	2.44	0.56
5:R:53:ASN:O	5:R:57:GLN:HG3	2.06	0.56
1:A:233:PRO:O	5:E:22:THR:HA	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:77:TYR:HA	8:H:47:ARG:HH21	1.70	0.56
4:Q:204:MET:HG2	16:Q:506:PEE:H2	1.88	0.56
3:C:220:PHE:CD1	3:C:224:TYR:HB2	2.41	0.55
3:C:75:TYR:CD2	5:E:57:GLN:HG2	2.40	0.55
7:G:79:ASN:CG	8:H:52:GLU:HB2	2.27	0.55
10:N:41:ILE:HG12	10:N:195:MET:HG2	1.88	0.55
11:O:109:VAL:HB	11:O:119:LEU:HD12	1.89	0.55
5:R:163:SER:HA	5:R:174:GLY:O	2.06	0.55
3:C:10:LEU:HD13	3:P:202:GLU:HG3	1.88	0.55
3:C:38:GLY:O	3:C:39:ILE:C	2.44	0.55
3:P:29:SER:O	3:P:32:ASN:HB2	2.07	0.55
1:A:77:LYS:HE3	2:B:291:ALA:HB1	1.89	0.55
5:R:75:GLU:HA	5:R:75:GLU:OE1	2.07	0.55
4:D:93:LYS:NZ	4:D:93:LYS:CD	2.67	0.55
8:U:17:LEU:HD11	8:U:21:ARG:NE	2.22	0.55
2:B:133:ARG:HD3	2:B:135:TRP:CZ2	2.42	0.55
3:C:70:CYS:SG	3:C:80:ARG:HD3	2.47	0.55
5:E:27:GLU:N	5:E:27:GLU:OE1	2.40	0.55
3:P:103:TYR:HD1	3:P:325:PHE:HD2	1.53	0.55
4:Q:165:TYR:N	4:Q:165:TYR:CD1	2.75	0.55
3:C:103:TYR:HB2	3:C:325:PHE:CE2	2.41	0.55
10:N:328:HIS:CE1	7:T:5:GLY:O	2.59	0.55
11:O:299:VAL:HG11	11:O:336:VAL:HG13	1.88	0.55
3:C:75:TYR:HE2	5:E:57:GLN:HG2	1.68	0.54
11:O:124:LEU:HD11	11:O:219:VAL:HG13	1.89	0.54
7:T:59:TYR:CD1	7:T:59:TYR:C	2.80	0.54
2:B:51:ILE:HG12	2:B:204:MET:HG2	1.88	0.54
4:Q:149:PHE:HE1	4:Q:156:GLN:HB3	1.72	0.54
2:B:254:HIS:ND1	2:B:325:TYR:OH	2.28	0.54
3:C:184:ILE:CD1	3:P:187:PHE:CZ	2.90	0.54
2:B:70:ARG:HE	5:I:68:VAL:HG23	1.71	0.54
5:I:64:LEU:HA	5:I:78:TYR:C	2.28	0.54
10:N:21:ASN:HB2	10:N:221:GLY:CA	2.38	0.54
5:R:156:TYR:HB2	5:R:165:TYR:HB2	1.87	0.54
5:R:95:PRO:HB2	5:R:137:GLY:HA3	1.88	0.54
8:U:38:GLU:HA	8:U:41:ASP:HB2	1.89	0.54
10:N:27:SER:HA	10:N:199:ALA:O	2.08	0.54
4:Q:40:CYS:SG	17:Q:501:HEC:HBC3	2.47	0.54
5:R:16:PRO:HA	5:R:19:LEU:HD12	1.90	0.54
12:V:65:VAL:HB	12:V:77:ARG:HB2	1.90	0.54
7:G:59:TYR:HD1	7:G:59:TYR:C	2.10	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:75:ALA:CB	8:H:43:ARG:HH11	2.19	0.54
3:P:70:CYS:SG	3:P:80:ARG:HD3	2.48	0.54
1:A:29:GLN:HE22	1:A:204:GLU:HG3	1.71	0.53
10:N:58:PHE:CZ	10:N:127:ILE:HG12	2.42	0.53
2:B:87:ARG:HB3	6:S:107:TRP:CZ2	2.43	0.53
12:V:62:ARG:HB2	12:V:78:TYR:HD1	1.67	0.53
17:D:501:HEC:HMB1	17:D:501:HEC:CBB	2.38	0.53
6:F:21:TYR:C	6:F:21:TYR:CD1	2.81	0.53
3:P:18:PHE:O	3:P:220:PHE:HD2	1.92	0.53
10:N:347:THR:HG21	10:N:443:TRP:CD1	2.43	0.53
6:F:40:ASN:OD1	6:F:40:ASN:C	2.45	0.53
5:R:171:ILE:CD1	5:R:176:ALA:HB3	2.38	0.53
3:P:144:THR:O	3:P:148:ASN:HB2	2.08	0.53
1:A:46:ARG:NH1	1:A:93:GLU:OE2	2.38	0.53
2:B:243:GLU:HA	2:B:424:MET:O	2.09	0.53
11:O:305:GLU:O	11:O:306:PRO:C	2.46	0.53
4:Q:211:MET:HE1	9:W:31:PHE:CZ	2.44	0.53
5:R:97:PHE:O	5:R:134:ILE:HA	2.09	0.53
1:A:27:SER:HA	1:A:199:ALA:O	2.07	0.52
2:B:124:LEU:HD11	2:B:219:VAL:HG13	1.90	0.52
4:D:37:CYS:SG	17:D:501:HEC:HBB3	2.49	0.52
11:O:220:ALA:HA	11:O:224:LEU:HG	1.91	0.52
1:A:123:GLU:HB2	1:A:126:GLN:HB2	1.91	0.52
1:A:442:PHE:C	1:A:443:TRP:O	2.46	0.52
4:Q:37:CYS:HB3	17:Q:501:HEC:HHC	1.90	0.52
8:U:66:ASP:HA	8:U:69:VAL:HB	1.92	0.52
10:N:444:LEU:N	10:N:445:LYS:N	2.57	0.52
11:O:329:GLN:HB2	11:O:332:SER:HB2	1.91	0.52
6:S:18:LYS:HA	6:S:83:TYR:CE2	2.45	0.52
1:A:41:ILE:HG12	1:A:195:MET:HG2	1.91	0.52
1:A:443:TRP:NE1	1:A:444:LEU:CD2	2.73	0.52
2:B:154:ASN:ND2	5:I:76:VAL:HG11	2.24	0.52
2:B:325:TYR:CE2	5:I:59:ALA:CB	2.93	0.52
4:Q:211:MET:HG2	9:W:35:PHE:CE2	2.45	0.52
7:G:75:ALA:HB1	8:H:43:ARG:HH11	1.75	0.52
3:C:179:PHE:HE2	3:P:179:PHE:HE2	1.58	0.52
7:G:18:LEU:HD23	7:G:23:GLN:HB3	1.92	0.51
7:G:73:ASN:CB	7:G:74:PRO:CD	2.85	0.51
2:B:329:GLN:HB2	2:B:332:SER:HB2	1.93	0.51
2:B:87:ARG:HB3	6:S:107:TRP:CE2	2.46	0.51
3:P:104:TYR:CD1	3:P:208:PRO:HA	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:31:TRP:NE1	13:C:502:HEM:O1D	2.43	0.51
3:C:187:PHE:CZ	3:P:184:ILE:HD11	2.46	0.51
2:B:101:THR:HG22	2:B:102:ARG:N	2.25	0.51
2:B:109:VAL:HB	2:B:119:LEU:HD12	1.92	0.51
3:C:205:SER:OG	14:C:503:G8U:C27	2.59	0.51
4:Q:216:LEU:N	4:Q:217:PRO:HD2	2.26	0.51
4:Q:11:PRO:HA	4:Q:15:ARG:HD2	1.92	0.51
10:N:159:GLN:HB3	5:R:7:VAL:HG21	1.93	0.51
3:P:375:LYS:O	6:S:17:ARG:NH1	2.44	0.51
8:U:44:VAL:HG12	8:U:45:SER:N	2.26	0.51
5:R:41:ALA:HB2	9:W:20:PHE:HE1	1.75	0.51
3:C:51:LEU:HD13	13:C:501:HEM:HBD1	1.93	0.51
4:D:211:MET:HG2	9:J:35:PHE:CE2	2.46	0.51
10:N:375:VAL:O	10:N:379:ILE:HG13	2.11	0.51
4:Q:225:HIS:CE1	7:T:20:PRO:HB2	2.46	0.51
3:C:104:TYR:CE1	3:C:208:PRO:HA	2.46	0.51
11:O:28:ARG:NH1	11:O:32:GLY:HA2	2.25	0.51
1:A:58:PHE:CZ	1:A:127:ILE:HG23	2.47	0.50
8:U:34:ARG:O	8:U:37:LEU:HB3	2.11	0.50
1:A:260:PRO:HB2	1:A:264:HIS:CB	2.41	0.50
3:C:187:PHE:HZ	3:P:184:ILE:CD1	2.24	0.50
13:P:501:HEM:HBA1	13:P:501:HEM:CHA	2.41	0.50
3:C:144:THR:O	3:C:148:ASN:HB2	2.10	0.50
1:A:21:ASN:HB2	1:A:221:GLY:CA	2.39	0.50
3:C:103:TYR:CD1	3:C:325:PHE:CD2	3.00	0.50
5:R:140:THR:HG21	5:R:178:LEU:HB2	1.93	0.50
1:A:443:TRP:CD1	1:A:444:LEU:HD22	2.47	0.50
3:C:18:PHE:O	3:C:220:PHE:CD2	2.64	0.50
3:C:77:TRP:CE3	3:C:78:ILE:HG13	2.47	0.50
7:G:49:ALA:N	7:G:50:PRO:HD2	2.27	0.50
10:N:288:ALA:O	10:N:296:SER:HB2	2.12	0.50
11:O:101:THR:HG22	11:O:102:ARG:N	2.26	0.50
3:C:11:MET:SD	3:P:198:LEU:HD12	2.52	0.50
4:Q:181:GLN:HB2	8:U:77:LEU:HD22	1.92	0.50
8:H:66:ASP:HA	8:H:69:VAL:HB	1.93	0.49
3:C:18:PHE:HZ	14:C:503:G8U:C11	2.21	0.49
11:O:52:LYS:HB2	11:O:203:ARG:HB3	1.95	0.49
3:C:184:ILE:HD12	3:P:187:PHE:CZ	2.47	0.49
5:I:61:GLY:O	5:I:78:TYR:CB	2.58	0.49
11:O:46:ARG:NH2	11:O:110:GLU:OE2	2.46	0.49
9:W:4:THR:HG22	9:W:5:LEU:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:122:THR:HB	3:P:189:ILE:HG12	1.95	0.49
5:R:171:ILE:HD13	5:R:176:ALA:HB3	1.95	0.49
3:C:319:PRO:HA	7:G:47:ARG:NH1	2.27	0.49
16:P:505:PEE:H54	18:T:501:CDL:H542	1.95	0.49
4:Q:164:ILE:HG22	4:Q:168:VAL:HG11	1.93	0.49
4:Q:97:ASN:HB2	4:Q:98:PRO:HD2	1.94	0.49
1:A:443:TRP:CD1	1:A:444:LEU:HD23	2.48	0.49
2:B:308:ASP:OD1	5:I:57:GLY:N	2.37	0.49
3:C:38:GLY:O	3:C:41:LEU:N	2.46	0.49
3:P:22:PRO:HG2	7:T:3:GLN:HA	1.94	0.49
8:U:40:CYS:O	8:U:43:ARG:HB2	2.12	0.49
1:A:442:PHE:HD1	1:A:442:PHE:C	2.16	0.49
2:B:325:TYR:CD2	5:I:59:ALA:CB	2.96	0.49
2:B:87:ARG:HD2	6:S:107:TRP:HE1	1.78	0.49
4:D:165:TYR:CD1	4:D:165:TYR:N	2.80	0.49
7:G:38:LEU:HA	7:G:41:THR:OG1	2.13	0.49
16:P:505:PEE:O5	18:T:501:CDL:HA32	2.13	0.49
11:O:71:LEU:CD2	12:V:68:VAL:HG21	2.40	0.49
8:U:40:CYS:SG	8:U:43:ARG:NH2	2.86	0.48
2:B:70:ARG:HG2	5:I:68:VAL:HB	1.95	0.48
3:C:220:PHE:CE2	3:C:225:THR:HG22	2.47	0.48
8:H:38:GLU:CA	8:H:41:ASP:HB2	2.42	0.48
11:O:51:ILE:HG12	11:O:204:MET:HG2	1.95	0.48
11:O:166:ALA:HB2	11:O:244:ILE:HG13	1.94	0.48
10:N:58:PHE:HZ	10:N:127:ILE:HG23	1.77	0.48
11:O:37:SER:HA	11:O:208:GLY:O	2.14	0.48
2:B:166:ALA:HB2	2:B:244:ILE:HG13	1.95	0.48
10:N:328:HIS:CD2	10:N:328:HIS:C	2.85	0.48
6:S:18:LYS:HA	6:S:83:TYR:CD2	2.49	0.48
1:A:375:VAL:O	1:A:379:ILE:HG13	2.13	0.48
7:G:34:ILE:N	7:G:35:PRO:HD2	2.28	0.48
3:P:333:LEU:HD13	16:P:505:PEE:H68	1.94	0.48
4:D:137:PRO:HA	4:D:149:PHE:CD2	2.48	0.48
7:G:75:ALA:HB1	8:H:43:ARG:HD2	1.94	0.48
7:T:30:PHE:HD1	7:T:34:ILE:HD11	1.79	0.48
3:C:277:ALA:HB1	3:C:294:LEU:HD12	1.95	0.48
3:C:106:SER:CB	13:C:502:HEM:HBD2	2.34	0.48
6:F:18:LYS:HG3	6:F:83:TYR:CD2	2.45	0.48
11:O:26:PHE:HZ	11:O:390:GLY:O	1.96	0.48
4:Q:27:ARG:HB2	4:Q:55:CYS:HB2	1.96	0.48
7:T:67:GLU:OE1	7:T:67:GLU:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:324:LEU:O	3:C:327:ALA:HB3	2.13	0.48
11:O:227:ARG:HA	11:O:227:ARG:HE	1.79	0.48
3:P:69:ILE:HA	3:P:73:VAL:CG2	2.44	0.48
2:B:52:LYS:HB2	2:B:203:ARG:HB3	1.96	0.48
13:C:501:HEM:HBC2	13:C:501:HEM:HMC2	1.96	0.48
4:D:149:PHE:HD1	4:D:156:GLN:O	1.97	0.48
6:F:13:LEU:HA	6:F:16:ILE:HD12	1.96	0.48
7:G:34:ILE:O	7:G:38:LEU:HG	2.13	0.48
1:A:328:HIS:HB2	1:A:427:PRO:HB2	1.95	0.48
2:B:56:ARG:NH2	2:B:235:ALA:O	2.47	0.48
3:C:379:TRP:CZ3	6:F:37:ILE:HD12	2.49	0.48
13:P:501:HEM:HBC2	13:P:501:HEM:CMC	2.36	0.48
6:S:13:LEU:HA	6:S:16:ILE:HD12	1.95	0.48
1:A:280:TYR:HB3	1:A:307:PHE:CE2	2.48	0.47
2:B:261:SER:OG	2:B:262:ALA:N	2.46	0.47
7:G:81:ARG:HD2	8:H:47:ARG:HD3	1.94	0.47
10:N:29:GLN:HE22	10:N:204:GLU:HG3	1.79	0.47
1:A:32:GLN:O	1:A:202:GLY:HA3	2.14	0.47
4:D:27:ARG:HB2	4:D:55:CYS:HB2	1.95	0.47
5:E:45:VAL:HG13	9:J:28:ALA:HA	1.95	0.47
4:Q:37:CYS:SG	17:Q:501:HEC:CBB	3.02	0.47
9:W:52:TRP:O	9:W:56:LYS:HB2	2.14	0.47
3:C:25:SER:O	6:F:70:MET:HG3	2.14	0.47
10:N:65:LYS:NZ	11:O:287:ARG:O	2.47	0.47
11:O:95:LYS:HB3	11:O:110:GLU:HB2	1.95	0.47
3:P:329:VAL:HG22	16:P:505:PEE:H30	1.95	0.47
16:Q:506:PEE:H14	5:R:54:VAL:HG13	1.95	0.47
7:T:49:ALA:N	7:T:50:PRO:HD2	2.29	0.47
1:A:431:LEU:HD12	1:A:432:PRO:HD2	1.95	0.47
3:P:131:TYR:HA	13:P:501:HEM:HAA1	1.96	0.47
3:P:50:PHE:HE2	5:R:58:PHE:O	1.98	0.47
11:O:181:TYR:CZ	11:O:182:ARG:HG2	2.50	0.47
5:R:34:GLY:HA3	9:W:10:TYR:HB2	1.96	0.47
3:C:13:ILE:O	3:C:16:ASN:ND2	2.48	0.47
3:C:193:ALA:O	3:C:196:HIS:HB3	2.15	0.47
8:H:52:GLU:HG2	8:H:53:ASP:N	2.30	0.47
3:P:51:LEU:HD13	13:P:501:HEM:HBD1	1.95	0.47
11:O:141:GLN:HE22	11:O:186:VAL:HB	1.79	0.47
5:R:135:LEU:HD13	5:R:180:LEU:HD12	1.96	0.47
1:A:21:ASN:O	1:A:221:GLY:O	2.33	0.47
3:P:310:SER:HA	3:P:374:ASN:HD21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:18:LYS:HG3	6:S:83:TYR:CD2	2.50	0.47
5:E:27:GLU:OE1	5:E:27:GLU:CA	2.59	0.47
10:N:148:VAL:HG12	10:N:152:TYR:CE2	2.50	0.47
1:A:442:PHE:CD1	1:A:442:PHE:C	2.88	0.47
5:E:11:SER:HA	5:E:14:ARG:HD2	1.97	0.47
11:O:101:THR:HG22	11:O:103:GLU:H	1.79	0.47
7:T:18:LEU:HD23	7:T:23:GLN:HB3	1.97	0.47
7:T:34:ILE:O	7:T:38:LEU:HG	2.15	0.47
1:A:443:TRP:CG	1:A:444:LEU:N	2.83	0.46
7:G:67:GLU:HA	7:G:67:GLU:OE1	2.15	0.46
10:N:46:ARG:NH1	10:N:93:GLU:OE2	2.47	0.46
3:C:18:PHE:O	3:C:220:PHE:HD2	1.99	0.46
2:B:154:ASN:ND2	5:I:76:VAL:CG1	2.78	0.46
3:P:278:TYR:CE2	3:P:282:ARG:HD3	2.50	0.46
1:A:40:TRP:HB3	1:A:384:LEU:HD11	1.97	0.46
3:C:13:ILE:O	3:C:13:ILE:HG22	2.15	0.46
4:D:231:LYS:O	6:F:71:ARG:HD3	2.16	0.46
3:P:13:ILE:O	3:P:13:ILE:CG2	2.63	0.46
1:A:30:SER:OG	1:A:32:GLN:HG3	2.15	0.46
11:O:261:SER:OG	11:O:262:ALA:N	2.48	0.46
5:E:72:SER:HB2	3:P:168:PHE:CE2	2.50	0.46
3:P:234:LEU:CD2	4:Q:216:LEU:HD11	2.46	0.46
1:A:159:GLN:CB	5:E:7:VAL:HG21	2.45	0.46
14:P:503:G8U:F1	14:P:503:G8U:C9	2.46	0.46
5:R:91:TRP:HZ3	5:R:136:ILE:HD11	1.81	0.46
5:R:34:GLY:CA	9:W:10:TYR:HB2	2.46	0.46
1:A:444:LEU:C	1:A:444:LEU:HD23	2.36	0.46
3:C:374:ASN:HB3	3:C:379:TRP:HB2	1.96	0.46
11:O:49:LEU:HD23	11:O:127:THR:HG21	1.97	0.46
5:R:175:PRO:CD	19:R:501:FES:S1	3.04	0.46
8:U:24:CYS:C	8:U:26:GLN:H	2.19	0.46
2:B:301:LYS:HZ2	2:B:301:LYS:HD2	1.77	0.46
8:H:36:ARG:O	8:H:36:ARG:HG2	2.15	0.46
3:P:13:ILE:O	3:P:13:ILE:HG22	2.15	0.46
3:P:277:ALA:HB1	3:P:294:LEU:HD12	1.97	0.46
5:R:137:GLY:O	5:R:146:PRO:HD2	2.16	0.46
4:D:184:LYS:HG3	8:H:74:PHE:CE2	2.51	0.46
3:P:186:PRO:HG2	13:P:501:HEM:HMC3	1.98	0.46
8:U:69:VAL:CG1	8:U:73:LEU:HD12	2.46	0.46
3:C:22:PRO:HG2	7:G:3:GLN:HA	1.98	0.46
3:C:75:TYR:HD2	5:E:57:GLN:CB	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:18:LEU:CD2	7:G:23:GLN:HB3	2.46	0.46
8:H:44:VAL:CG1	8:H:45:SER:N	2.79	0.46
10:N:40:TRP:HB3	10:N:384:LEU:HD11	1.98	0.46
10:N:41:ILE:HG21	10:N:190:TYR:CD1	2.51	0.46
3:P:37:LEU:HD23	3:P:90:PHE:CD1	2.51	0.46
4:Q:10:TYR:O	4:Q:15:ARG:NH1	2.49	0.46
5:R:175:PRO:HD2	19:R:501:FES:S1	2.56	0.46
7:G:76:ALA:O	7:G:77:TYR:CD1	2.66	0.45
7:G:77:TYR:HA	8:H:47:ARG:NH2	2.31	0.45
11:O:334:GLY:HA2	11:O:434:PRO:HD3	1.99	0.45
13:P:502:HEM:HBB2	13:P:502:HEM:CMB	2.45	0.45
4:D:97:ASN:HB2	4:D:98:PRO:HD2	1.98	0.45
3:P:45:ILE:HA	13:P:501:HEM:HMC2	1.98	0.45
10:N:159:GLN:CB	5:R:7:VAL:HG21	2.46	0.45
1:A:184:GLU:HG2	1:A:188:ARG:HD3	1.99	0.45
4:D:164:ILE:HG22	4:D:168:VAL:HG11	1.96	0.45
4:D:43:MET:HG2	4:D:46:VAL:HG23	1.98	0.45
3:P:284:ILE:HD12	3:P:293:ALA:HB2	1.97	0.45
6:S:40:ASN:C	6:S:40:ASN:OD1	2.55	0.45
3:C:150:LEU:HD13	3:C:160:LEU:HD22	1.98	0.45
8:H:24:CYS:C	8:H:26:GLN:H	2.20	0.45
10:N:30:SER:OG	10:N:32:GLN:HG3	2.16	0.45
5:E:72:SER:HB2	3:P:168:PHE:HE2	1.81	0.45
5:R:83:GLU:HA	5:R:100:HIS:HB3	1.99	0.45
5:R:134:ILE:HD11	5:R:185:TYR:CG	2.52	0.45
6:S:18:LYS:HG3	6:S:83:TYR:HD2	1.81	0.45
1:A:298:ALA:HA	1:A:303:LEU:HB2	1.99	0.45
5:R:118:ARG:NH2	5:R:173:LYS:O	2.41	0.45
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.51	0.45
2:B:37:SER:HA	2:B:208:GLY:O	2.16	0.45
2:B:26:PHE:HZ	2:B:390:GLY:O	1.99	0.45
3:C:138:MET:HE2	3:C:138:MET:HA	1.99	0.45
3:P:103:TYR:CD1	3:P:325:PHE:CD2	3.01	0.45
3:C:181:PHE:HA	3:C:184:ILE:HG22	1.98	0.45
3:C:278:TYR:CE2	3:C:282:ARG:HD3	2.52	0.45
3:P:379:TRP:CZ3	6:S:33:ARG:HD3	2.51	0.45
13:P:502:HEM:HHD	13:P:502:HEM:HBC2	1.98	0.45
