



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:02 PM UTC

PDB ID : 4D6U / pdb_00004d6u
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

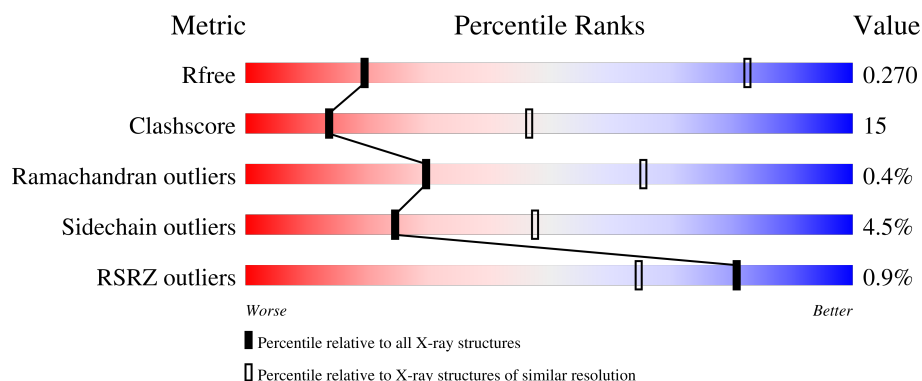
1 Overall quality at a glance

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}	180053	1243 (4.40-3.80)
Clashscore	190562	1293 (4.40-3.80)
Ramachandran outliers	187476	1206 (4.40-3.80)
Sidechain outliers	187428	1193 (4.40-3.80)
RSRZ outliers	180081	1240 (4.40-3.80)

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

Mol	Chain	Length	Quality of chain
1	A	480	
2	B	453	
3	C	379	
3	P	379	
4	D	325	

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Mol	Chain	Length	Quality of chain
4	Q	325	
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	-
14	G8U	P	503	-	-	X	-
16	PEE	C	505	X	-	-	-
16	PEE	D	506	X	-	-	-
16	PEE	P	505	X	-	-	-
16	PEE	Q	506	X	-	-	-
19	FES	R	501	-	-	X	-

2 Entry composition

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
1	A	444	Total	C	N	O	S	0	0	0
			3439	2148	607	664	20			

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

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

- Molecule 3 is a protein called CYTOCHROME B.

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

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

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

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

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

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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
9	W	59	Total	C	N	O	0	0	0
			487	320	84	83			

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

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

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
11	O	419	Total	C	N	O	S	0	0	0
			3140	1972	555	606	7			

There is a discrepancy between the modelled and reference sequences:

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

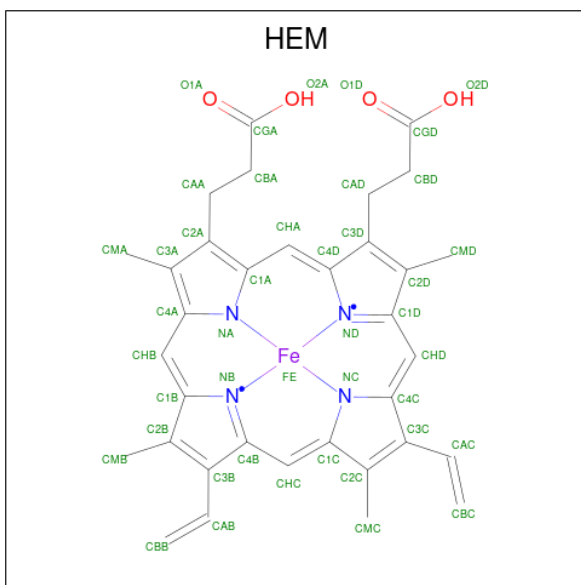
- Molecule 12 is a protein called CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL.

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

There is a discrepancy between the modelled and reference sequences:

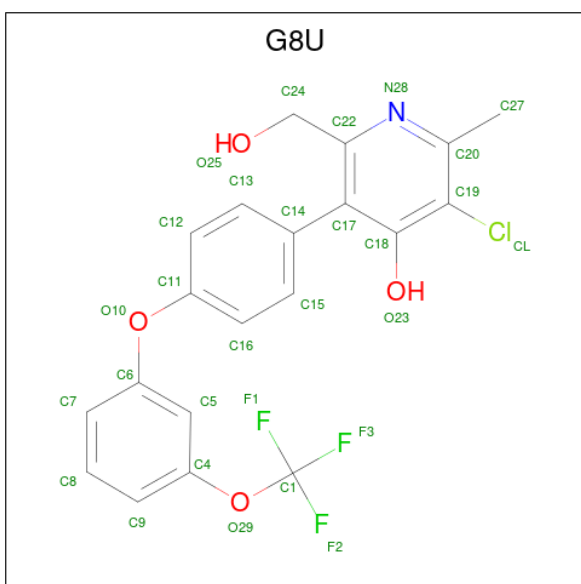
Chain	Residue	Modelled	Actual	Comment	Reference
V	64	VAL	LEU	conflict	UNP P13272