11:O:354:ASN:N	11:O:355:PRO:HD2	2.32	0.45
11:O:76:THR:HG23	11:O:81:SER:HA	1.99	0.45
3:P:324:LEU:O	3:P:327:ALA:HB3	2.17	0.45
3:P:75:TYR:CD2	5:R:57:GLN:HG2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:198:LEU:HD12	3:P:11:MET:SD	2.57	0.45
2:B:334:GLY:HA2	2:B:434:PRO:HD3	1.99	0.45
3:C:77:TRP:CZ3	3:C:78:ILE:HG13	2.52	0.45
3:P:94:LEU:O	3:P:98:VAL:HG23	2.16	0.45
4:Q:131:LEU:HD21	17:Q:501:HEC:HMB2	1.98	0.45
8:U:52:GLU:HG2	8:U:53:ASP:N	2.32	0.45
2:B:230:LEU:CD1	2:B:233:SER:HB3	2.47	0.44
5:E:41:ALA:HB2	9:J:20:PHE:HE1	1.82	0.44
10:N:70:ARG:HB3	10:N:74:ALA:HB3	1.99	0.44
4:Q:110:PRO:HA	4:Q:111:PRO:HD2	1.90	0.44
1:A:391:PRO:HG2	1:A:394:GLU:HB2	1.99	0.44
2:B:101:THR:HG22	2:B:103:GLU:H	1.82	0.44
3:C:303:LEU:HD23	3:C:306:LEU:HD12	1.98	0.44
11:O:83:PHE:CE1	11:O:87:ARG:HG3	2.51	0.44
2:B:160:ILE:HG21	5:I:64:LEU:HB2	1.99	0.44
4:Q:17:LEU:HD12	4:Q:18:LEU:HD23	1.98	0.44
4:Q:211:MET:HE3	5:R:49:TYR:CD2	2.52	0.44
2:B:437:ASP:OD2	11:O:169:ARG:NH2	2.50	0.44
3:C:233:LEU:CD1	4:D:219:VAL:HG21	2.47	0.44
4:D:37:CYS:SG	17:D:501:HEC:CAB	3.05	0.44
3:P:379:TRP:CD2	6:S:33:ARG:HD3	2.52	0.44
5:R:166:ASP:OD1	5:R:170:ARG:N	2.50	0.44
2:B:227:ARG:HE	2:B:227:ARG:HA	1.81	0.44
3:C:13:ILE:HG23	3:C:16:ASN:HD21	1.82	0.44
3:C:234:LEU:CD2	4:D:216:LEU:HD11	2.46	0.44
4:D:11:PRO:HA	4:D:15:ARG:HD2	1.98	0.44
10:N:431:LEU:HD12	10:N:432:PRO:HD2	1.98	0.44
3:P:137:GLN:OE1	3:P:260:ASN:N	2.48	0.44
3:P:90:PHE:HE2	3:P:123:VAL:HG13	1.77	0.44
12:V:76:VAL:O	12:V:76:VAL:CG1	2.65	0.44
2:B:26:PHE:CE2	2:B:391:SER:HA	2.53	0.44
2:B:76:THR:HG23	2:B:81:SER:HA	1.99	0.44
13:C:501:HEM:HBC2	13:C:501:HEM:CMC	2.47	0.44
3:P:319:PRO:HA	7:T:47:ARG:NH1	2.33	0.44
9:W:4:THR:CG2	9:W:5:LEU:N	2.80	0.44
1:A:432:PRO:HB2	1:A:437:ILE:HG13	1.99	0.44
3:C:8:HIS:N	3:C:9:PRO:CD	2.77	0.44
5:I:65:VAL:HB	5:I:77:ARG:HB2	1.99	0.44
7:T:28:HIS:HB3	7:T:32:LYS:HG3	2.00	0.44
1:A:140:GLU:OE2	5:I:53:GLU:CB	2.61	0.44
11:O:56:ARG:NH2	11:O:235:ALA:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:303:LEU:HD23	3:P:306:LEU:HD12	1.99	0.44
1:A:58:PHE:HD2	1:A:182:LEU:HD22	1.83	0.43
1:A:113:LEU:HA	1:A:116:ILE:HD12	2.00	0.43
3:C:284:ILE:HD12	3:C:293:ALA:HB2	2.00	0.43
6:F:51:PRO:HD2	6:F:54:LEU:HB2	1.99	0.43
10:N:32:GLN:O	10:N:202:GLY:HA3	2.17	0.43
10:N:8:LEU:HB3	10:N:393:ALA:HB2	2.00	0.43
10:N:88:ALA:CB	10:N:97:TYR:HD1	2.31	0.43
7:T:67:GLU:O	7:T:71:ARG:HG3	2.18	0.43
2:B:129:ALA:N	2:B:130:PRO:CD	2.81	0.43
2:B:305:GLN:HA	2:B:305:GLN:HE21	1.82	0.43
11:O:150:VAL:O	11:O:153:GLN:HG2	2.19	0.43
4:Q:56:TYR:CE1	4:Q:64:LEU:HD11	2.54	0.43
5:R:44:THR:HG21	9:W:24:ILE:HD13	2.00	0.43
5:R:86:ASN:HB2	5:R:99:ARG:HD2	2.00	0.43
6:S:83:TYR:O	6:S:83:TYR:HD1	2.01	0.43
8:U:36:ARG:O	8:U:40:CYS:HB3	2.18	0.43
8:U:73:LEU:HD23	8:U:73:LEU:O	2.18	0.43
2:B:95:LYS:HB3	2:B:110:GLU:HB2	2.01	0.43
4:D:204:MET:HE2	16:D:506:PEE:H7	2.00	0.43
8:H:35:GLU:O	8:H:39:LEU:HD12	2.17	0.43
10:N:23:LEU:HA	10:N:192:ALA:O	2.18	0.43
3:P:77:TRP:CZ3	3:P:78:ILE:CD1	2.99	0.43
5:R:146:PRO:HA	5:R:158:CYS:HA	2.00	0.43
2:B:37:SER:HB3	2:B:216:LEU:HD12	2.01	0.43
3:C:138:MET:CE	3:C:138:MET:HA	2.49	0.43
3:C:13:ILE:O	3:C:13:ILE:CG2	2.65	0.43
6:F:18:LYS:HA	6:F:83:TYR:CE2	2.54	0.43
10:N:223:TYR:CB	10:N:228:VAL:HG21	2.48	0.43
3:P:27:ILE:HG13	3:P:224:TYR:CZ	2.54	0.43
1:A:260:PRO:HB2	1:A:264:HIS:HB2	2.01	0.43
2:B:49:LEU:HD23	2:B:127:THR:HG21	2.01	0.43
10:N:149:VAL:HG23	10:N:425:PHE:HB2	2.00	0.43
3:P:165:TRP:NE1	3:P:170:VAL:HG22	2.33	0.43
3:C:378:LYS:HE3	6:F:33:ARG:HH21	1.82	0.43
4:D:216:LEU:N	4:D:217:PRO:HD2	2.33	0.43
11:O:133:ARG:HD3	11:O:135:TRP:CZ2	2.53	0.43
3:P:36:LEU:HB3	3:P:235:LEU:HD22	2.01	0.43
4:Q:162:PRO:HA	4:Q:163:PRO:HD3	1.93	0.43
17:Q:501:HEC:CBB	17:Q:501:HEC:HMB1	2.49	0.43
3:C:102:LEU:HD21	3:C:304:ILE:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:83:ARG:HB2	4:D:84:PRO:HD2	2.01	0.43
11:O:304:HIS:ND1	11:O:304:HIS:N	2.66	0.43
4:Q:117:VAL:CG2	4:Q:190:LEU:HB3	2.49	0.43
3:C:264:THR:HG21	5:R:144:CYS:HA	2.01	0.43
4:D:40:CYS:SG	17:D:501:HEC:CAC	3.07	0.43
4:D:40:CYS:SG	17:D:501:HEC:CBC	3.04	0.43
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.54	0.43
2:B:87:ARG:HD2	6:S:107:TRP:NE1	2.33	0.43
2:B:144:LEU:HB2	2:B:183:ILE:HG23	2.00	0.43
3:P:226:ILE:HD12	3:P:229:ILE:HD12	2.01	0.43
3:P:312:GLN:HB2	3:P:318:ARG:HD2	2.01	0.43
7:T:18:LEU:CD2	7:T:23:GLN:HB3	2.48	0.43
8:H:44:VAL:HG12	8:H:45:SER:N	2.34	0.42
3:P:13:ILE:O	3:P:16:ASN:ND2	2.51	0.42
5:R:144:CYS:HB2	19:R:501:FES:S2	2.59	0.42
2:B:354:ASN:N	2:B:355:PRO:HD2	2.34	0.42
3:C:18:PHE:HZ	14:C:503:G8U:O10	1.97	0.42
3:P:69:ILE:O	3:P:73:VAL:HB	2.19	0.42
7:T:59:TYR:HD1	7:T:59:TYR:C	2.22	0.42
8:H:73:LEU:O	8:H:73:LEU:HD23	2.19	0.42
2:B:283:PRO:HG3	5:I:56:ARG:O	2.19	0.42
10:N:280:TYR:HB3	10:N:307:PHE:CE2	2.54	0.42
3:P:221:HIS:CG	3:P:222:PRO:HA	2.53	0.42
3:C:35:SER:O	3:C:39:ILE:HD12	2.18	0.42
3:C:228:ASP:OD2	14:C:503:G8U:O23	2.37	0.42
11:O:37:SER:HB3	11:O:216:LEU:HD12	2.02	0.42
1:A:45:SER:OG	1:A:92:ARG:HG2	2.19	0.42
3:C:75:TYR:HD2	5:E:57:GLN:HB3	1.85	0.42
7:G:44:CYS:HA	7:G:47:ARG:HD2	2.02	0.42
10:N:293:PRO:O	10:N:297:ILE:HG12	2.19	0.42
3:P:57:SER:HB2	3:P:176:THR:HA	2.02	0.42
3:P:66:VAL:O	3:P:69:ILE:HB	2.20	0.42
4:Q:138:PRO:HG3	8:U:55:THR:HA	2.02	0.42
5:R:49:TYR:CE1	5:R:53:ASN:ND2	2.87	0.42
3:P:30:TRP:CH2	18:T:501:CDL:H711	2.55	0.42
8:U:36:ARG:HG2	8:U:36:ARG:O	2.20	0.42
1:A:303:LEU:HB3	1:A:334:MET:HG2	2.02	0.42
1:A:98:TYR:HE2	1:A:373:THR:HG23	1.85	0.42
3:C:304:ILE:HB	3:C:305:PRO:HD3	2.01	0.42
10:N:113:LEU:HA	10:N:116:ILE:HD12	2.02	0.42
10:N:40:TRP:C	10:N:41:ILE:HG13	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:O:144:LEU:HB2	11:O:183:ILE:HG23	2.00	0.42
11:O:213:HIS:N	11:O:214:PRO:CD	2.82	0.42
2:B:134:ARG:NH2	6:S:49:ARG:O	2.53	0.42
3:P:29:SER:HB2	18:T:501:CDL:HB61	2.02	0.42
9:W:2:ALA:HA	9:W:3:PRO:HD3	1.79	0.42
1:A:148:VAL:HG12	1:A:152:TYR:CE2	2.55	0.42
2:B:213:HIS:N	2:B:214:PRO:CD	2.82	0.42
10:N:106:LEU:O	10:N:110:VAL:HG23	2.19	0.42
5:R:147:ILE:HD13	5:R:159:PRO:HG3	2.02	0.42
10:N:161:THR:HB	10:N:162:PRO:HD2	2.01	0.42
11:O:172:LEU:HD13	11:O:316:TYR:HD2	1.83	0.42
3:P:140:PHE:CD1	3:P:140:PHE:C	2.93	0.42
3:P:27:ILE:HG13	3:P:224:TYR:OH	2.20	0.42
4:Q:229:VAL:HG22	7:T:20:PRO:HD3	2.01	0.42
2:B:181:TYR:CZ	2:B:182:ARG:HG2	2.53	0.42
2:B:83:PHE:CE1	2:B:87:ARG:HG3	2.55	0.42
4:D:165:TYR:CE1	4:D:168:VAL:HG23	2.49	0.42
4:D:181:GLN:OE1	8:H:77:LEU:HB3	2.20	0.42
4:D:47:ALA:O	4:D:50:HIS:HB2	2.20	0.42
11:O:129:ALA:N	11:O:130:PRO:CD	2.83	0.42
1:A:45:SER:OG	1:A:92:ARG:HA	2.20	0.42
3:C:276:PHE:CD1	3:C:277:ALA:N	2.88	0.42
3:P:138:MET:HA	3:P:138:MET:HE2	2.00	0.42
3:C:276:PHE:C	3:C:276:PHE:CD1	2.92	0.41
3:C:94:LEU:O	3:C:98:VAL:HG23	2.19	0.41
10:N:40:TRP:CZ2	10:N:377:GLU:HA	2.55	0.41
1:A:23:LEU:HA	1:A:192:ALA:O	2.20	0.41
7:G:37:VAL:O	7:G:41:THR:OG1	2.34	0.41
2:B:290:ASN:ND2	5:I:56:ARG:HB3	2.35	0.41
9:J:52:TRP:O	9:J:56:LYS:HB2	2.20	0.41
10:N:21:ASN:O	10:N:221:GLY:O	2.38	0.41
3:P:103:TYR:HB2	3:P:325:PHE:HE2	1.85	0.41
5:R:143:GLY:O	5:R:144:CYS:SG	2.78	0.41
2:B:29:LEU:CD2	2:B:30:PRO:HD2	2.51	0.41
4:D:56:TYR:CE1	4:D:64:LEU:HD11	2.55	0.41
5:I:68:VAL:HG12	5:I:69:SER:N	2.35	0.41
11:O:200:THR:OG1	11:O:203:ARG:HD3	2.20	0.41
11:O:272:PHE:CD1	11:O:413:ALA:HB1	2.55	0.41
3:P:150:LEU:HD13	3:P:160:LEU:HD22	2.03	0.41
13:P:501:HEM:HBB2	13:P:501:HEM:CMB	2.50	0.41
4:Q:208:MET:HA	16:Q:506:PEE:H48	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:109:GLU:O	5:R:112:VAL:HB	2.20	0.41
6:S:102:LYS:O	6:S:106:GLU:HG2	2.20	0.41
1:A:41:ILE:HG21	1:A:190:TYR:CD1	2.55	0.41
3:C:18:PHE:CZ	14:C:503:G8U:C12	3.02	0.41
10:N:192:ALA:N	10:N:193:PRO:HD2	2.36	0.41
4:Q:178:THR:HG21	8:U:16:PRO:HD2	2.02	0.41
4:Q:6:HIS:HA	4:Q:7:PRO:HD3	1.97	0.41
3:C:103:TYR:HD1	3:C:325:PHE:HD2	1.64	0.41
4:D:162:PRO:HA	4:D:163:PRO:HD3	1.94	0.41
4:D:37:CYS:SG	17:D:501:HEC:CBB	3.08	0.41
4:Q:211:MET:HE3	5:R:49:TYR:HD2	1.85	0.41
1:A:58:PHE:CD2	1:A:182:LEU:CD2	3.03	0.41
1:A:65:LYS:NZ	2:B:287:ARG:O	2.54	0.41
2:B:378:PHE:O	2:B:382:VAL:HG23	2.20	0.41
4:D:17:LEU:HD12	4:D:18:LEU:HD23	2.03	0.41
7:G:80:ASP:HB3	8:H:47:ARG:HD2	2.02	0.41
5:R:72:SER:OG	5:R:73:LYS:N	2.53	0.41
5:R:83:GLU:HG3	5:R:100:HIS:CD2	2.55	0.41
4:Q:3:LEU:CD2	8:U:56:GLU:HG3	2.51	0.41
3:C:211:ILE:HD11	6:F:36:THR:HG22	2.03	0.41
5:I:76:VAL:CG1	5:I:76:VAL:O	2.67	0.41
11:O:230:LEU:CD1	11:O:233:SER:HB3	2.50	0.41
4:Q:17:LEU:HD12	4:Q:18:LEU:CD2	2.51	0.41
4:Q:191:ARG:HA	4:Q:191:ARG:HD2	1.90	0.41
1:A:70:ARG:HB3	1:A:74:ALA:HB3	2.03	0.41
2:B:141:GLN:HE22	2:B:186:VAL:HB	1.85	0.41
3:C:92:ILE:HG13	3:C:272:TRP:CH2	2.56	0.41
5:I:54:SER:HA	5:I:56:ARG:HH11	1.84	0.41
10:N:60:GLU:OE2	11:O:287:ARG:NH1	2.52	0.41
11:O:393:THR:HG22	11:O:397:THR:HB	2.02	0.41
10:N:291:SER:HA	11:O:87:ARG:NE	2.35	0.41
3:C:378:LYS:HG3	6:F:33:ARG:NH2	2.36	0.41
3:C:69:ILE:HA	3:C:73:VAL:CG2	2.51	0.41
4:D:37:CYS:C	4:D:39:SER:H	2.24	0.41
10:N:298:ALA:HA	10:N:303:LEU:HB2	2.03	0.41
10:N:416:TYR:CE1	10:N:442:PHE:HA	2.55	0.41
4:Q:102:ARG:O	4:Q:105:ASN:O	2.39	0.41
8:U:17:LEU:HD13	8:U:73:LEU:HD11	2.02	0.41
3:C:366:MET:HB2	3:C:367:PRO:HD3	2.03	0.41
11:O:56:ARG:HB2	11:O:171:ALA:HB1	2.02	0.41
11:O:26:PHE:CZ	11:O:391:SER:HA	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:126:TYR:C	4:Q:126:TYR:CD1	2.94	0.41
4:D:106:ASN:HD22	4:D:106:ASN:HA	1.57	0.41
7:G:50:PRO:HG2	7:G:51:PRO:HD3	2.03	0.41
10:N:184:GLU:CG	10:N:188:ARG:HD3	2.50	0.41
3:P:181:PHE:HA	3:P:184:ILE:HG22	2.02	0.41
4:Q:25:SER:HB3	4:Q:188:THR:HG21	2.01	0.41
4:Q:83:ARG:HB2	4:Q:84:PRO:HD2	2.03	0.41
1:A:354:VAL:HG21	1:A:404:ALA:HA	2.03	0.40
3:C:122:THR:HB	3:C:189:ILE:HG12	2.03	0.40
3:C:36:LEU:HB3	3:C:235:LEU:HD22	2.03	0.40
3:C:140:PHE:CE2	3:C:261:PRO:HB3	2.56	0.40
3:C:310:SER:HA	3:C:374:ASN:HD21	1.85	0.40
10:N:184:GLU:HG2	10:N:188:ARG:HD3	2.02	0.40
10:N:391:PRO:HG2	10:N:394:GLU:HB2	2.01	0.40
3:P:138:MET:CE	3:P:138:MET:HA	2.50	0.40
5:R:158:CYS:HB3	5:R:163:SER:HB2	2.03	0.40
2:B:56:ARG:HB2	2:B:171:ALA:HB1	2.03	0.40
3:C:66:VAL:O	3:C:69:ILE:HB	2.20	0.40
5:I:64:LEU:HD11	5:I:76:VAL:CG2	2.51	0.40
3:P:17:ALA:HA	3:P:21:LEU:HB2	2.02	0.40
5:R:165:TYR:CE1	5:R:171:ILE:HD13	2.57	0.40
5:R:75:GLU:HB3	5:R:195:VAL:H	1.86	0.40
4:Q:140:GLY:HA3	8:U:53:ASP:HA	2.03	0.40
1:A:26:ALA:HB1	1:A:379:ILE:CG2	2.51	0.40
10:N:316:ASP:N	10:N:316:ASP:OD1	2.51	0.40
3:P:140:PHE:CE2	3:P:261:PRO:HB3	2.56	0.40
3:P:174:THR:O	3:P:177:ARG:HG2	2.21	0.40
4:Q:43:MET:HG2	4:Q:46:VAL:HG23	2.04	0.40
6:S:83:TYR:CD1	6:S:83:TYR:C	2.94	0.40
4:Q:180:SER:OG	8:U:15:ASP:OD1	2.33	0.40
1:A:100:LYS:HD2	1:A:373:THR:OG1	2.20	0.40
2:B:169:ARG:NH2	2:B:240:HIS:CD2	2.86	0.40
2:B:417:PHE:C	2:B:417:PHE:CD1	2.94	0.40
3:C:226:ILE:HD12	3:C:229:ILE:HD12	2.02	0.40
3:C:374:ASN:HA	3:C:379:TRP:HD1	1.86	0.40
4:D:138:PRO:HD3	4:D:149:PHE:CE2	2.55	0.40
7:G:28:HIS:HB3	7:G:32:LYS:HG3	2.04	0.40
9:J:9:LEU:HD13	9:J:13:LEU:HD13	2.03	0.40
5:R:121:GLN:NE2	5:R:126:ARG:HG2	2.37	0.40
6:S:96:GLU:OE1	6:S:96:GLU:HA	2.21	0.40
8:U:24:CYS:O	8:U:26:GLN:N	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:TYR:HB3	1:A:241:ILE:HG21	2.03	0.40
3:C:220:PHE:CZ	14:C:503:G8U:H15	2.56	0.40
4:D:149:PHE:CD1	4:D:156:GLN:HB3	2.56	0.40
4:D:43:MET:HG2	4:D:46:VAL:CG2	2.52	0.40
8:H:17:LEU:HD11	8:H:21:ARG:HE	1.86	0.40
11:O:270:ASN:HB3	11:O:405:VAL:HG21	2.03	0.40
11:O:304:HIS:O	11:O:305:GLU:HG2	2.22	0.40
3:P:282:ARG:NH2	3:P:338:ILE:O	2.49	0.40
2:B:83:PHE:CE2	6:S:104:ARG:HA	2.56	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	442/480 (92%)	401 (91%)	38 (9%)	3 (1%)	22	60
2	B	420/453 (93%)	377 (90%)	43 (10%)	0	100	100
3	C	372/379 (98%)	334 (90%)	37 (10%)	1 (0%)	41	75
3	P	368/379 (97%)	331 (90%)	36 (10%)	1 (0%)	41	75
4	D	238/325 (73%)	219 (92%)	18 (8%)	1 (0%)	34	71
4	Q	239/325 (74%)	221 (92%)	16 (7%)	2 (1%)	19	58
5	E	71/274 (26%)	62 (87%)	8 (11%)	1 (1%)	11	45
5	I	23/274 (8%)	20 (87%)	3 (13%)	0	100	100
5	R	194/274 (71%)	168 (87%)	25 (13%)	1 (0%)	29	67
6	F	96/111 (86%)	88 (92%)	8 (8%)	0	100	100
6	S	97/111 (87%)	90 (93%)	7 (7%)	0	100	100
7	G	78/82 (95%)	71 (91%)	7 (9%)	0	100	100
7	T	72/82 (88%)	66 (92%)	6 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	63/91 (69%)	53 (84%)	9 (14%)	1 (2%)	9	43
8	U	64/91 (70%)	54 (84%)	9 (14%)	1 (2%)	9	43
9	J	56/64 (88%)	47 (84%)	9 (16%)	0	100	100
9	W	57/64 (89%)	49 (86%)	8 (14%)	0	100	100
10	N	442/480 (92%)	402 (91%)	38 (9%)	2 (0%)	29	67
11	O	417/453 (92%)	378 (91%)	38 (9%)	1 (0%)	47	80
12	V	15/274 (6%)	12 (80%)	3 (20%)	0	100	100
All	All	3824/5066 (76%)	3443 (90%)	366 (10%)	15 (0%)	34	71