- Molecule 13 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



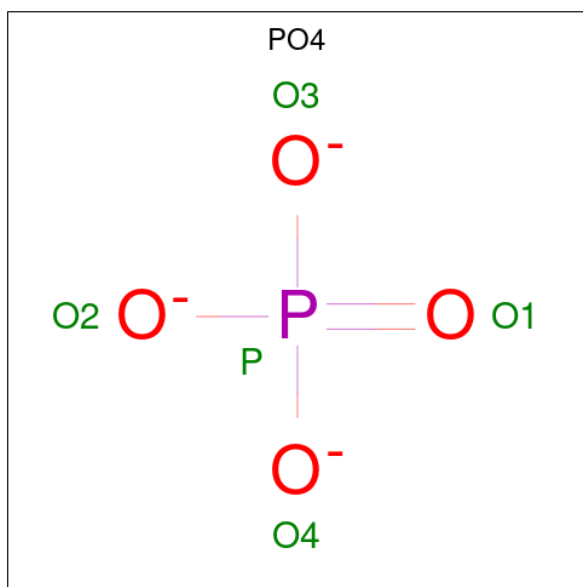
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
13	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
13	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
13	P	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 14 is 3-chloro-6-(hydroxymethyl)-2-methyl-5-{4-[3-(trifluoromethoxy)phenoxy]phenyl}pyridin-4-ol (CCD ID: G8U) (formula: $\text{C}_{20}\text{H}_{15}\text{ClF}_3\text{NO}_4$).



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

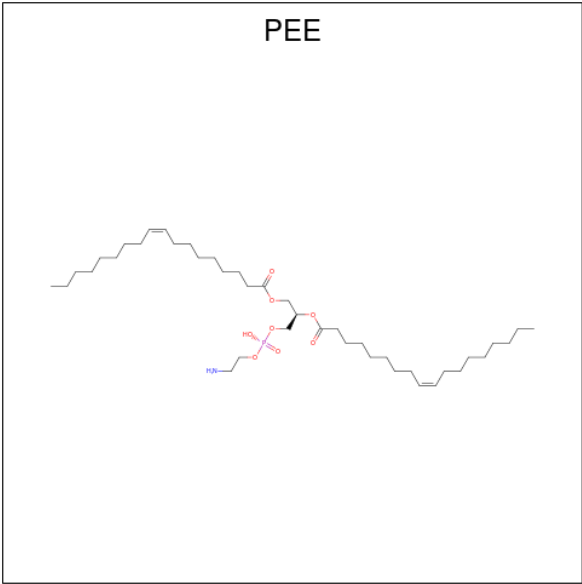
- Molecule 15 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

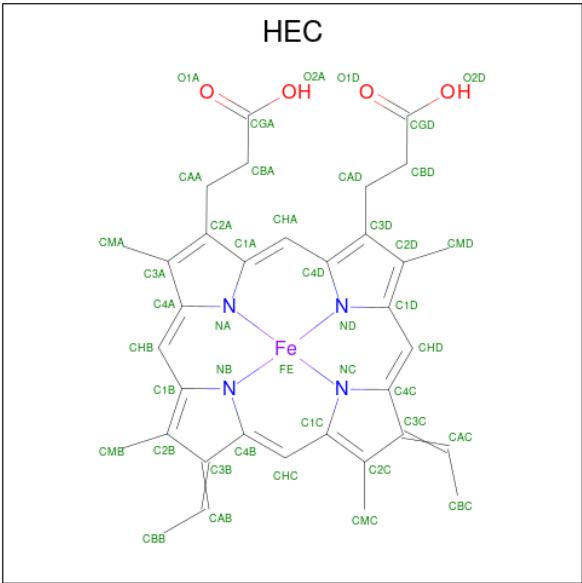
- Molecule 16 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula:

C₄₁H₇₈NO₈P).



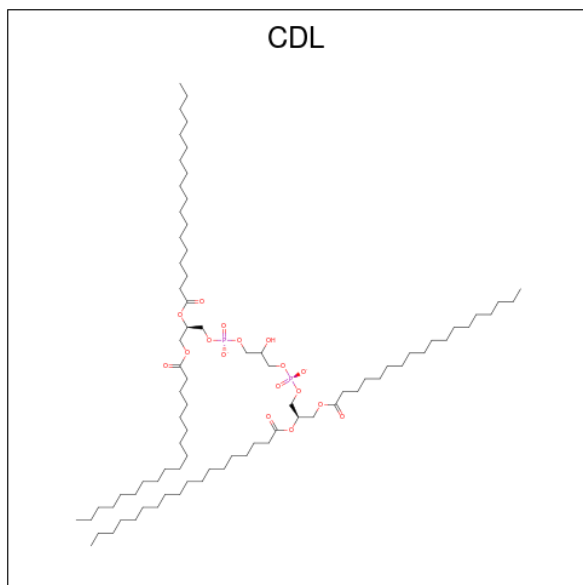
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
16	D	1	Total	C	N	O	P	0	0
			26	16	1	8	1		
16	P	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
16	Q	1	Total	C	N	O	P	0	0
			51	41	1	8	1		

- Molecule 17 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄).



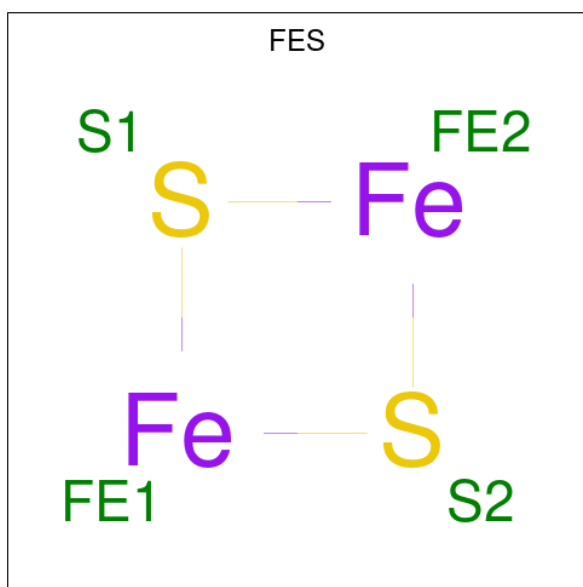
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	
17	Q	1	Total	C	Fe	N	O	
			43	34	1	4	4	

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



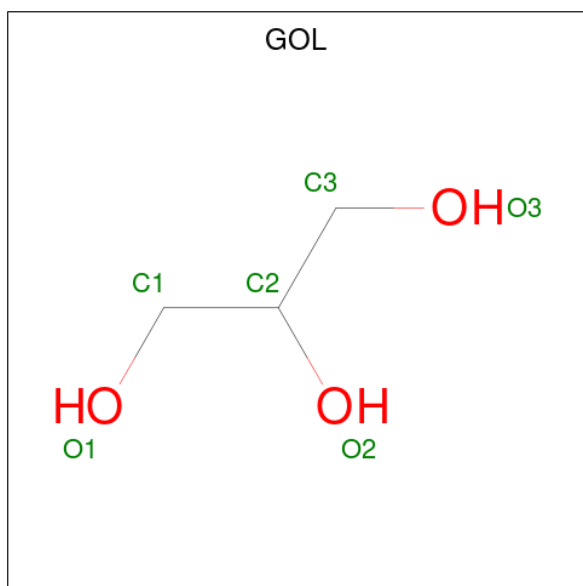
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	D	1	Total	C	O	P		
			39	24	13	2	0	0
18	G	1	Total	C	O	P		
			44	25	17	2	0	0
18	Q	1	Total	C	O	P		
			39	24	13	2	0	0
18	T	1	Total	C	O	P		
			49	30	17	2	0	0

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 20 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