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	443	TRP
8	H	25	GLU
8	U	25	GLU
5	E	61	SER
1	A	267	ASN
5	R	61	SER
1	A	260	PRO
3	C	13	ILE
10	N	267	ASN
10	N	260	PRO
3	P	13	ILE
11	O	306	PRO
4	Q	176	PRO
4	D	176	PRO
4	Q	217	PRO

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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%)	351 (95%)	17 (5%)	27	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	331/355 (93%)	324 (98%)	7 (2%)	53	72
3	C	322/327 (98%)	310 (96%)	12 (4%)	34	59
3	P	318/327 (97%)	305 (96%)	13 (4%)	30	57
4	D	205/257 (80%)	200 (98%)	5 (2%)	49	69
4	Q	206/257 (80%)	202 (98%)	4 (2%)	57	75
5	E	63/228 (28%)	59 (94%)	4 (6%)	18	46
5	I	21/228 (9%)	20 (95%)	1 (5%)	25	53
5	R	168/228 (74%)	161 (96%)	7 (4%)	30	56
6	F	90/99 (91%)	83 (92%)	7 (8%)	12	39
6	S	91/99 (92%)	84 (92%)	7 (8%)	13	40
7	G	71/72 (99%)	62 (87%)	9 (13%)	4	22
7	T	66/72 (92%)	59 (89%)	7 (11%)	6	27
8	H	62/85 (73%)	55 (89%)	7 (11%)	6	25
8	U	63/85 (74%)	58 (92%)	5 (8%)	12	39
9	J	49/54 (91%)	47 (96%)	2 (4%)	30	57
9	W	49/54 (91%)	48 (98%)	1 (2%)	55	73
10	N	367/394 (93%)	352 (96%)	15 (4%)	30	57
11	O	328/355 (92%)	318 (97%)	10 (3%)	41	64
12	V	15/228 (7%)	14 (93%)	1 (7%)	16	44
All	All	3253/4198 (78%)	3112 (96%)	141 (4%)	29	56

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	PRO
1	A	149	VAL
1	A	156	THR
1	A	185	TYR
1	A	203	LEU
1	A	223	TYR
1	A	230	THR
1	A	305	GLN
1	A	328	HIS
1	A	338	LEU
1	A	348	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	365	LEU
1	A	388	ARG
1	A	392	LEU
1	A	416	TYR
1	A	442	PHE
1	A	444	LEU
2	B	33	LEU
2	B	99	THR
2	B	116	VAL
2	B	126	VAL
2	B	226	ILE
2	B	230	LEU
2	B	436	ILE
3	C	10	LEU
3	C	18	PHE
3	C	39	ILE
3	C	90	PHE
3	C	122	THR
3	C	140	PHE
3	C	156	ILE
3	C	161	VAL
3	C	233	LEU
3	C	257	THR
3	C	296	PHE
3	C	377	LEU
4	D	37	CYS
4	D	42	SER
4	D	165	TYR
4	D	178	THR
4	D	211	MET
5	E	7	VAL
5	E	27	GLU
5	E	54	VAL
5	E	72	SER
6	F	13	LEU
6	F	21	TYR
6	F	40	ASN
6	F	83	TYR
6	F	91	GLU
6	F	94	LEU
6	F	95	LYS
7	G	2	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	72	LYS
7	G	74	PRO
8	H	14	VAL
8	H	36	ARG
8	H	38	GLU
8	H	39	LEU
8	H	40	CYS
8	H	41	ASP
8	H	44	VAL
5	I	65	VAL
9	J	4	THR
9	J	9	LEU
10	N	146	ARG
10	N	149	VAL
10	N	156	THR
10	N	185	TYR
10	N	203	LEU
10	N	230	THR
10	N	305	GLN
10	N	328	HIS
10	N	348	SER
10	N	365	LEU
10	N	388	ARG
10	N	392	LEU
10	N	416	TYR
10	N	442	PHE
10	N	443	TRP
11	O	24	LEU
11	O	33	LEU
11	O	99	THR
11	O	126	VAL
11	O	224	LEU
11	O	226	ILE
11	O	230	LEU
11	O	301	LYS
11	O	304	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
11	O	436	ILE
3	P	10	LEU
3	P	18	PHE
3	P	35	SER
3	P	39	ILE
3	P	63	PHE
3	P	122	THR
3	P	140	PHE
3	P	156	ILE
3	P	161	VAL
3	P	257	THR
3	P	296	PHE
3	P	378	LYS
3	P	379	TRP
4	Q	37	CYS
4	Q	165	TYR
4	Q	178	THR
4	Q	211	MET
5	R	7	VAL
5	R	54	VAL
5	R	72	SER
5	R	76	ILE
5	R	113	GLU
5	R	140	THR
5	R	182	VAL
6	S	13	LEU
6	S	40	ASN
6	S	83	TYR
6	S	91	GLU
6	S	94	LEU
6	S	95	LYS
6	S	109	LYS
7	T	2	ARG
7	T	9	ARG
7	T	17	SER
7	T	18	LEU
7	T	41	THR
7	T	46	LEU
7	T	59	TYR
8	U	14	VAL
8	U	36	ARG
8	U	40	CYS

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Mol	Chain	Res	Type
8	U	43	ARG
8	U	50	THR
12	V	71	ASN
9	W	9	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	118	GLN
1	A	271	GLN
1	A	328	HIS
2	B	104	ASN
2	B	154	ASN
2	B	156	GLN
2	B	240	HIS
2	B	277	HIS
2	B	290	ASN
2	B	305	GLN
2	B	400	GLN
3	C	16	ASN
3	C	32	ASN
3	C	312	GLN
3	C	352	GLN
4	D	105	ASN
4	D	225	HIS
5	E	57	GLN
6	F	79	GLN
10	N	29	GLN
10	N	61	HIS
10	N	118	GLN
10	N	271	GLN
10	N	328	HIS
11	O	104	ASN
11	O	154	ASN
11	O	240	HIS
11	O	400	GLN
3	P	16	ASN
3	P	32	ASN
3	P	312	GLN
3	P	374	ASN
4	Q	105	ASN

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Mol	Chain	Res	Type
4	Q	225	HIS
5	R	57	GLN
5	R	141	HIS
6	S	79	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

27 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	$\# Z  > 2$
15	PO4	D	502	-	4,4,4	0.83	0	6,6,6	0.44	0
15	PO4	F	501	-	4,4,4	0.92	0	6,6,6	0.51	0
17	HEC	Q	501	4	26,50,50	2.51	12 (46%)	18,82,82	2.68	7 (38%)
15	PO4	D	503	-	4,4,4	0.93	0	6,6,6	0.46	0
15	PO4	S	501	-	4,4,4	0.88	0	6,6,6	0.36	0
18	CDL	Q	505	-	38,38,99	1.19	2 (5%)	43,47,111	1.14	3 (6%)
16	PEE	C	505	-	48,48,50	0.99	2 (4%)	51,53,55	0.84	2 (3%)
17	HEC	D	501	4	26,50,50	2.46	12 (46%)	18,82,82	2.59	5 (27%)
15	PO4	E	501	-	4,4,4	0.81	0	6,6,6	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	FES	R	501	5	0,4,4	0.00	-	-	-	-
13	HEM	P	501	3	27,50,50	0.90	2 (7%)	17,82,82	1.08	1 (5%)
20	GOL	R	502	-	5,5,5	0.30	0	5,5,5	0.30	0
16	PEE	P	505	-	48,48,50	0.98	2 (4%)	51,53,55	0.88	2 (3%)
15	PO4	C	504	-	4,4,4	1.01	0	6,6,6	0.21	0
13	HEM	C	502	3	27,50,50	0.96	0	17,82,82	1.56	3 (17%)
14	G8U	C	503	3	31,31,31	2.25	6 (19%)	41,45,45	1.66	8 (19%)
16	PEE	Q	506	-	50,50,50	1.02	2 (4%)	53,55,55	0.89	3 (5%)
13	HEM	C	501	3	27,50,50	0.99	2 (7%)	17,82,82	1.39	1 (5%)
14	G8U	P	503	3	31,31,31	2.16	6 (19%)	41,45,45	1.80	6 (14%)
13	HEM	P	502	3	27,50,50	0.89	2 (7%)	17,82,82	1.54	2 (11%)
15	PO4	D	504	-	4,4,4	0.92	0	6,6,6	0.41	0
18	CDL	T	501	-	48,48,99	1.32	4 (8%)	54,60,111	1.25	4 (7%)
18	CDL	G	501	-	43,43,99	1.50	4 (9%)	49,55,111	1.44	6 (12%)
15	PO4	P	504	-	4,4,4	0.86	0	6,6,6	0.68	0
18	CDL	D	505	-	38,38,99	1.20	2 (5%)	43,47,111	1.08	4 (9%)
16	PEE	D	506	-	25,25,50	1.42	2 (8%)	28,30,55	1.22	3 (10%)
15	PO4	N	501	-	4,4,4	0.93	0	6,6,6	0.39	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
17	HEC	D	501	4	-	0/6/54/54	-
14	G8U	C	503	3	-	5/15/15/15	0/3/3/3
17	HEC	Q	501	4	-	1/6/54/54	-
18	CDL	T	501	-	-	29/57/57/110	-
16	PEE	Q	506	-	1/1/4/4	28/54/54/54	-
13	HEM	P	501	3	-	4/6/54/54	-
18	CDL	G	501	-	-	32/52/52/110	-
20	GOL	R	502	-	-	3/4/4/4	-
16	PEE	P	505	-	1/1/4/4	31/52/52/54	-
13	HEM	C	501	3	-	1/6/54/54	-
13	HEM	C	502	3	-	1/6/54/54	-
13	HEM	P	502	3	-	2/6/54/54	-
14	G8U	P	503	3	-	4/15/15/15	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	PEE	D	506	-	1/1/4/4	13/29/29/54	-
19	FES	R	501	5	-	-	0/1/1/1
18	CDL	Q	505	-	-	13/43/43/110	-
18	CDL	D	505	-	-	24/43/43/110	-
16	PEE	C	505	-	1/1/4/4	29/52/52/54	-

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	503	G8U	C19-C20	7.20	1.48	1.38
17	Q	501	HEC	C3C-C2C	6.77	1.47	1.40
17	D	501	HEC	C3C-C2C	6.71	1.47	1.40
14	P	503	G8U	C19-C20	6.55	1.47	1.38
17	Q	501	HEC	C3B-C2B	5.84	1.46	1.40
14	C	503	G8U	C17-C18	5.56	1.47	1.40
18	G	501	CDL	OA6-CA5	5.43	1.47	1.35
17	D	501	HEC	C3B-C2B	5.35	1.46	1.40
14	P	503	G8U	O23-C18	-5.30	1.24	1.37
14	P	503	G8U	C17-C18	5.26	1.46	1.40
14	C	503	G8U	O23-C18	-5.14	1.25	1.37
18	T	501	CDL	OA6-CA5	4.95	1.46	1.35
18	G	501	CDL	OB6-CB5	4.92	1.48	1.34
16	Q	506	PEE	O2-C10	4.76	1.47	1.34
18	D	505	CDL	OA6-CA5	4.72	1.47	1.34
16	D	506	PEE	O3-C30	4.71	1.47	1.33
16	P	505	PEE	O2-C10	4.66	1.47	1.34
18	G	501	CDL	OB8-CB7	4.66	1.47	1.33
18	Q	505	CDL	OA6-CA5	4.59	1.47	1.34
18	T	501	CDL	OB6-CB5	4.51	1.47	1.34
16	D	506	PEE	O2-C10	4.43	1.46	1.34
16	C	505	PEE	O2-C10	4.39	1.46	1.34
18	D	505	CDL	OA8-CA7	4.36	1.46	1.33
18	Q	505	CDL	OA8-CA7	4.35	1.46	1.33
16	Q	506	PEE	O3-C30	4.28	1.45	1.33
18	T	501	CDL	OB8-CB7	4.18	1.45	1.33
16	C	505	PEE	O3-C30	4.18	1.45	1.33
16	P	505	PEE	O3-C30	4.08	1.45	1.33
14	C	503	G8U	C18-C19	3.84	1.45	1.39
14	P	503	G8U	C17-C22	3.77	1.49	1.40
17	D	501	HEC	C3B-C4B	3.73	1.49	1.43
14	P	503	G8U	C18-C19	3.64	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	501	HEC	C3D-C2D	3.54	1.48	1.37
17	Q	501	HEC	C2A-C3A	3.49	1.48	1.37
17	D	501	HEC	C3D-C2D	3.35	1.47	1.37
14	C	503	G8U	C17-C22	3.28	1.48	1.40
13	C	501	HEM	C3B-C2B	-3.27	1.35	1.40
17	Q	501	HEC	C4A-C3A	3.15	1.49	1.42
17	Q	501	HEC	C3B-C4B	3.11	1.48	1.43
17	D	501	HEC	C2A-C3A	3.06	1.46	1.37
17	D	501	HEC	C1C-CHC	2.91	1.49	1.41
17	D	501	HEC	C3C-C4C	2.81	1.48	1.43
17	Q	501	HEC	C1B-CHB	2.78	1.48	1.41
18	G	501	CDL	OA8-CA7	2.77	1.47	1.33
17	D	501	HEC	C4A-C3A	2.74	1.48	1.42
17	Q	501	HEC	C1C-CHC	2.69	1.48	1.41
17	Q	501	HEC	C1A-C2A	2.66	1.48	1.42
17	D	501	HEC	C1A-C2A	2.58	1.48	1.42
17	D	501	HEC	C4D-CHA	2.47	1.47	1.41
18	T	501	CDL	OA8-CA7	2.45	1.45	1.33
13	P	501	HEM	C4D-C3D	2.44	1.48	1.42
14	C	503	G8U	C19-CL	2.44	1.78	1.72
17	Q	501	HEC	C1D-CHD	2.41	1.47	1.41
17	D	501	HEC	C1B-CHB	2.32	1.47	1.41
17	D	501	HEC	C1D-CHD	2.26	1.47	1.41
17	Q	501	HEC	C4D-CHA	2.25	1.47	1.41
13	C	501	HEM	C4D-C3D	2.23	1.47	1.42
13	P	502	HEM	C4D-C3D	2.18	1.47	1.42
14	P	503	G8U	C19-CL	2.13	1.77	1.72
13	P	502	HEM	C3B-C2B	-2.07	1.37	1.40
17	Q	501	HEC	C3C-C4C	2.07	1.46	1.43
13	P	501	HEM	C3B-C2B	-2.04	1.37	1.40