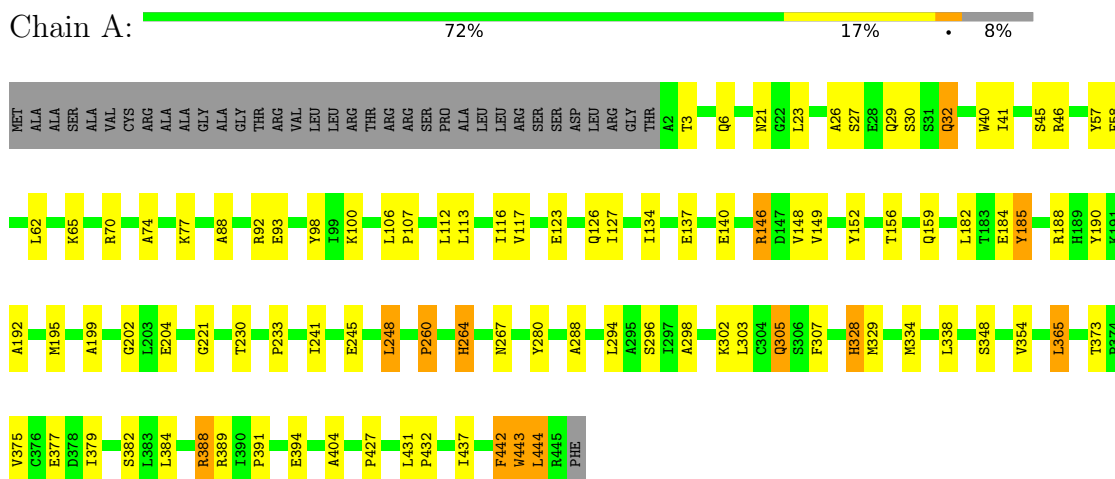


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	R	1	Total	C	O	0	0
			6	3	3		

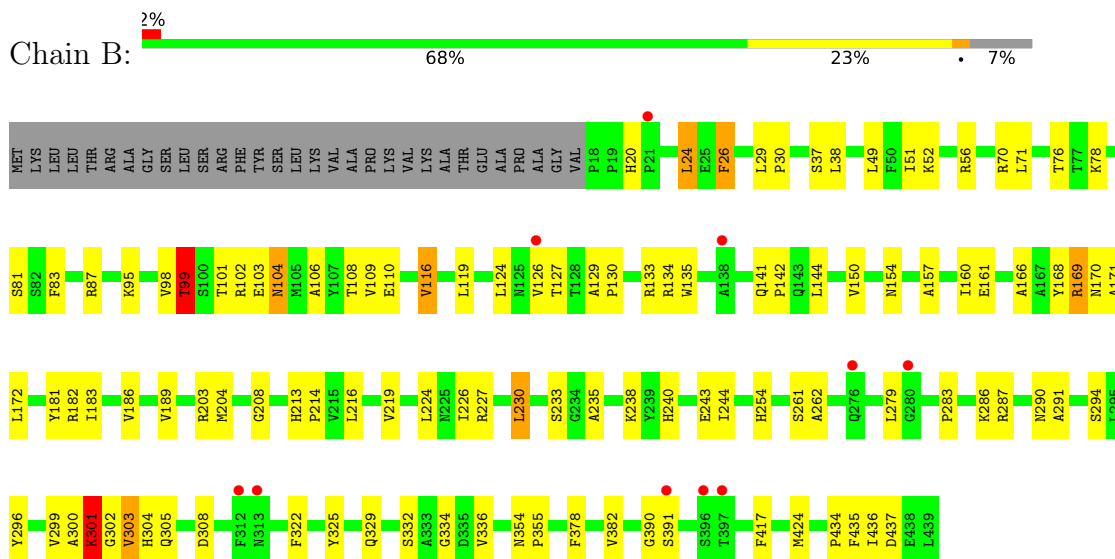
3 Residue-property plots [i](#)