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Q	501	HEC	C1D-C2D-C3D	-7.34	101.89	107.00
14	P	503	G8U	C27-C20-C19	-6.01	119.56	123.01
17	D	501	HEC	C1D-C2D-C3D	-5.77	102.98	107.00
14	P	503	G8U	C18-C19-C20	-5.71	119.16	122.79
18	G	501	CDL	OA6-CA5-C11	5.69	121.56	111.09
18	T	501	CDL	OA6-CA5-C11	5.57	121.34	111.09
14	C	503	G8U	C18-C19-C20	-5.38	119.38	122.79
17	D	501	HEC	CMB-C2B-C3B	5.04	131.74	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	501	HEC	CAA-CBA-CGA	-4.87	104.50	112.67
13	C	501	HEM	CBA-CAA-C2A	-4.70	103.82	112.49
17	Q	501	HEC	CMB-C2B-C3B	4.43	131.03	125.82
18	G	501	CDL	OB6-CB5-C51	4.33	122.87	110.80
14	P	503	G8U	C20-N28-C22	4.31	123.67	118.99
14	C	503	G8U	C27-C20-C19	-4.30	120.54	123.01
13	C	502	HEM	C4A-C3A-C2A	4.28	109.97	107.00
17	D	501	HEC	CMC-C2C-C3C	4.15	130.71	125.82
18	Q	505	CDL	OA6-CA5-C11	4.15	120.45	111.50
14	C	503	G8U	C20-N28-C22	4.09	123.42	118.99
16	D	506	PEE	O2-C10-C11	4.07	120.27	111.50
17	Q	501	HEC	CMC-C2C-C3C	3.96	130.48	125.82
18	T	501	CDL	OB6-CB5-C51	3.94	119.98	111.50
18	D	505	CDL	OA6-CA5-C11	3.92	119.95	111.50
13	P	502	HEM	CAD-CBD-CGD	-3.75	106.38	112.67
16	C	505	PEE	O2-C10-C11	3.45	118.95	111.50
16	P	505	PEE	O2-C10-C11	3.44	118.91	111.50
13	P	502	HEM	CBD-CAD-C3D	3.11	118.21	112.48
16	Q	506	PEE	O2-C10-C11	3.00	117.97	111.50
18	D	505	CDL	OA8-CA7-C31	2.97	121.22	111.91
18	G	501	CDL	OB8-CB7-C71	2.89	120.98	111.91
18	Q	505	CDL	OA8-CA7-C31	2.76	120.58	111.91
17	Q	501	HEC	CMD-C2D-C3D	2.68	130.00	124.94
14	P	503	G8U	C14-C17-C22	2.67	125.62	123.46
14	C	503	G8U	C20-C19-CL	2.65	124.90	121.14
16	D	506	PEE	O3-C30-C31	2.64	120.19	111.91
17	Q	501	HEC	CBD-CAD-C3D	-2.58	107.72	112.49
14	P	503	G8U	C17-C22-N28	-2.52	120.51	123.61
17	Q	501	HEC	CAA-CBA-CGA	-2.49	108.50	112.67
14	P	503	G8U	C14-C17-C18	-2.43	115.86	120.05
13	C	502	HEM	CMA-C3A-C4A	-2.40	124.78	128.46
18	T	501	CDL	OB8-CB7-C71	2.34	119.27	111.91
16	Q	506	PEE	C2-O2-C10	2.34	123.55	117.79
18	T	501	CDL	OA6-CA5-OA7	-2.34	118.32	122.96
13	C	502	HEM	CAA-CBA-CGA	-2.32	108.78	112.67
18	Q	505	CDL	OB4-PB2-OB3	2.31	119.72	110.68
18	G	501	CDL	OB6-CB5-OB7	-2.30	118.14	123.70
14	C	503	G8U	C15-C14-C17	-2.30	116.98	120.79
16	C	505	PEE	O3-C30-C31	2.27	119.03	111.91
14	C	503	G8U	C17-C18-C19	-2.24	116.52	119.27
16	Q	506	PEE	O3-C30-C31	2.19	118.79	111.91
16	D	506	PEE	O3-C30-O5	-2.18	118.08	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	501	HEC	CMD-C2D-C3D	2.17	129.04	124.94
16	P	505	PEE	O3-C30-C31	2.17	118.71	111.91
18	D	505	CDL	OA8-CA7-OA9	-2.17	118.13	123.59
18	D	505	CDL	OB4-PB2-OB3	2.12	118.98	110.68
14	C	503	G8U	C18-C19-CL	-2.10	115.72	118.08
18	G	501	CDL	CA6-OA8-CA7	2.10	122.37	117.10
17	Q	501	HEC	C4C-C3C-C2C	-2.07	104.12	106.35
13	P	501	HEM	C1D-C2D-C3D	-2.03	105.58	107.00
14	C	503	G8U	C17-C22-N28	-2.03	121.10	123.61
18	G	501	CDL	OA8-CA7-C31	2.00	121.11	112.38

All (4) chirality outliers are listed below:

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

All (220) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	Q	505	CDL	CA2-OA2-PA1-OA3
13	P	501	HEM	C1A-C2A-CAA-CBA
13	P	501	HEM	C3A-C2A-CAA-CBA
13	P	501	HEM	C3D-CAD-CBD-CGD
20	R	502	GOL	C1-C2-C3-O3
16	P	505	PEE	O4P-C4-C5-N
18	T	501	CDL	CA2-OA2-PA1-OA3
18	T	501	CDL	CB3-OB5-PB2-OB3
16	Q	506	PEE	O4P-C4-C5-N
16	Q	506	PEE	C1-O3P-P-O1P
16	Q	506	PEE	C1-O3P-P-O2P
13	C	501	HEM	C3D-CAD-CBD-CGD
13	P	502	HEM	C2D-C3D-CAD-CBD
13	P	502	HEM	C4D-C3D-CAD-CBD
18	G	501	CDL	CB2-C1-CA2-OA2
18	G	501	CDL	CA2-OA2-PA1-OA4
18	G	501	CDL	CA3-OA5-PA1-OA2
18	G	501	CDL	CB3-OB5-PB2-OB4
18	G	501	CDL	OB7-CB5-OB6-CB4
18	G	501	CDL	C51-CB5-OB6-CB4

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Mol	Chain	Res	Type	Atoms
18	D	505	CDL	CA2-C1-CB2-OB2
18	D	505	CDL	CB2-OB2-PB2-OB4
18	D	505	CDL	CB2-OB2-PB2-OB5
16	D	506	PEE	O4P-C4-C5-N
16	D	506	PEE	C4-O4P-P-O1P
16	D	506	PEE	C4-O4P-P-O3P
18	T	501	CDL	C11-CA5-OA6-CA4
18	G	501	CDL	C11-CA5-OA6-CA4
18	T	501	CDL	OA7-CA5-OA6-CA4
18	G	501	CDL	OA7-CA5-OA6-CA4
18	T	501	CDL	C31-CA7-OA8-CA6
18	Q	505	CDL	OA9-CA7-OA8-CA6
18	T	501	CDL	OA9-CA7-OA8-CA6
18	T	501	CDL	O1-C1-CA2-OA2
18	T	501	CDL	O1-C1-CB2-OB2
18	G	501	CDL	O1-C1-CA2-OA2
18	G	501	CDL	O1-C1-CB2-OB2
18	D	505	CDL	O1-C1-CB2-OB2
18	Q	505	CDL	C31-CA7-OA8-CA6
18	G	501	CDL	C31-CA7-OA8-CA6
18	G	501	CDL	CA2-C1-CB2-OB2
16	C	505	PEE	C30-C31-C32-C33
18	Q	505	CDL	CA7-C31-C32-C33
16	C	505	PEE	C10-C11-C12-C13
16	P	505	PEE	C10-C11-C12-C13
16	P	505	PEE	C30-C31-C32-C33
16	Q	506	PEE	C10-C11-C12-C13
14	C	503	G8U	F3-C1-O29-C4
16	P	505	PEE	C11-C10-O2-C2
16	P	505	PEE	C1-O3P-P-O4P
18	T	501	CDL	CB3-OB5-PB2-OB2
16	Q	506	PEE	C1-O3P-P-O4P
18	T	501	CDL	CA2-C1-CB2-OB2
16	P	505	PEE	O4-C10-O2-C2
18	D	505	CDL	C31-CA7-OA8-CA6
18	T	501	CDL	C71-C72-C73-C74
16	C	505	PEE	C11-C10-O2-C2
18	Q	505	CDL	C38-C39-C40-C41
16	Q	506	PEE	C31-C32-C33-C34
18	G	501	CDL	OA9-CA7-OA8-CA6
16	C	505	PEE	O4-C10-O2-C2
16	C	505	PEE	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
18	G	501	CDL	CB4-CB3-OB5-PB2
18	T	501	CDL	C74-C75-C76-C77
16	D	506	PEE	C31-C30-O3-C3
16	Q	506	PEE	C41-C42-C43-C44
18	G	501	CDL	C74-C75-C76-C77
16	C	505	PEE	C38-C39-C40-C41
16	P	505	PEE	C19-C20-C21-C22
13	P	501	HEM	C2A-CAA-CBA-CGA
16	C	505	PEE	C42-C43-C44-C45
16	P	505	PEE	C41-C42-C43-C44
18	T	501	CDL	C53-C54-C55-C56
18	T	501	CDL	C73-C74-C75-C76
16	C	505	PEE	C31-C32-C33-C34
16	P	505	PEE	C18-C19-C20-C21
16	P	505	PEE	C42-C43-C44-C45
18	T	501	CDL	C52-C53-C54-C55
16	Q	506	PEE	C11-C12-C13-C14
18	Q	505	CDL	C34-C35-C36-C37
16	Q	506	PEE	C21-C22-C23-C24
18	D	505	CDL	OA9-CA7-OA8-CA6
16	C	505	PEE	C21-C22-C23-C24
18	D	505	CDL	C37-C38-C39-C40
18	Q	505	CDL	C37-C38-C39-C40
16	C	505	PEE	C15-C16-C17-C18
16	P	505	PEE	C21-C22-C23-C24
16	Q	506	PEE	C19-C20-C21-C22
16	Q	506	PEE	C32-C33-C34-C35
18	D	505	CDL	C38-C39-C40-C41
18	D	505	CDL	C11-CA5-OA6-CA4
16	P	505	PEE	C39-C40-C41-C42
16	Q	506	PEE	C17-C18-C19-C20
16	C	505	PEE	C18-C19-C20-C21
16	Q	506	PEE	C39-C40-C41-C42
16	C	505	PEE	C12-C13-C14-C15
16	D	506	PEE	C32-C33-C34-C35
18	D	505	CDL	OA7-CA5-OA6-CA4
16	P	505	PEE	C12-C13-C14-C15
16	Q	506	PEE	C34-C35-C36-C37
16	C	505	PEE	C13-C14-C15-C16
16	C	505	PEE	C19-C20-C21-C22
18	T	501	CDL	C51-C52-C53-C54
16	D	506	PEE	O5-C30-O3-C3

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Mol	Chain	Res	Type	Atoms
16	D	506	PEE	O4-C10-O2-C2
18	G	501	CDL	C71-CB7-OB8-CB6
16	C	505	PEE	C33-C34-C35-C36
16	P	505	PEE	C16-C17-C18-C19
16	Q	506	PEE	C40-C41-C42-C43
16	D	506	PEE	C11-C10-O2-C2
16	P	505	PEE	O2-C2-C3-O3
14	C	503	G8U	F2-C1-O29-C4
18	T	501	CDL	C72-C73-C74-C75
16	Q	506	PEE	C22-C23-C24-C25
16	C	505	PEE	C20-C21-C22-C23
16	Q	506	PEE	C4-O4P-P-O3P
16	Q	506	PEE	O3P-C1-C2-C3
18	G	501	CDL	OB5-CB3-CB4-CB6
16	P	505	PEE	C34-C35-C36-C37
16	C	505	PEE	C40-C41-C42-C43
16	C	505	PEE	C35-C36-C37-C38
18	T	501	CDL	CB2-C1-CA2-OA2
18	G	501	CDL	OB9-CB7-OB8-CB6
16	P	505	PEE	C1-C2-C3-O3
18	D	505	CDL	CA3-CA4-CA6-OA8
18	Q	505	CDL	C33-C34-C35-C36
16	P	505	PEE	C23-C24-C25-C26
16	Q	506	PEE	C36-C37-C38-C39
16	P	505	PEE	C33-C34-C35-C36
14	C	503	G8U	F1-C1-O29-C4
16	C	505	PEE	C1-C2-O2-C10
16	P	505	PEE	C1-C2-O2-C10
18	G	501	CDL	OA6-CA4-CA6-OA8
16	P	505	PEE	C37-C38-C39-C40
16	P	505	PEE	C13-C14-C15-C16
16	C	505	PEE	O3P-C1-C2-C3
16	D	506	PEE	O3P-C1-C2-C3
18	D	505	CDL	CA4-CA3-OA5-PA1
16	P	505	PEE	C35-C36-C37-C38
18	D	505	CDL	C36-C37-C38-C39
16	Q	506	PEE	C1-C2-C3-O3
18	G	501	CDL	CA3-CA4-CA6-OA8
16	D	506	PEE	C1-O3P-P-O4P
18	G	501	CDL	OB5-CB3-CB4-OB6
18	D	505	CDL	OA5-CA3-CA4-OA6
18	G	501	CDL	C73-C74-C75-C76

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Mol	Chain	Res	Type	Atoms
14	P	503	G8U	C17-C22-C24-O25
16	P	505	PEE	C20-C21-C22-C23
16	Q	506	PEE	O2-C2-C3-O3
16	Q	506	PEE	C35-C36-C37-C38
16	Q	506	PEE	C42-C43-C44-C45
18	D	505	CDL	C33-C34-C35-C36
16	C	505	PEE	O3P-C1-C2-O2
16	Q	506	PEE	O3P-C1-C2-O2
16	D	506	PEE	O3P-C1-C2-O2
20	R	502	GOL	O2-C2-C3-O3
16	P	505	PEE	C38-C39-C40-C41
16	C	505	PEE	C16-C17-C18-C19
18	T	501	CDL	C54-C55-C56-C57
16	Q	506	PEE	C13-C14-C15-C16
18	T	501	CDL	CA2-OA2-PA1-OA5
18	G	501	CDL	CB3-OB5-PB2-OB2
18	T	501	CDL	CB4-CB3-OB5-PB2
16	P	505	PEE	C1-O3P-P-O1P
18	T	501	CDL	CB3-OB5-PB2-OB4
18	G	501	CDL	CA3-OA5-PA1-OA4
18	G	501	CDL	CB3-OB5-PB2-OB3
18	T	501	CDL	OA5-CA3-CA4-CA6
18	T	501	CDL	OB5-CB3-CB4-CB6
18	D	505	CDL	OA5-CA3-CA4-CA6
16	P	505	PEE	C5-C4-O4P-P
18	T	501	CDL	OA5-CA3-CA4-OA6
18	T	501	CDL	OB5-CB3-CB4-OB6
18	D	505	CDL	C34-C35-C36-C37
16	Q	506	PEE	C18-C19-C20-C21
18	D	505	CDL	CB2-OB2-PB2-OB3
14	P	503	G8U	F2-C1-O29-C4
16	C	505	PEE	O2-C2-C3-O3
18	D	505	CDL	OA6-CA4-CA6-OA8
18	Q	505	CDL	CA3-OA5-PA1-OA2
16	C	505	PEE	C4-O4P-P-O3P
18	T	501	CDL	CB2-OB2-PB2-OB5
18	G	501	CDL	CA2-OA2-PA1-OA5
18	G	501	CDL	CB2-OB2-PB2-OB5
16	P	505	PEE	C31-C32-C33-C34
14	C	503	G8U	C5-C4-O29-C1
18	G	501	CDL	C71-C72-C73-C74
14	C	503	G8U	C9-C4-O29-C1

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Mol	Chain	Res	Type	Atoms
18	T	501	CDL	C75-C76-C77-C78
16	P	505	PEE	C14-C15-C16-C17
18	Q	505	CDL	CA2-OA2-PA1-OA5
18	D	505	CDL	CA5-C11-C12-C13
16	P	505	PEE	C43-C44-C45-C46
14	P	503	G8U	C5-C4-O29-C1
14	P	503	G8U	C9-C4-O29-C1
16	C	505	PEE	C39-C40-C41-C42
13	C	502	HEM	C3D-CAD-CBD-CGD
17	Q	501	HEC	C3D-CAD-CBD-CGD
18	D	505	CDL	C35-C36-C37-C38
18	D	505	CDL	C12-C11-CA5-OA6
16	Q	506	PEE	C1-C2-O2-C10
16	C	505	PEE	C14-C15-C16-C17
18	G	501	CDL	OA5-CA3-CA4-OA6
18	G	501	CDL	OA5-CA3-CA4-CA6
18	D	505	CDL	CA7-C31-C32-C33
20	R	502	GOL	O1-C1-C2-C3
18	D	505	CDL	C12-C11-CA5-OA7
18	Q	505	CDL	CA2-OA2-PA1-OA4
18	Q	505	CDL	CA3-OA5-PA1-OA3
16	C	505	PEE	C4-O4P-P-O1P
18	T	501	CDL	CB2-OB2-PB2-OB3
16	Q	506	PEE	C4-O4P-P-O1P
18	G	501	CDL	CA2-OA2-PA1-OA3
18	G	501	CDL	CB2-OB2-PB2-OB3
16	D	506	PEE	C1-O3P-P-O2P
16	C	505	PEE	O4P-C4-C5-N
16	C	505	PEE	C22-C23-C24-C25
16	D	506	PEE	C5-C4-O4P-P
18	Q	505	CDL	C35-C36-C37-C38
16	P	505	PEE	O3-C30-C31-C32

There are no ring outliers.