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

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

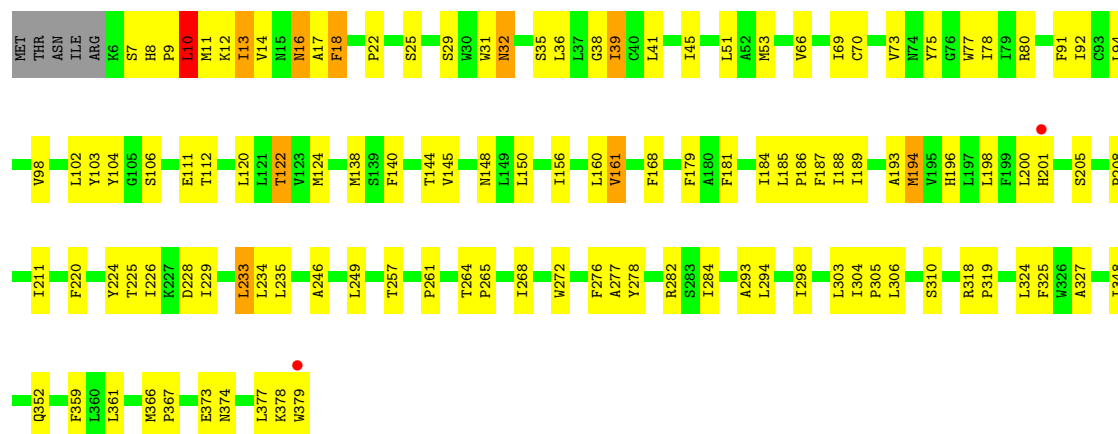


• Molecule 2: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL

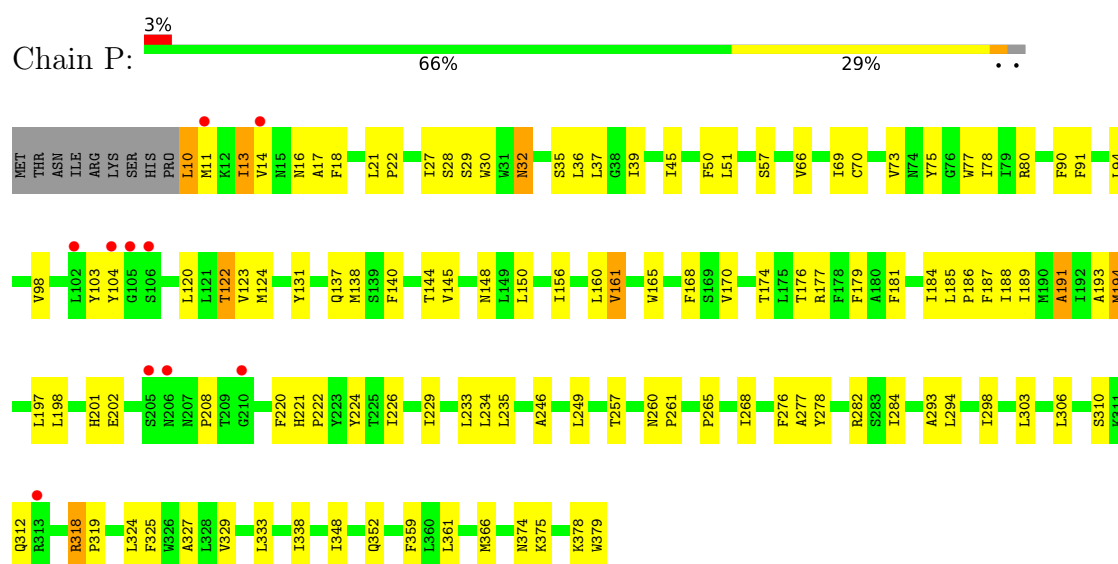


• Molecule 3: CYTOCHROME B

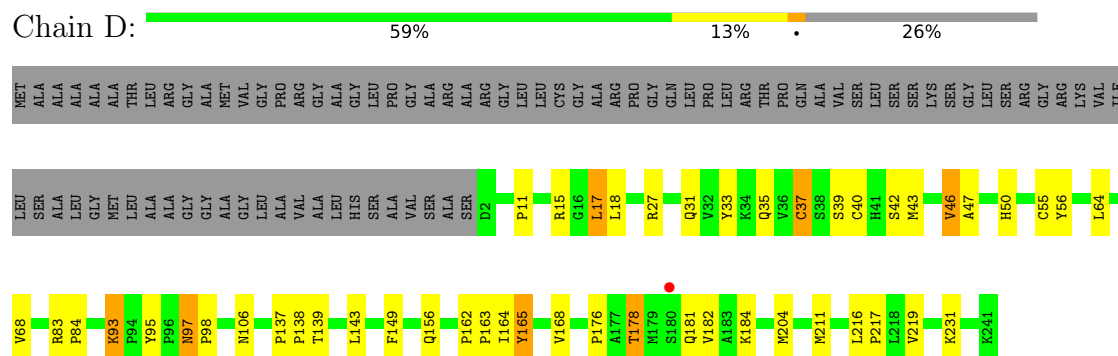




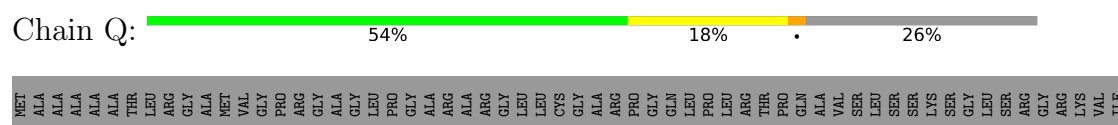
• Molecule 3: CYTOCHROME B

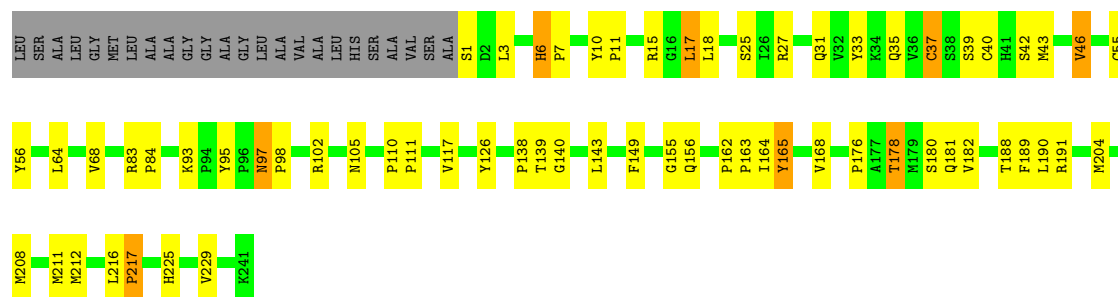


• Molecule 4: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL



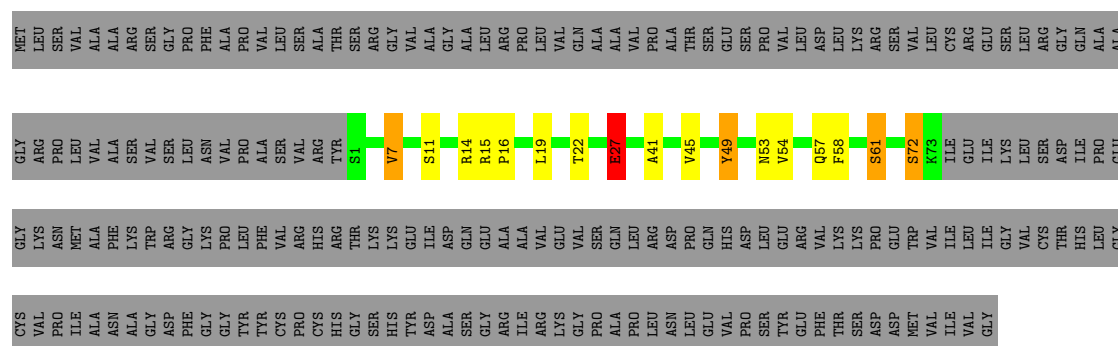
• Molecule 4: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL

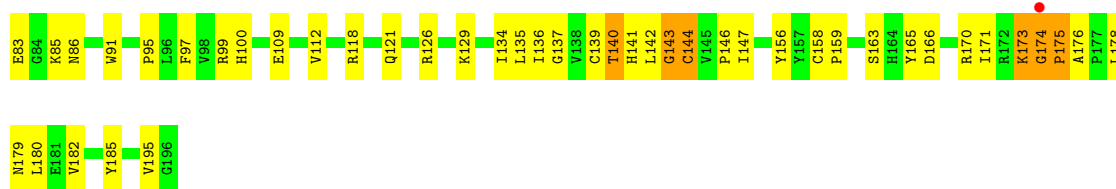




• Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

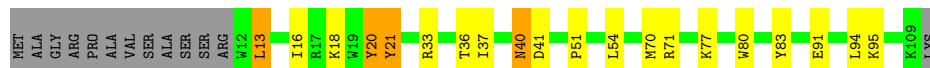
Chain E: 20% 73%





• Molecule 6: CYTOCHROME B-C1 COMPLEX SUBUNIT 7

Chain F: 70% 14% 12%



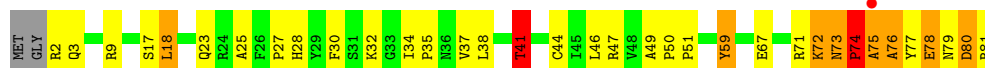
• Molecule 6: CYTOCHROME B-C1 COMPLEX SUBUNIT 7

Chain S: 71% 15% 11%



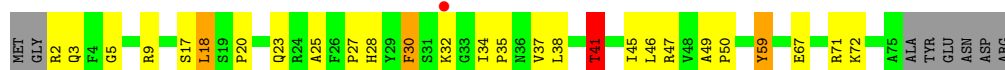
• Molecule 7: CYTOCHROME B-C1 COMPLEX SUBUNIT 8

Chain G: 55% 30% 10%



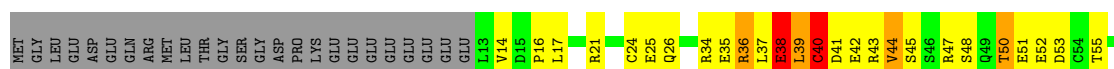
• Molecule 7: CYTOCHROME B-C1 COMPLEX SUBUNIT 8