13 monomers are involved in 72 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	Q	501	HEC	8	0
17	D	501	HEC	8	0
19	R	501	FES	3	0
13	P	501	HEM	10	0
16	P	505	PEE	4	0

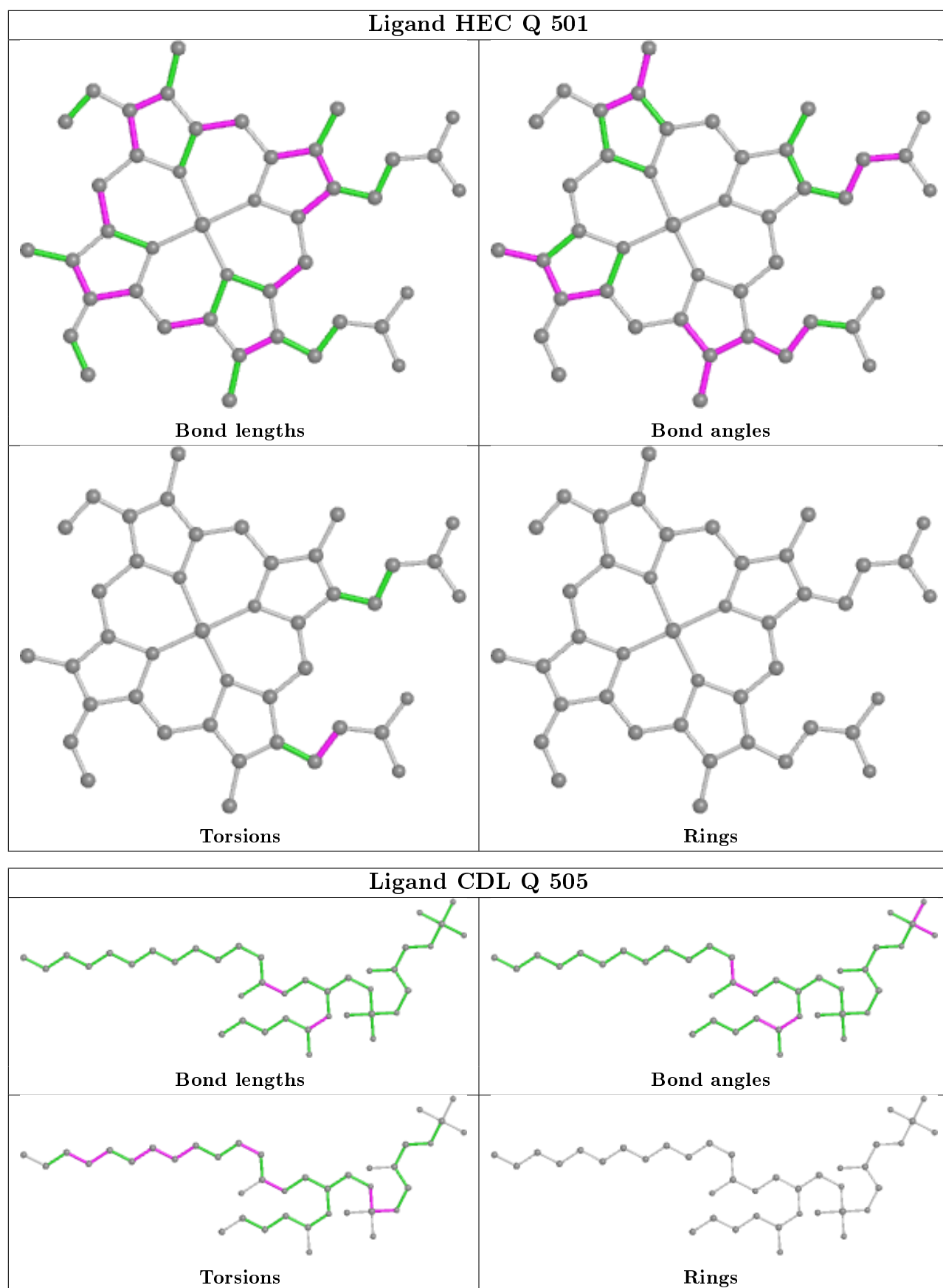
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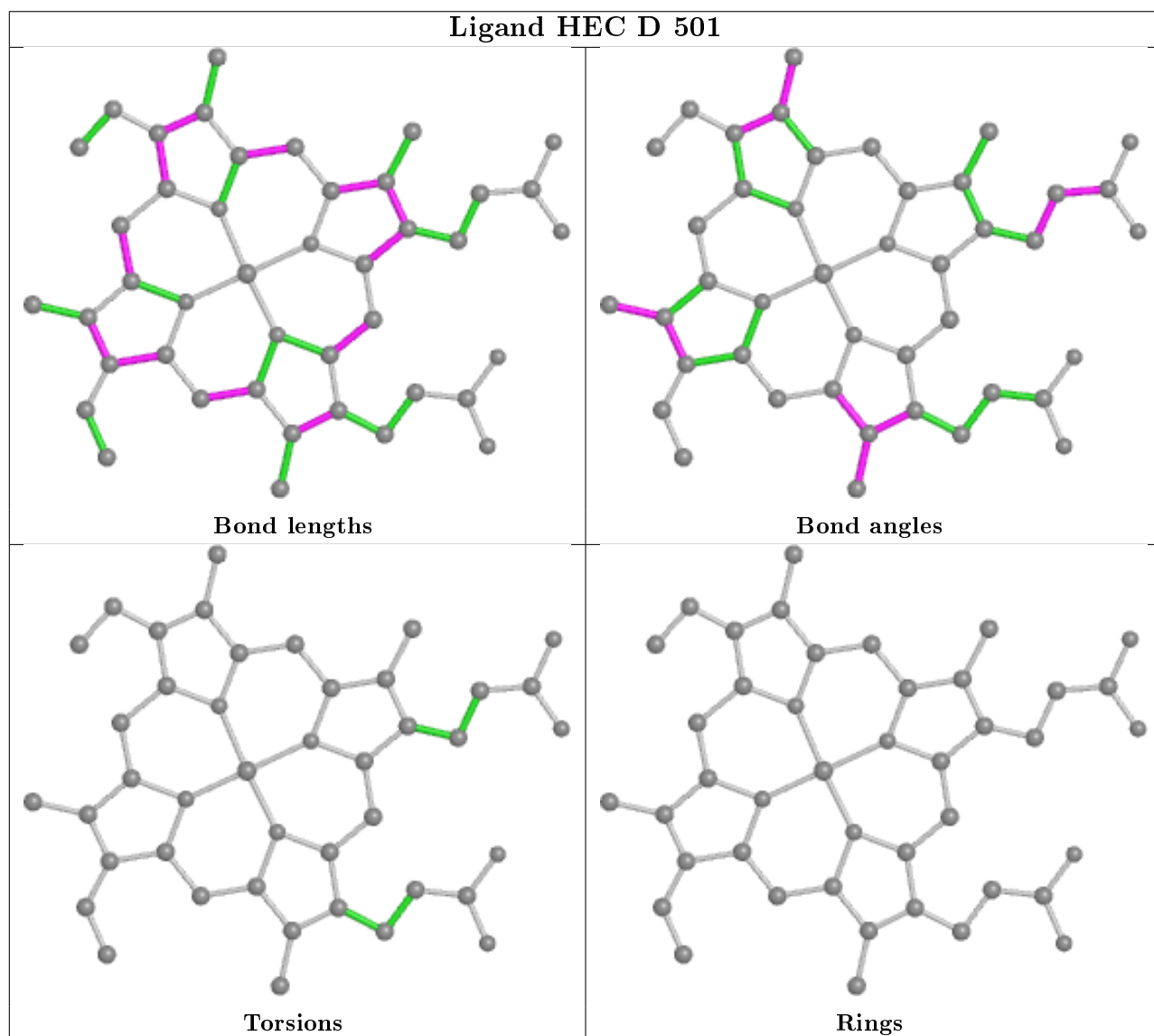
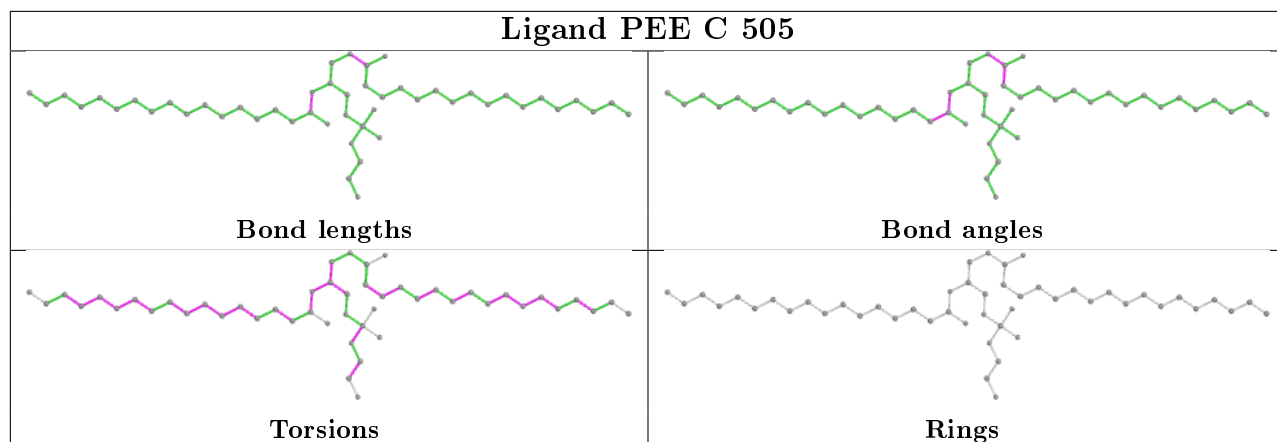


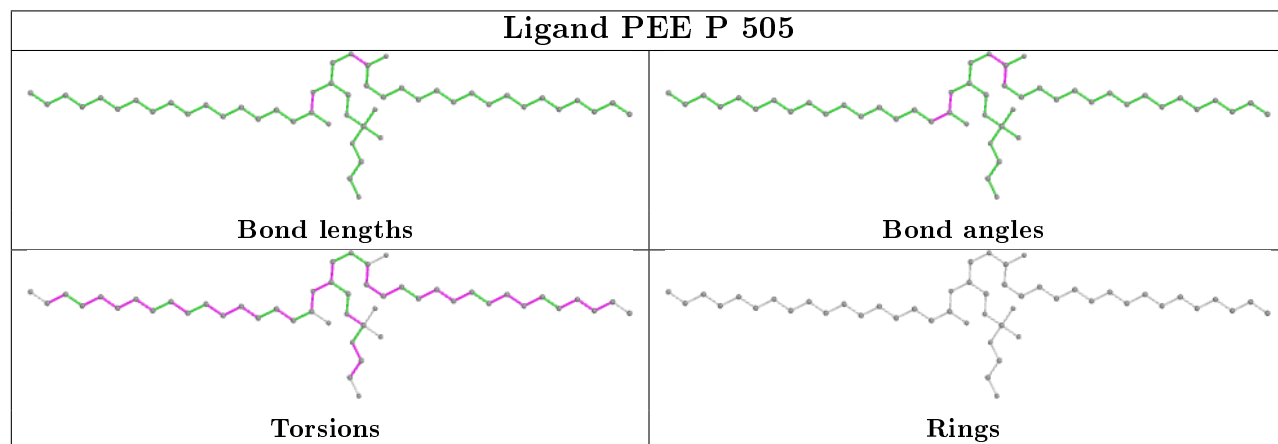
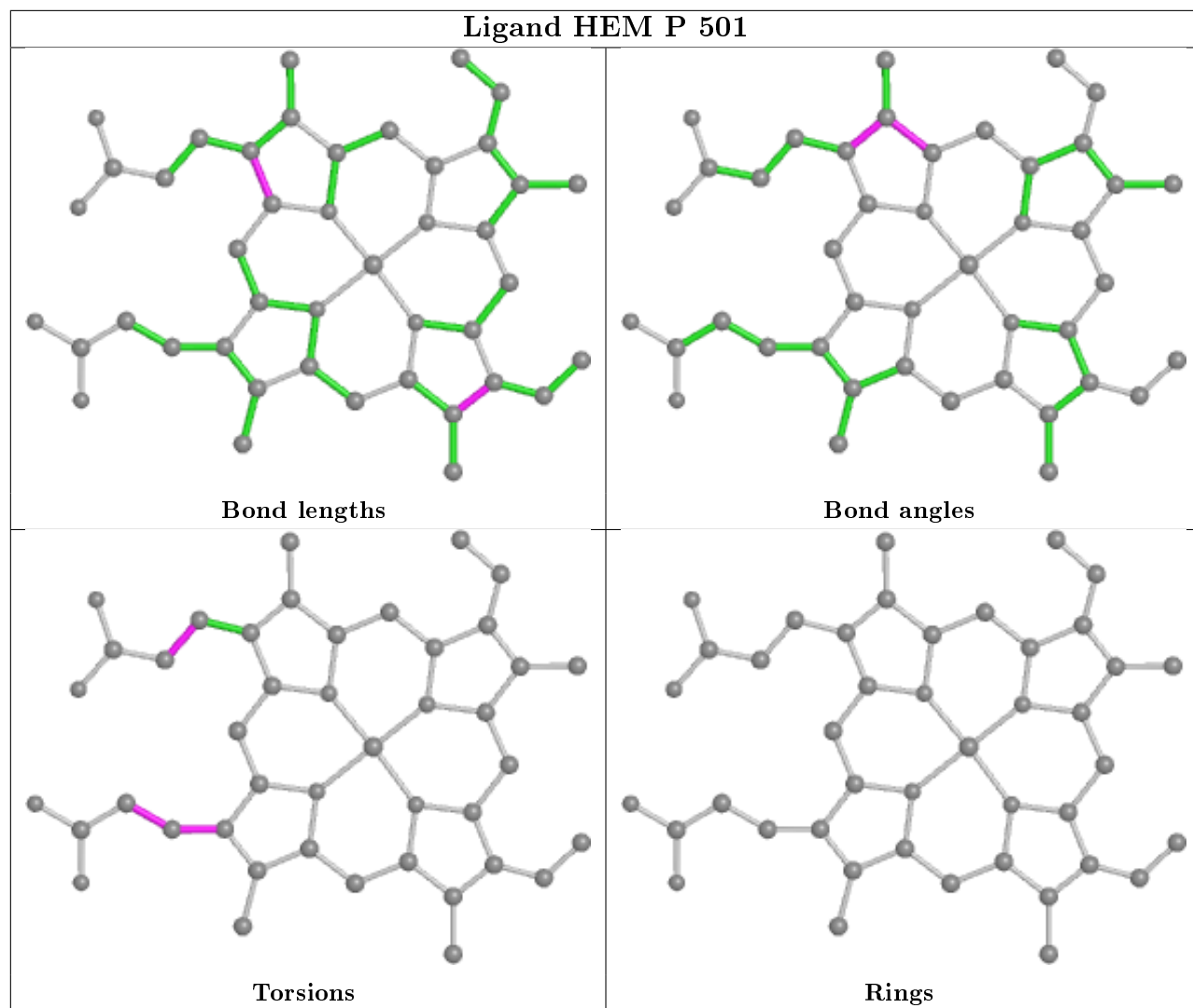
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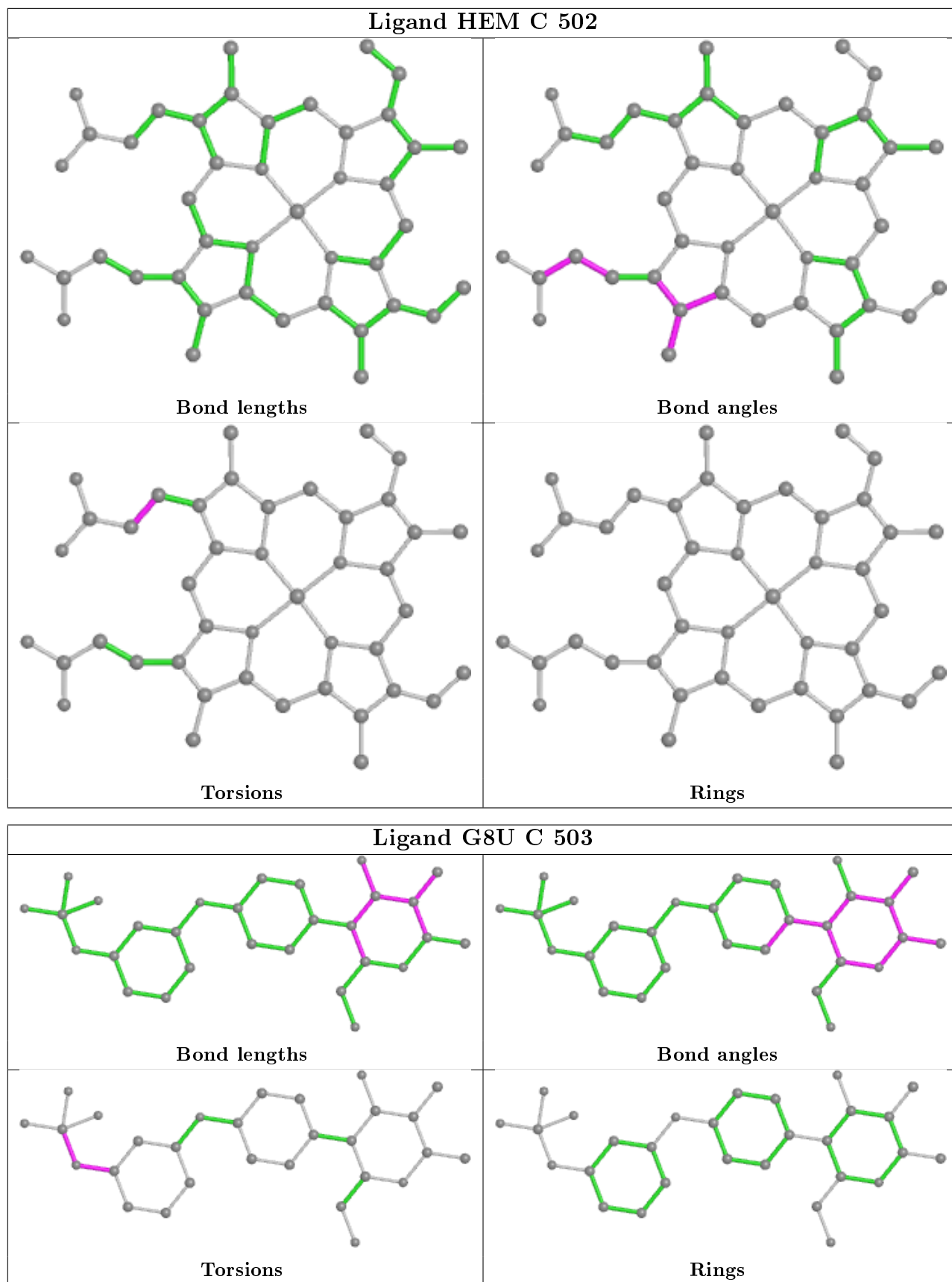
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	502	HEM	3	0
14	C	503	G8U	13	0
16	Q	506	PEE	3	0
13	C	501	HEM	5	0
14	P	503	G8U	9	0
13	P	502	HEM	2	0
18	T	501	CDL	5	0
16	D	506	PEE	1	0

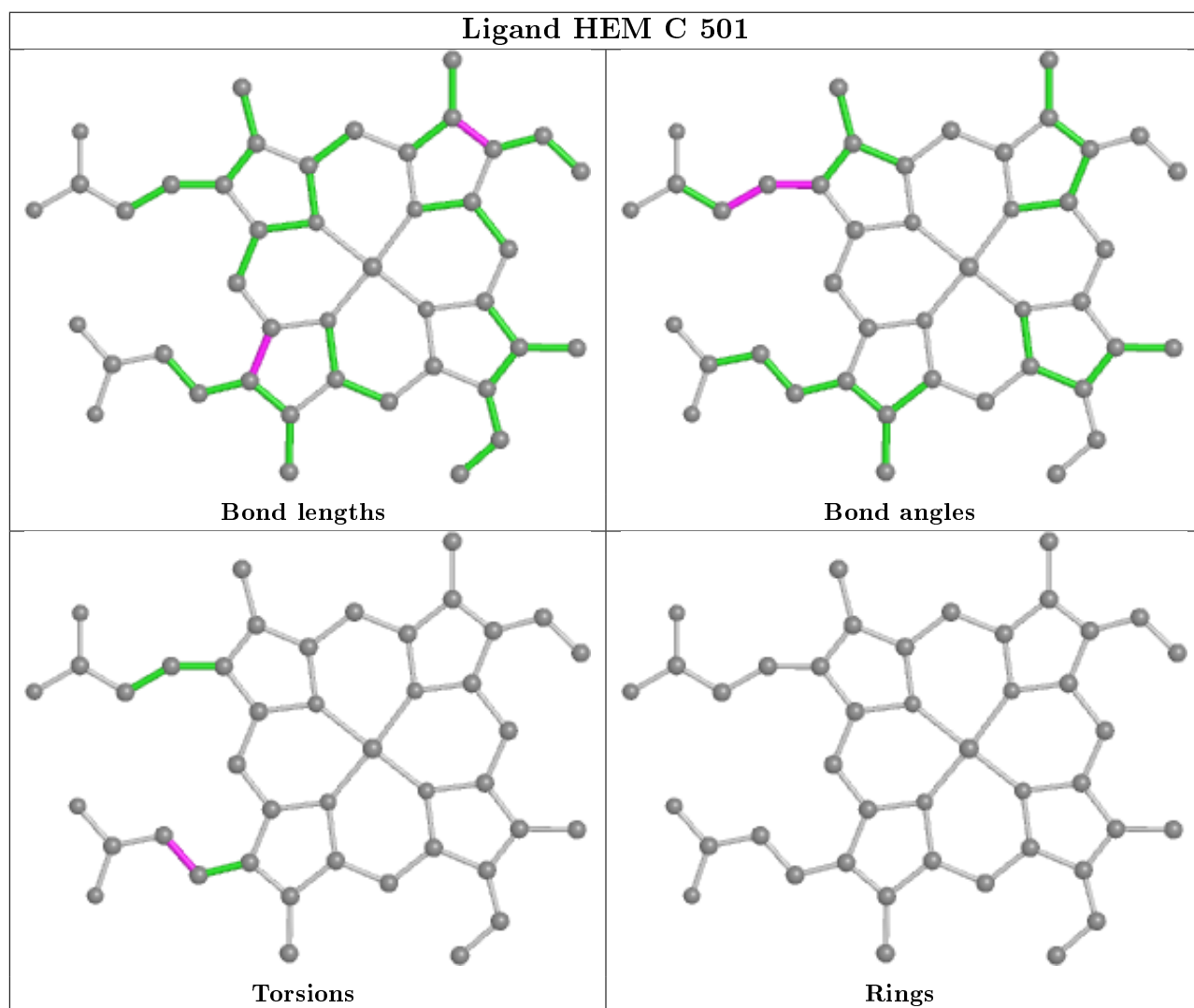
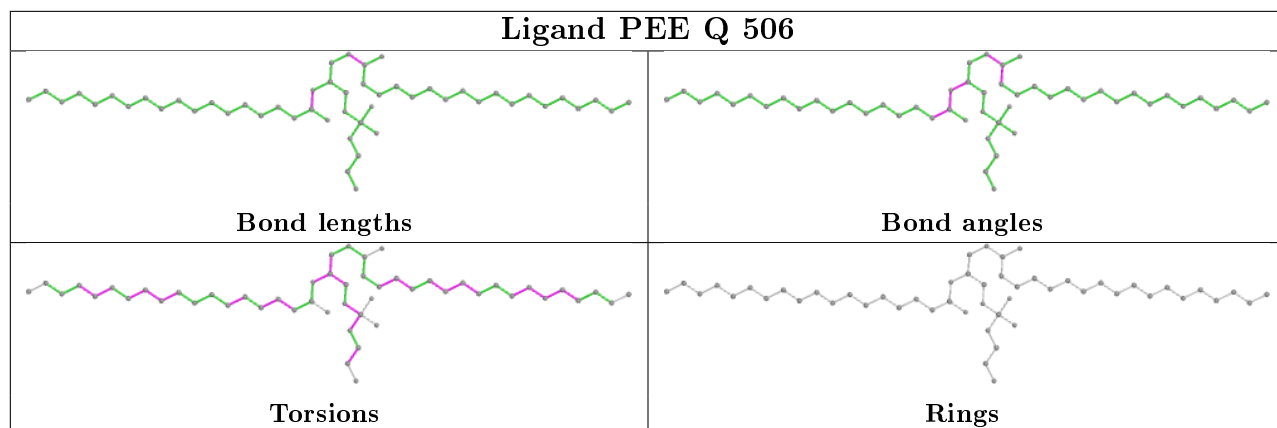
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