Chain T: 57% 28% 10%



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

Chain H: 35% 30% 29%



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

Chain U: 40% 22% 7% 27%





• Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT 9

Chain J: 77% 11% 9%



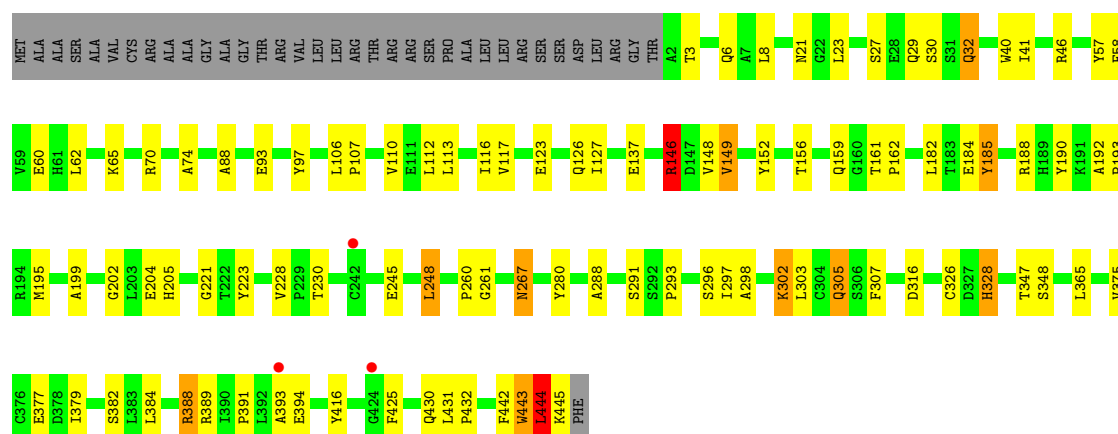
• Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT 9

Chain W: 67% 23% 8%



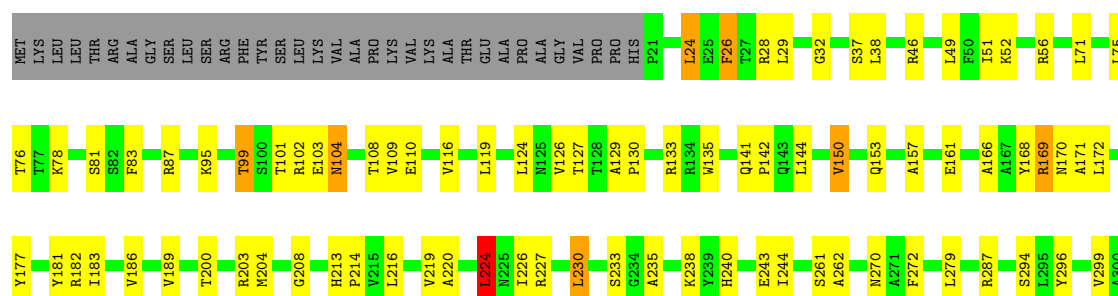
• Molecule 10: CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL

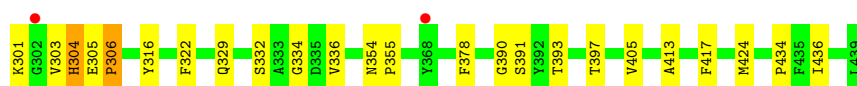
Chain N: 72% 18% 8%



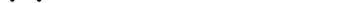
• Molecule 11: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL