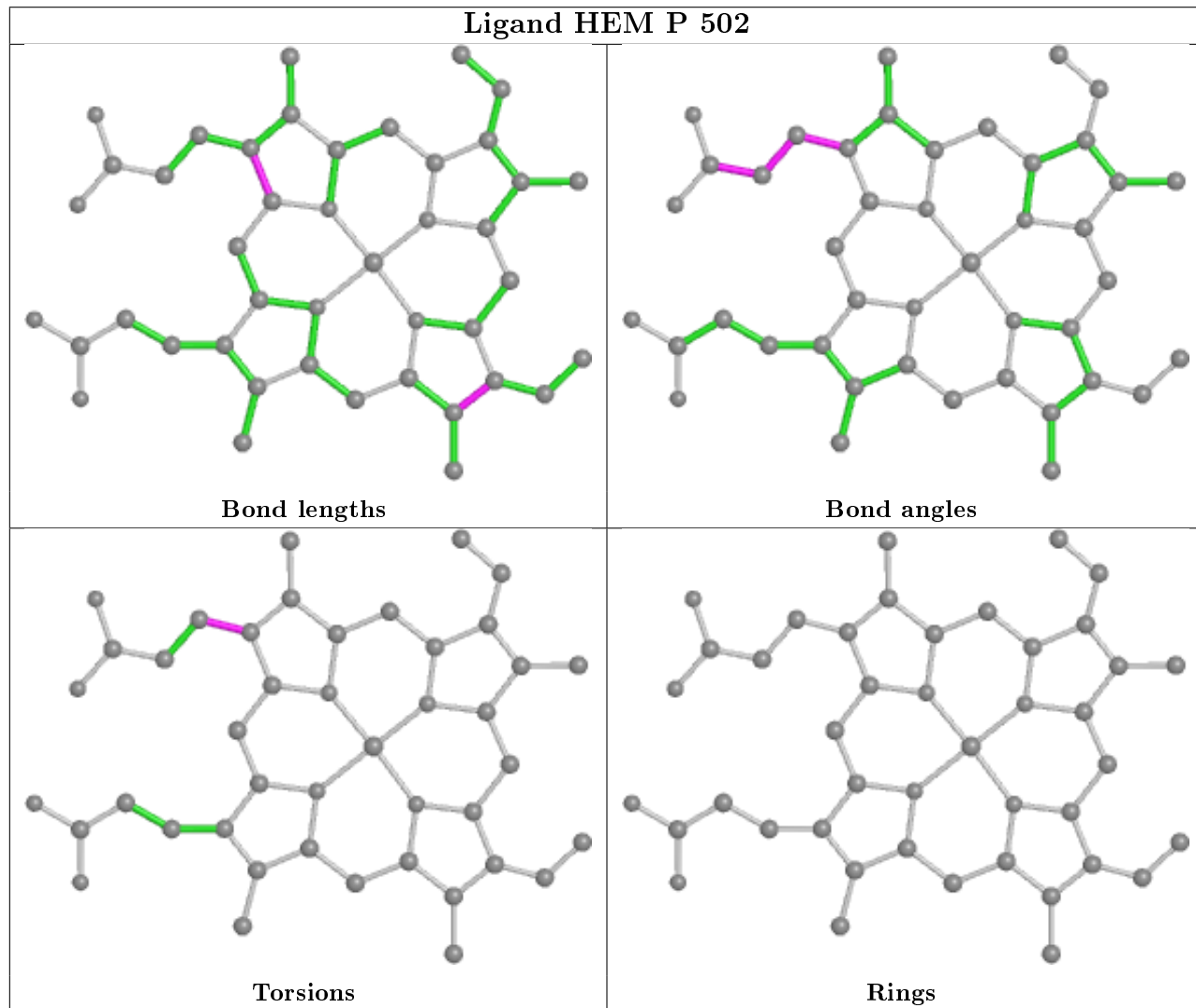
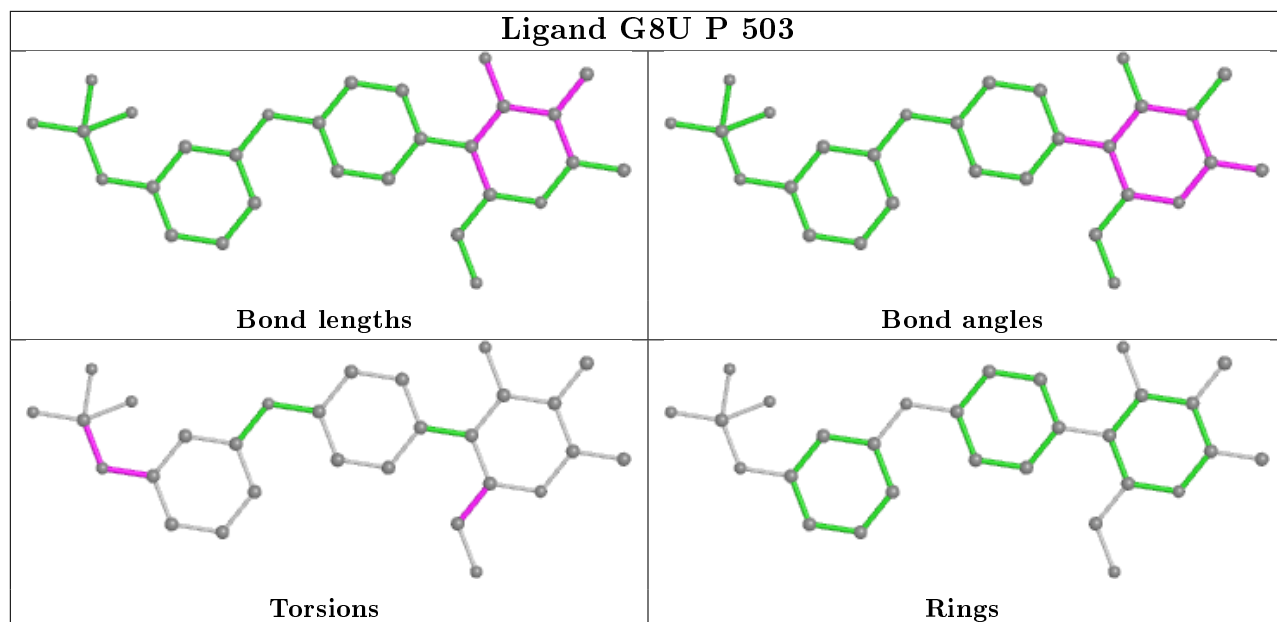


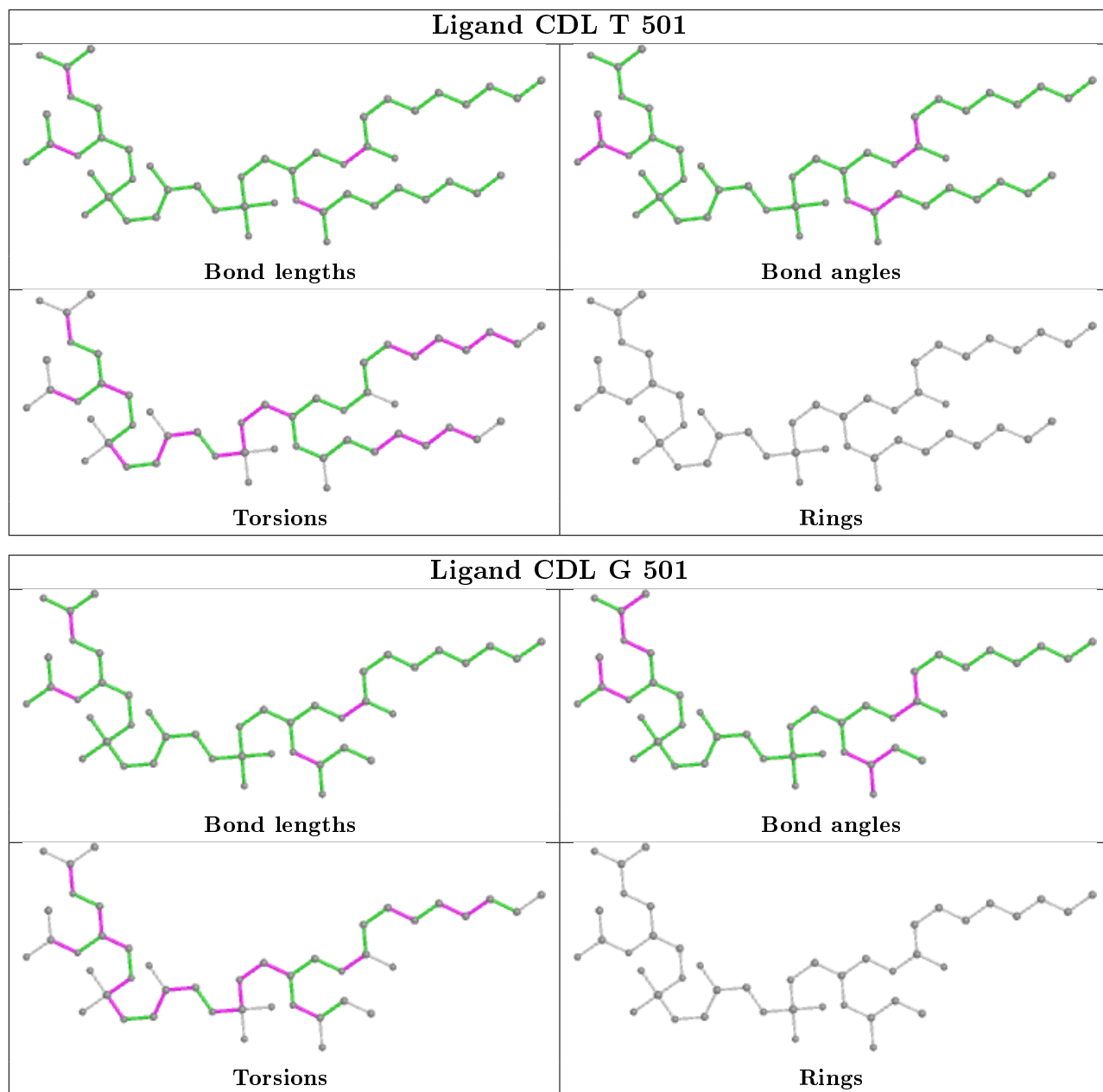




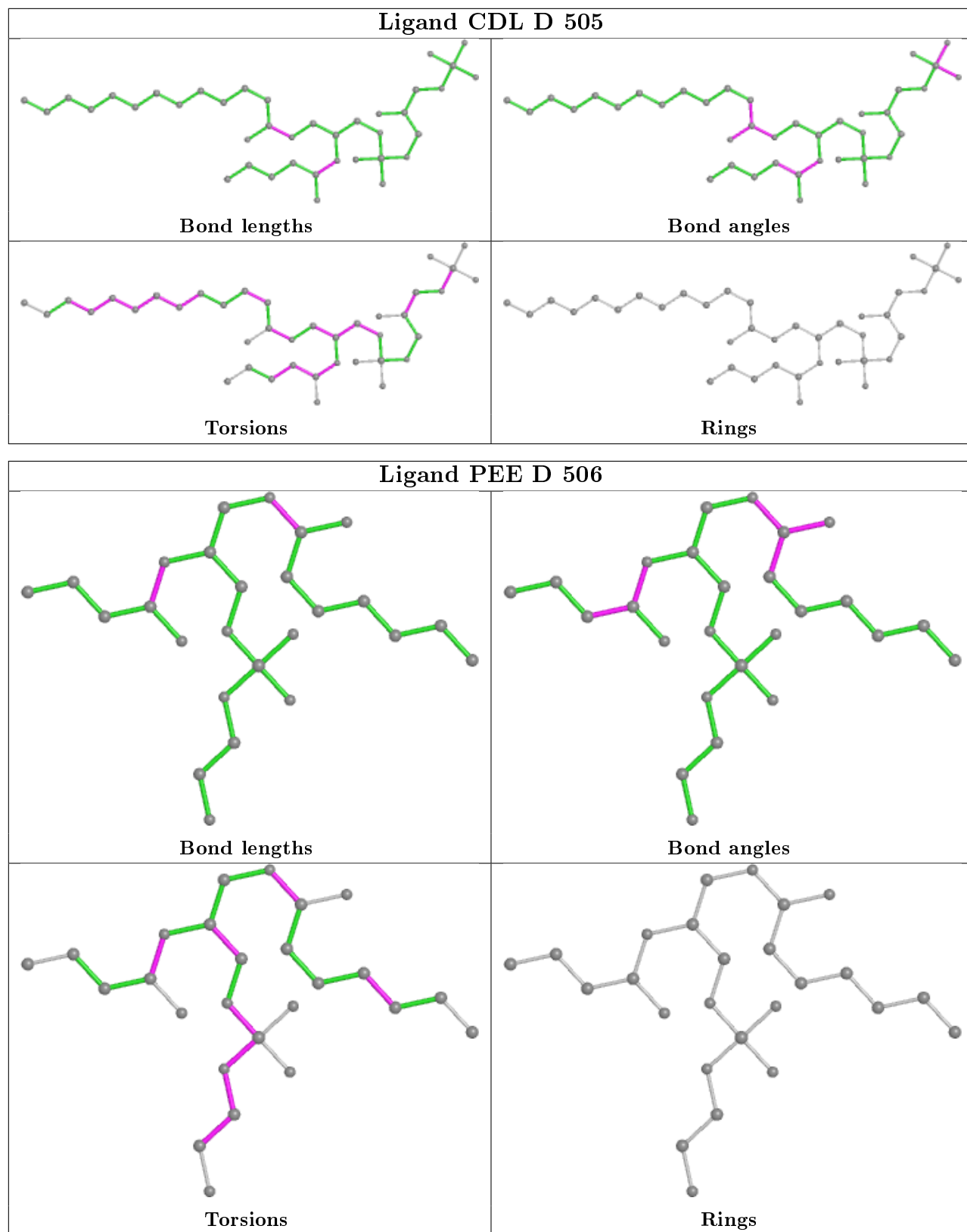












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
10	N	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	N	444:LEU	C	445:LYS	N	0.87

## 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%)	-0.06	7 (1%) 72 62	24, 182, 228, 270	0
2	B	422/453 (93%)	0.14	20 (4%) 31 26	126, 187, 223, 271	0
3	C	374/379 (98%)	-0.45	0 100 100	23, 131, 164, 249	0
3	P	370/379 (97%)	-0.39	0 100 100	99, 138, 177, 195	0
4	D	240/325 (73%)	-0.28	0 100 100	119, 149, 186, 210	0
4	Q	241/325 (74%)	-0.17	0 100 100	115, 162, 198, 232	0
5	E	73/274 (26%)	-0.34	0 100 100	123, 155, 194, 211	0
5	I	27/274 (9%)	0.29	1 (3%) 41 33	168, 214, 255, 306	0
5	R	196/274 (71%)	0.07	10 (5%) 28 24	30, 190, 238, 288	0
6	F	98/111 (88%)	-0.34	1 (1%) 82 74	121, 153, 190, 200	0
6	S	99/111 (89%)	-0.50	0 100 100	117, 148, 182, 208	0
7	G	80/82 (97%)	-0.23	2 (2%) 57 47	30, 149, 204, 273	0
7	T	74/82 (90%)	-0.26	0 100 100	114, 156, 198, 212	0
8	H	65/91 (71%)	-0.17	0 100 100	130, 160, 190, 202	0
8	U	66/91 (72%)	-0.35	1 (1%) 73 63	161, 190, 238, 284	0
9	J	58/64 (90%)	0.08	1 (1%) 70 60	131, 158, 191, 222	0
9	W	59/64 (92%)	-0.02	1 (1%) 70 60	115, 150, 186, 198	0
10	N	444/480 (92%)	-0.15	0 100 100	24, 162, 208, 261	0
11	O	419/453 (92%)	-0.09	6 (1%) 75 65	30, 176, 212, 247	0
12	V	17/274 (6%)	0.95	2 (11%) 4 5	174, 195, 225, 228	0
All	All	3866/5066 (76%)	-0.16	52 (1%) 77 68	23, 162, 216, 306	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	V	62	ARG	6.6
5	R	118	ARG	4.8
2	B	19	PRO	4.5
2	B	376	GLU	4.2
2	B	232	LEU	4.2
5	R	86	ASN	4.0
2	B	280	GLY	3.8
5	R	87	MET	3.6
11	O	232	LEU	3.5
2	B	21	PRO	3.5
12	V	77	ARG	3.3
7	G	76	ALA	3.3
2	B	18	PRO	3.2
11	O	231	GLY	3.1
5	R	180	LEU	3.1
5	R	98	VAL	3.0
2	B	313	ASN	2.9
2	B	274	VAL	2.8
5	R	181	GLU	2.7
11	O	227	ARG	2.6
7	G	75	ALA	2.6
11	O	233	SER	2.6
2	B	311	ALA	2.5
2	B	23	ASP	2.5
5	R	119	ASP	2.5
5	R	177	PRO	2.5
9	J	15	ARG	2.5
5	R	135	LEU	2.4
11	O	234	GLY	2.4
1	A	225	GLU	2.4
1	A	62	LEU	2.4
2	B	324	PHE	2.4
2	B	256	ALA	2.4
8	U	78	LYS	2.3
2	B	20	HIS	2.3
2	B	233	SER	2.3
2	B	276	GLN	2.3
1	A	370	ASP	2.2
2	B	426	ALA	2.2
9	W	2	ALA	2.2
1	A	177	LEU	2.2
2	B	391	SER	2.2
2	B	343	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	360	ALA	2.2
11	O	376	GLU	2.1
1	A	129	LYS	2.1
2	B	278	VAL	2.1
1	A	23	LEU	2.1
5	R	140	THR	2.1
1	A	226	ASP	2.1
6	F	14	GLU	2.0
5	I	71	ASN	2.0

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

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

## 6.3 Carbohydrates [\(i\)](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [\(i\)](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

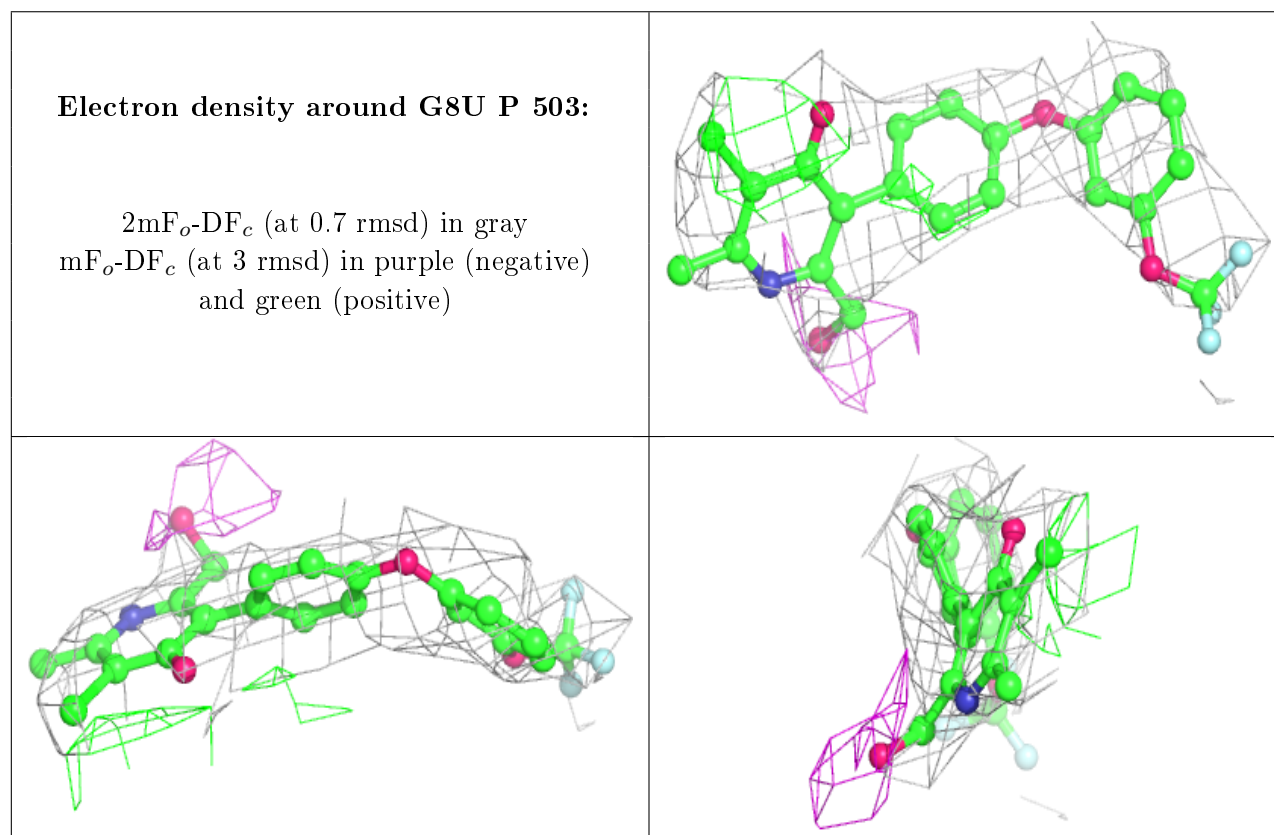
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
15	PO4	D	504	5/5	0.26	0.50	246,252,254,257	0
15	PO4	S	501	5/5	0.40	0.52	268,268,275,278	0
15	PO4	F	501	5/5	0.45	0.58	251,252,258,259	0
15	PO4	N	501	5/5	0.52	0.58	155,167,169,176	0
15	PO4	D	502	5/5	0.64	0.39	234,240,241,242	0
20	GOL	R	502	6/6	0.64	1.37	215,221,224,225	0
15	PO4	D	503	5/5	0.66	1.20	212,225,230,231	0
14	G8U	P	503	29/29	0.69	0.50	125,164,212,219	0
14	G8U	C	503	29/29	0.74	0.67	128,171,211,230	0
15	PO4	E	501	5/5	0.79	0.29	142,147,152,152	0
16	PEE	Q	506	51/51	0.80	0.55	125,148,166,171	0
15	PO4	C	504	5/5	0.80	0.35	156,159,161,168	0
18	CDL	D	505	39/100	0.81	0.37	112,152,165,174	0
18	CDL	Q	505	39/100	0.86	0.38	116,140,173,174	0

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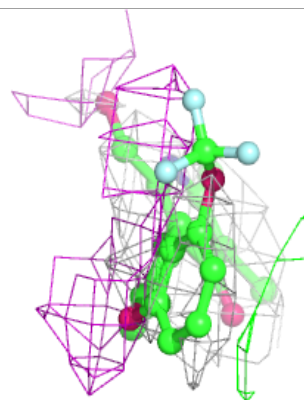
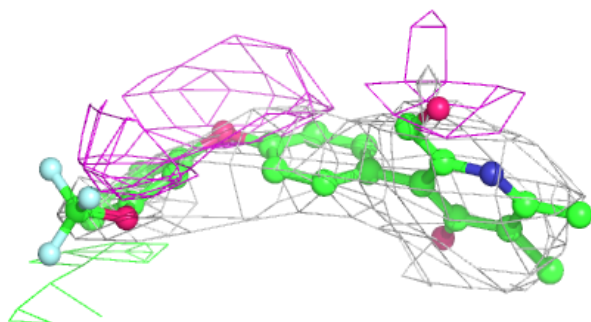
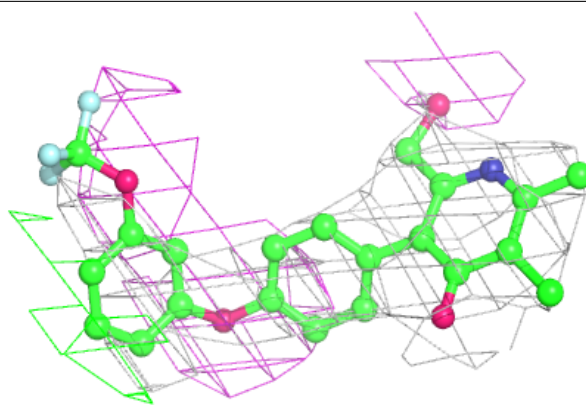
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
15	PO4	P	504	5/5	0.86	0.49	159,166,173,174	0
16	PEE	D	506	26/51	0.88	0.43	124,151,176,178	0
16	PEE	C	505	49/51	0.89	0.43	113,144,173,183	0
18	CDL	G	501	44/100	0.90	0.29	111,137,175,179	0
18	CDL	T	501	49/100	0.91	0.29	111,152,190,204	0
16	PEE	P	505	49/51	0.92	0.40	129,146,172,180	0
19	FES	R	501	4/4	0.94	0.10	200,213,218,224	0
17	HEC	D	501	43/43	0.96	0.30	125,134,153,161	0
17	HEC	Q	501	43/43	0.96	0.37	119,145,161,164	0
13	HEM	P	501	43/43	0.98	0.30	113,130,145,151	0
13	HEM	C	501	43/43	0.98	0.33	110,118,132,142	0
13	HEM	P	502	43/43	0.98	0.34	100,107,130,132	0
13	HEM	C	502	43/43	0.98	0.36	96,108,120,147	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.

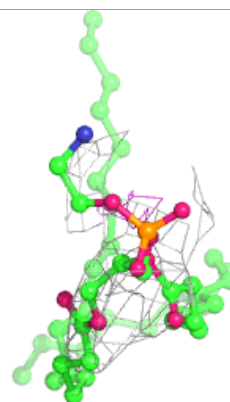
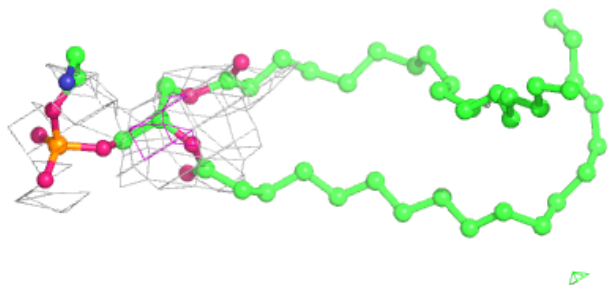
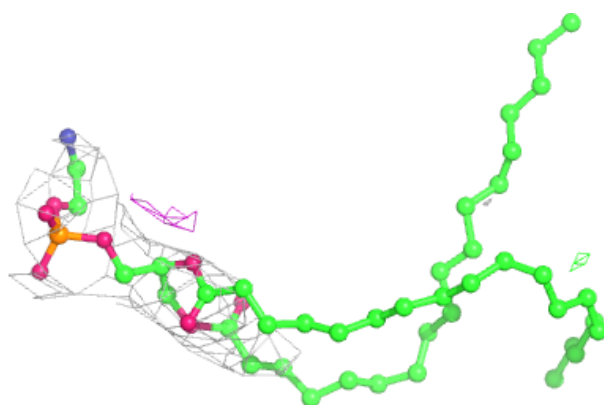


**Electron density around G8U C 503:**

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

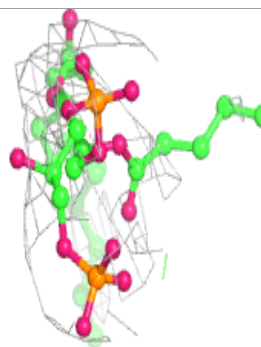
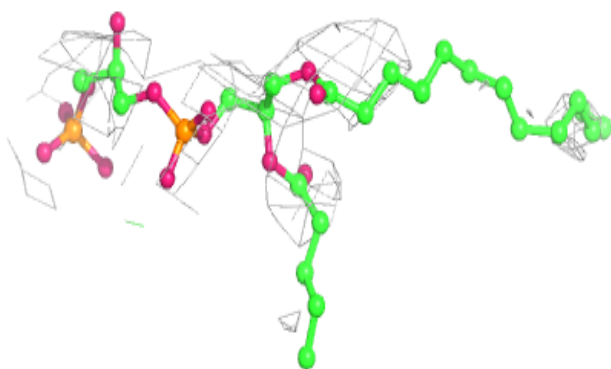
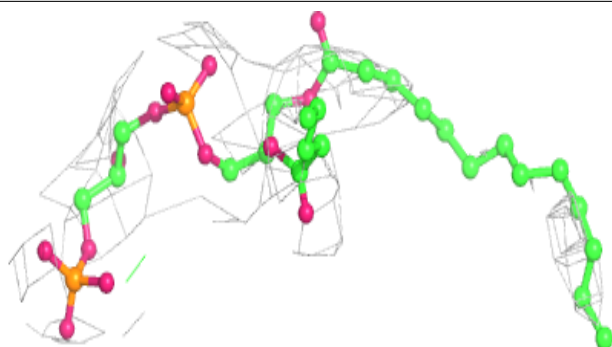
**Electron density around PEE Q 506:**

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and green (positive)

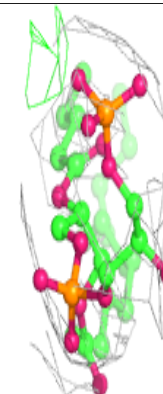
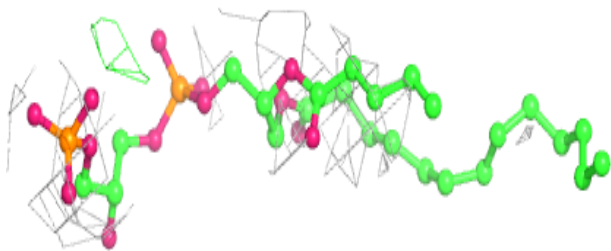
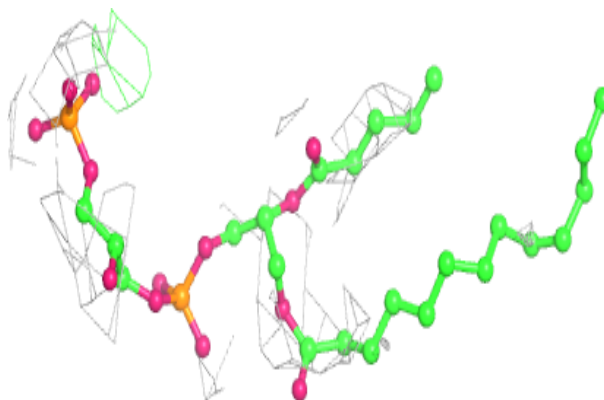


**Electron density around CDL D 505:**

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

**Electron density around CDL Q 505:**

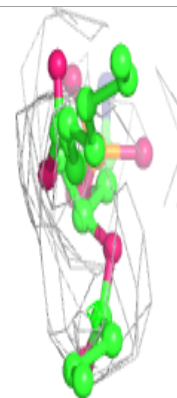
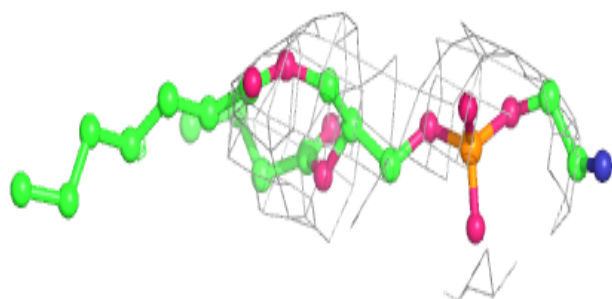
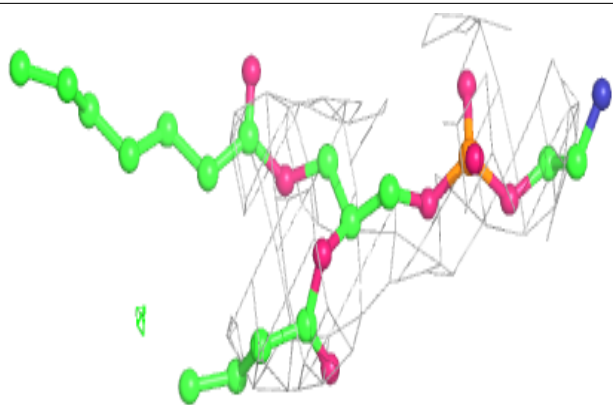
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



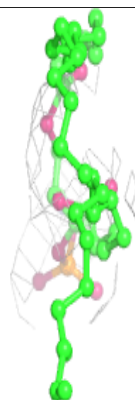
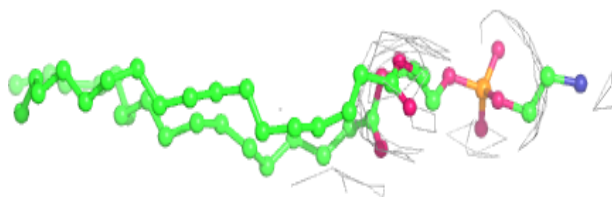
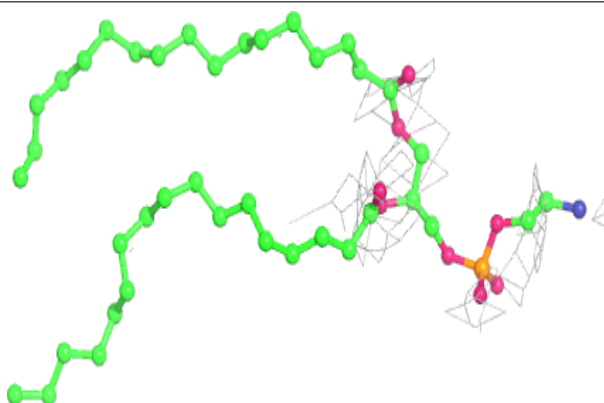


**Electron density around PEE D 506:**

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

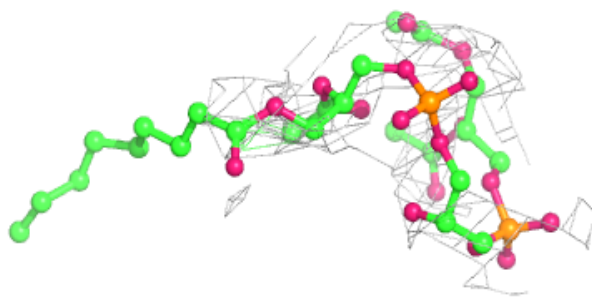
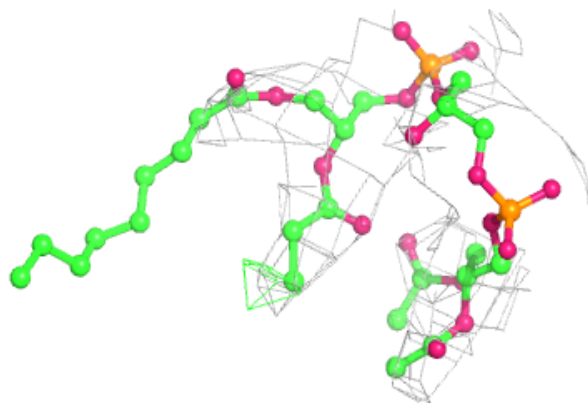
**Electron density around PEE C 505:**

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

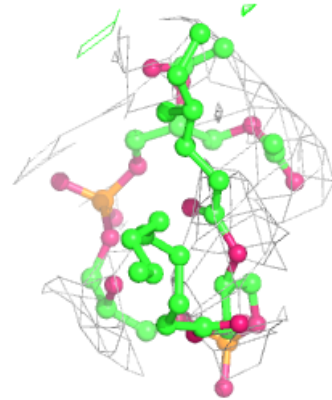
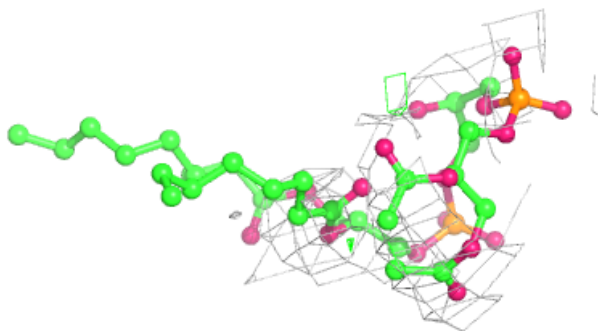
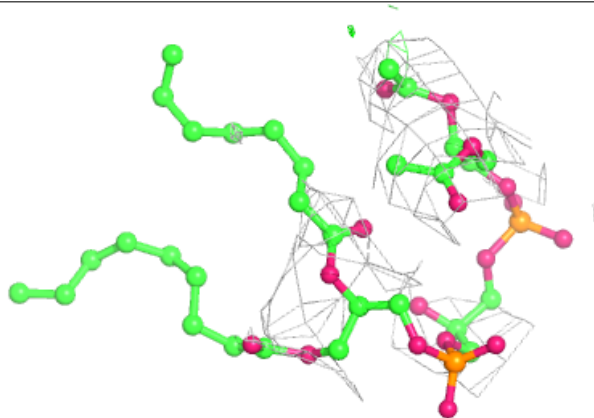


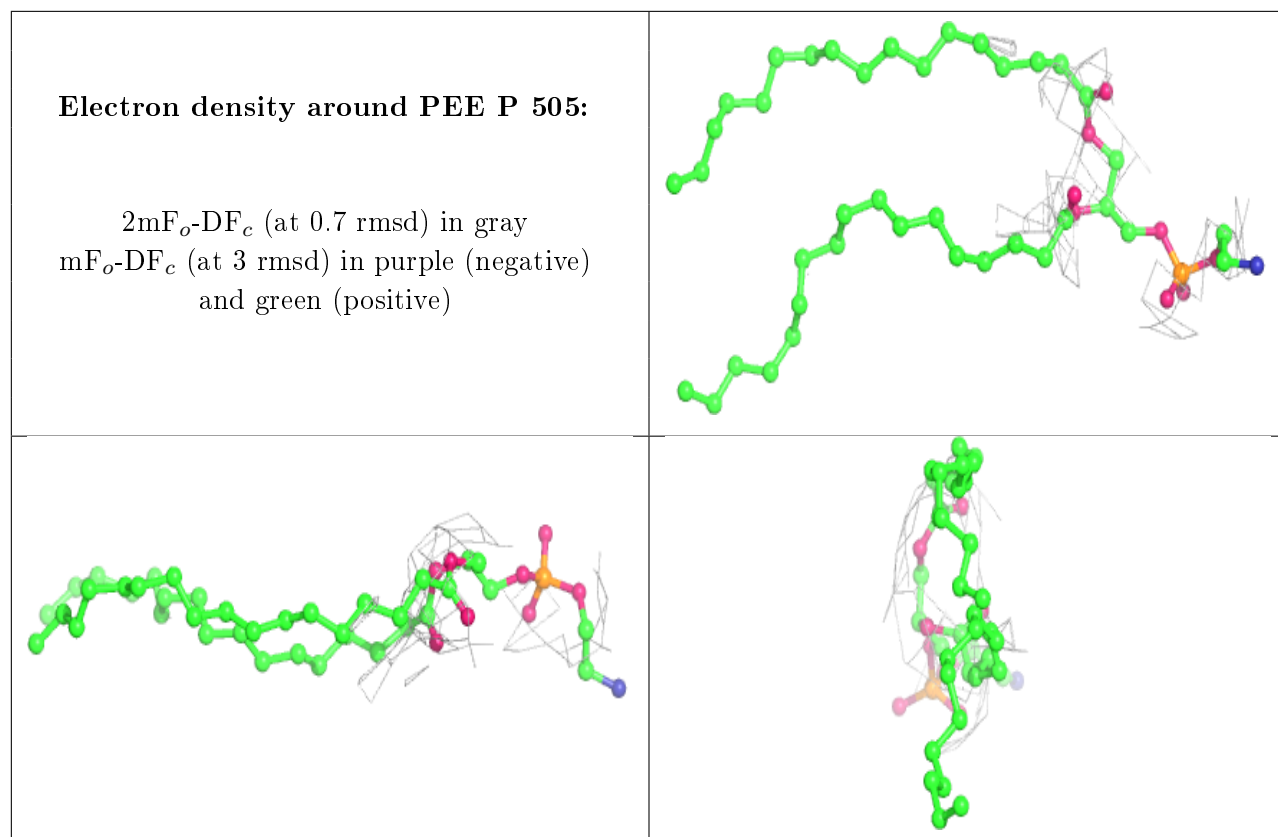
**Electron density around CDL G 501:**

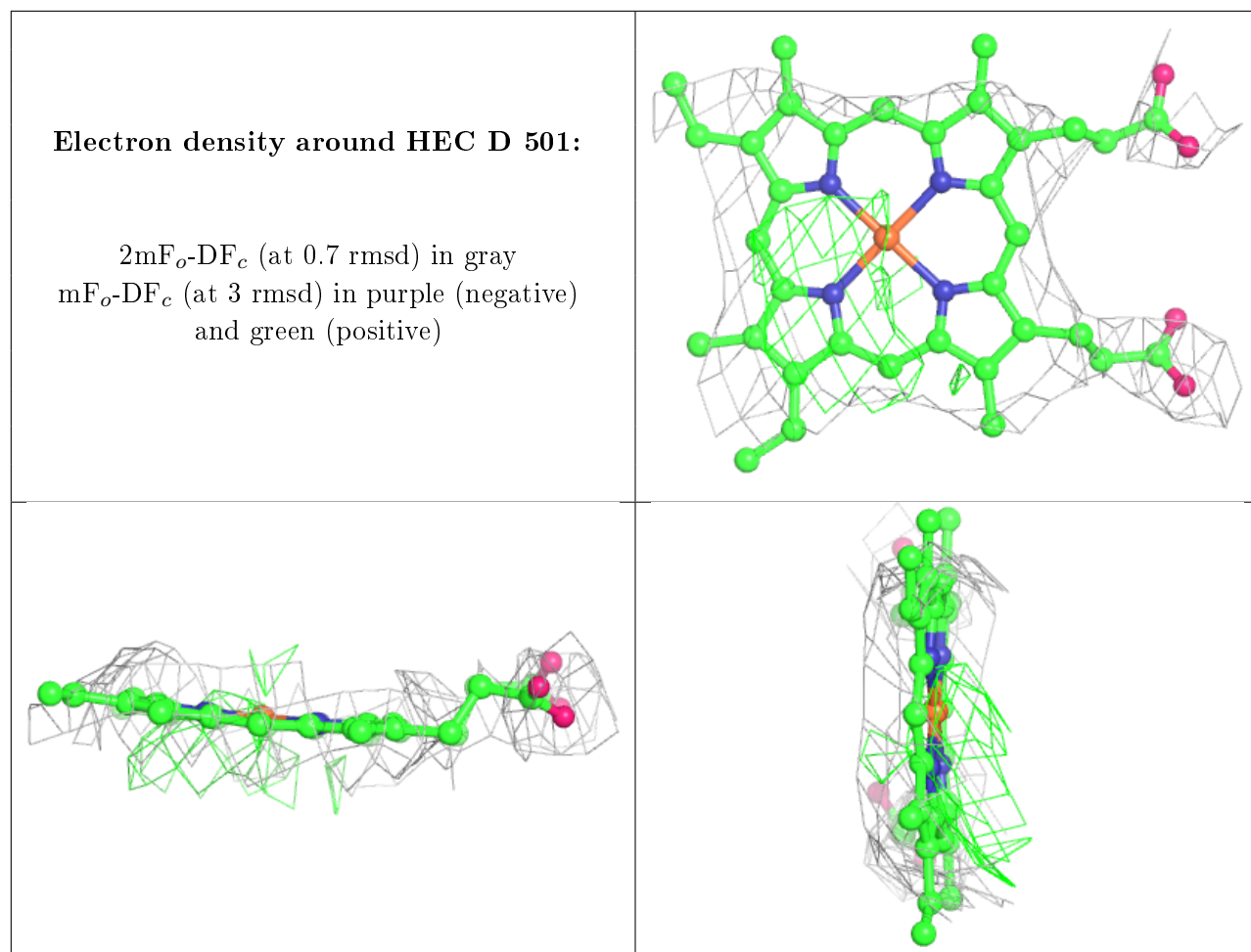
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

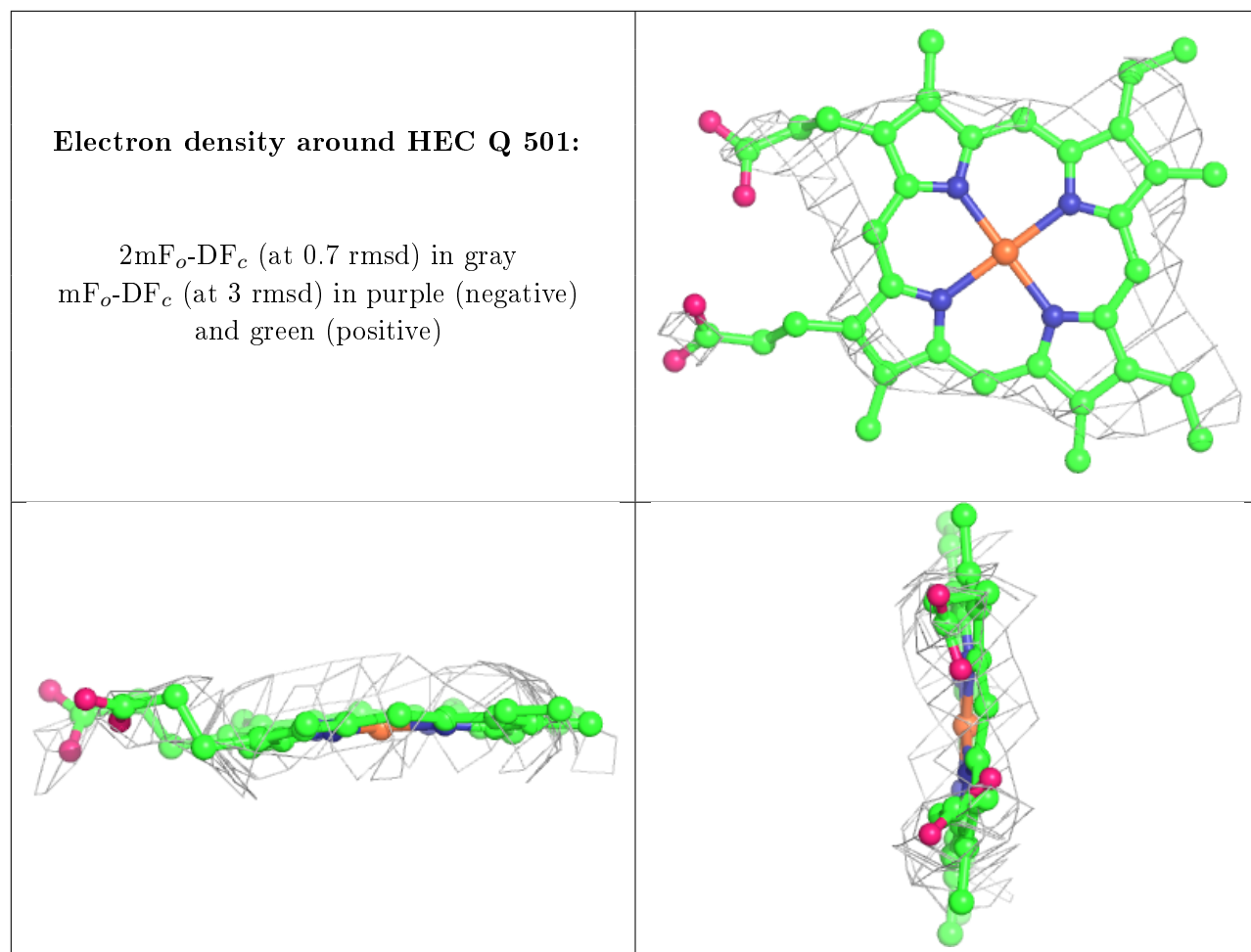
**Electron density around CDL T 501:**

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



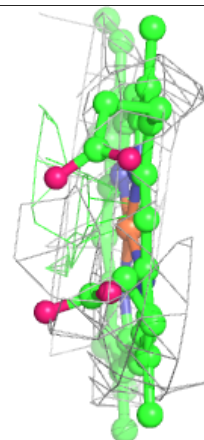
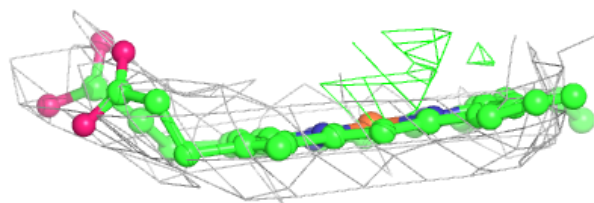
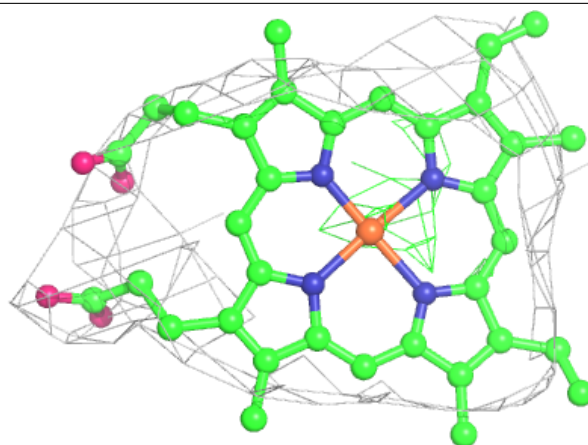


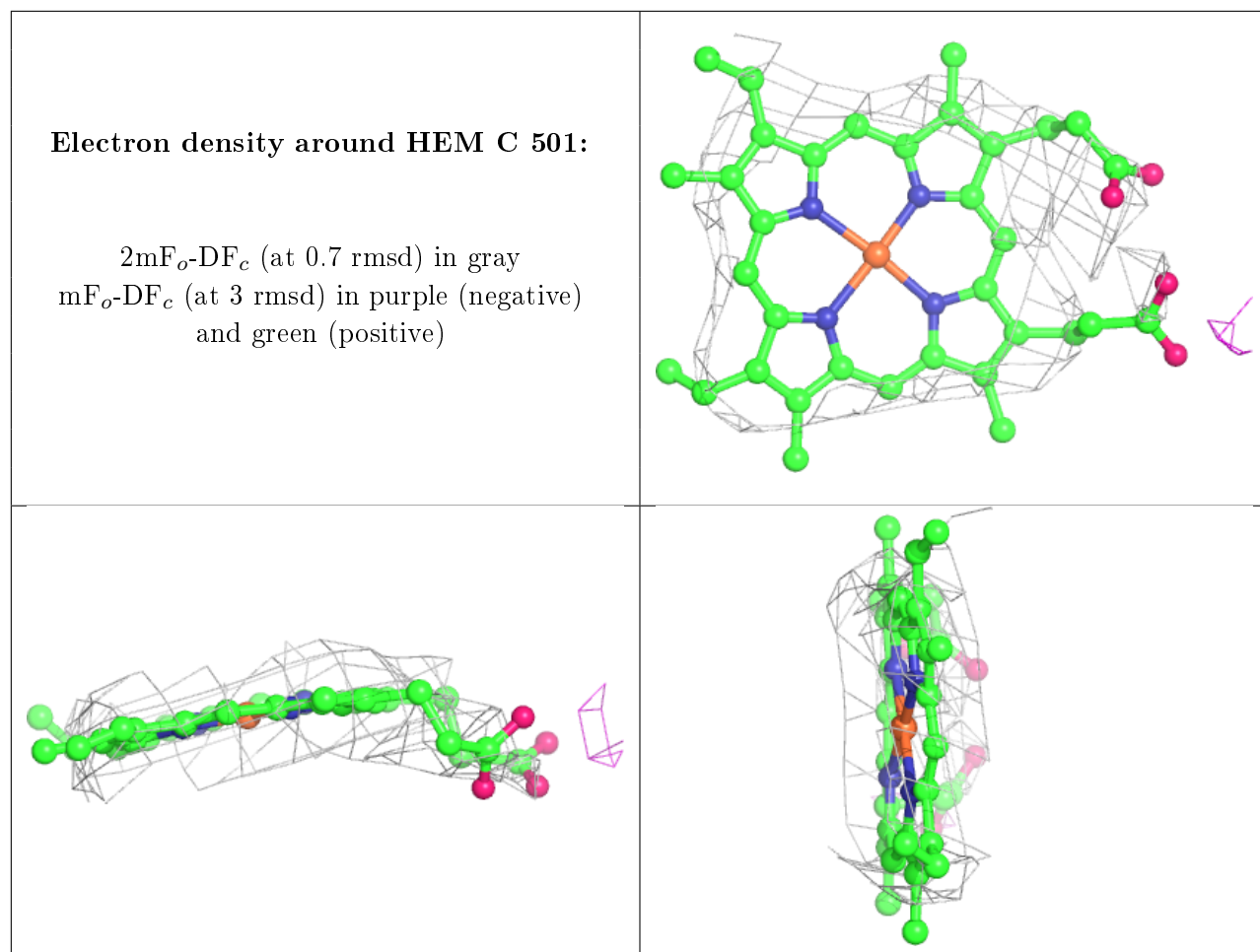




**Electron density around HEM P 501:**

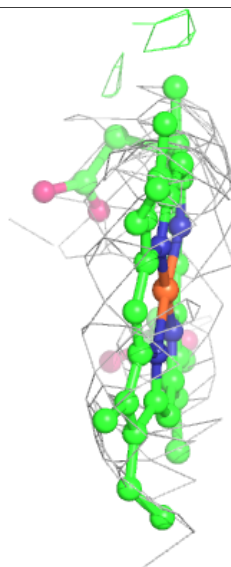
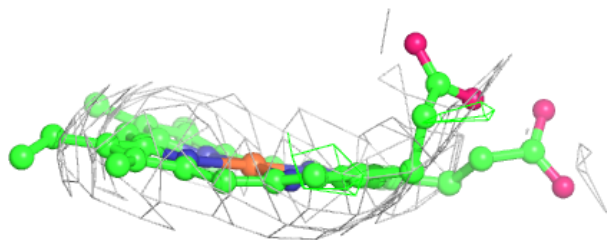
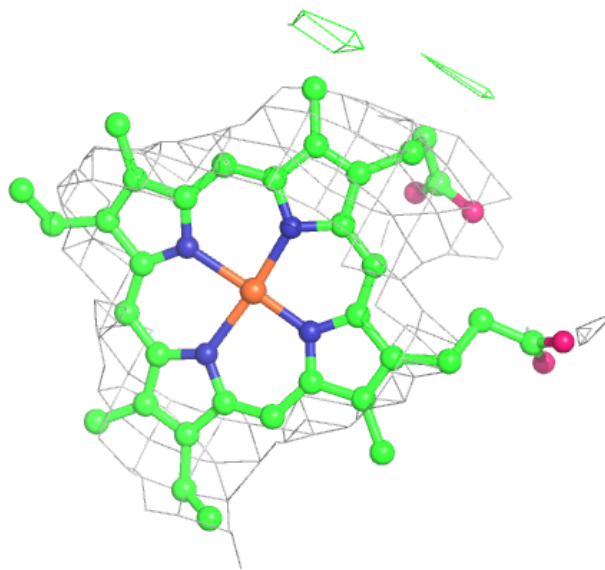
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



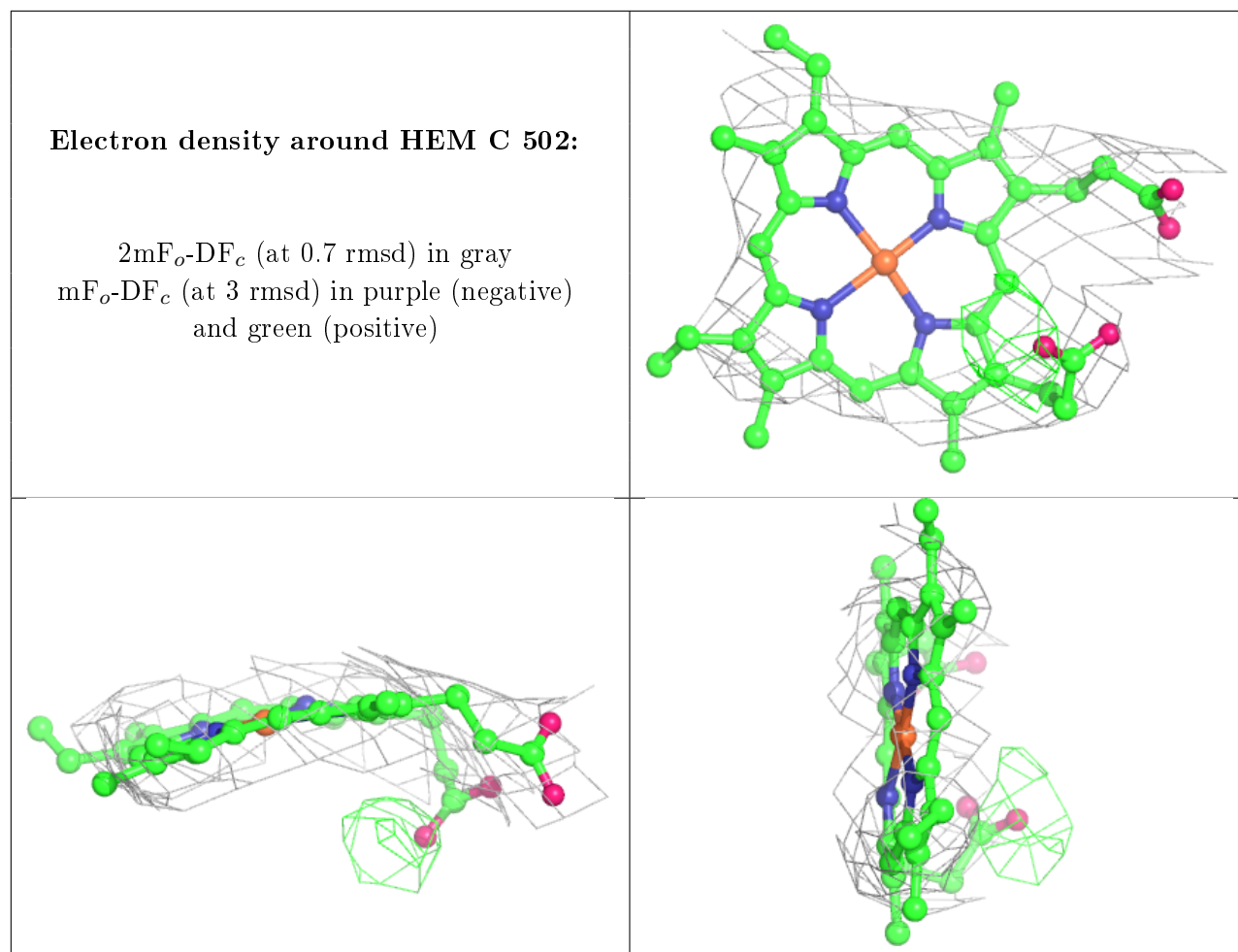


**Electron density around HEM P 502:**

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







## 6.5 Other polymers [i](#)

There are no such residues in this entry.