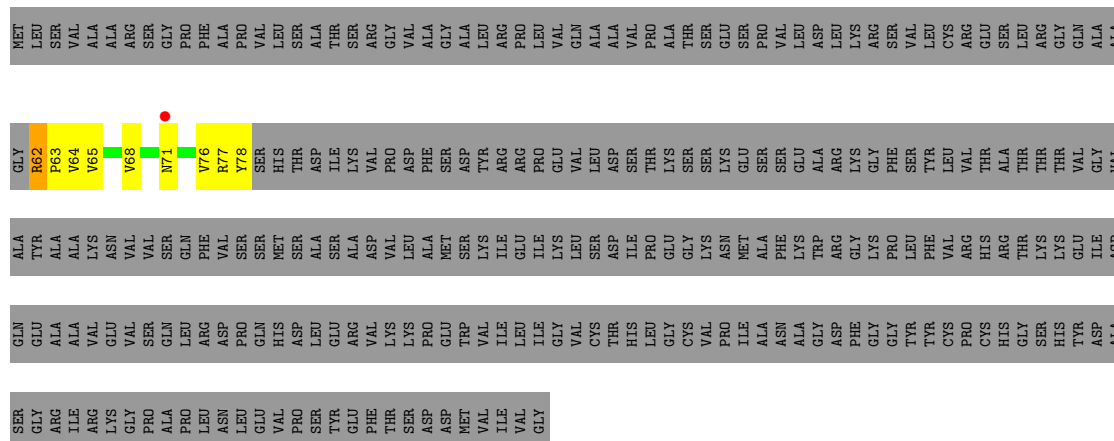
Chain O: 69% 22% 8%





● Molecule 12: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

Chain V:  94%



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	129.49Å 129.49Å 719.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 4.09 50.00 – 4.09	Depositor EDS
% Data completeness (in resolution range)	80.6 (50.00-4.09) 80.6 (50.00-4.09)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.57 (at 4.14Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.223 , 0.271 0.222 , 0.270	Depositor DCC
R_{free} test set	2147 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	123.3	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 156.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.086 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	31080	wwPDB-VP
Average B, all atoms (Å ²)	163.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.62	3/3511 (0.1%)	0.93	10/4766 (0.2%)
2	B	0.78	12/3224 (0.4%)	1.00	16/4375 (0.4%)
3	C	0.70	6/3065 (0.2%)	0.92	4/4196 (0.1%)
3	P	0.67	5/3031 (0.2%)	0.91	5/4150 (0.1%)
4	D	0.66	5/1971 (0.3%)	0.90	3/2676 (0.1%)
4	Q	0.65	4/1977 (0.2%)	0.91	7/2684 (0.3%)
5	E	0.97	5/557 (0.9%)	0.96	2/752 (0.3%)
5	I	0.95	0/196	1.45	4/263 (1.5%)
5	R	0.71	5/1552 (0.3%)	1.07	11/2100 (0.5%)
6	F	0.73	4/879 (0.5%)	0.89	0/1180
6	S	0.71	3/888 (0.3%)	0.86	1/1191 (0.1%)
7	G	0.90	5/699 (0.7%)	1.75	10/946 (1.1%)
7	T	0.82	3/645 (0.5%)	0.93	2/873 (0.2%)
8	H	0.99	2/534 (0.4%)	1.45	9/718 (1.3%)
8	U	1.00	4/543 (0.7%)	1.38	8/729 (1.1%)
9	J	0.70	1/495 (0.2%)	0.83	0/667
9	W	0.64	0/500	0.86	2/675 (0.3%)
10	N	0.82	2/3501 (0.1%)	0.94	13/4752 (0.3%)
11	O	0.71	9/3197 (0.3%)	0.90	6/4336 (0.1%)
12	V	0.95	1/129 (0.8%)	1.37	3/177 (1.7%)
All	All	0.74	79/31094 (0.3%)	0.99	116/42206 (0.3%)

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 (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	N	444	LEU	C-N	-32.90	0.87	1.33
2	B	169	ARG	CZ-NH1	14.43	1.52	1.32
4	D	93	LYS	CE-NZ	12.20	1.85	1.49
5	E	27	GLU	CD-OE1	11.86	1.47	1.25
3	P	194	MET	SD-CE	11.10	2.07	1.79
3	C	194	MET	SD-CE	10.88	2.06	1.79
7	G	74	PRO	N-CD	10.25	1.62	1.47
8	H	55	THR	CB-CG2	-10.19	1.19	1.52
11	O	169	ARG	CZ-NH1	9.70	1.46	1.32
5	E	27	GLU	CD-OE2	9.08	1.42	1.25
8	U	55	THR	CB-CG2	-8.80	1.23	1.52
8	U	50	THR	CB-CG2	-8.75	1.23	1.52
8	H	38	GLU	CD-OE1	8.62	1.41	1.25
7	T	41	THR	CB-OG1	8.23	1.56	1.43
2	B	99	THR	CB-OG1	8.03	1.56	1.43
3	C	10	LEU	CG-CD2	-7.85	1.26	1.52
9	J	4	THR	CB-OG1	7.81	1.56	1.43
2	B	169	ARG	NE-CZ	7.80	1.41	1.33
1	A	388	ARG	CZ-NH1	-7.56	1.22	1.32
2	B	108	THR	CB-CG2	-7.55	1.27	1.52
8	U	38	GLU	CD-OE1	7.35	1.39	1.25
7	G	73	ASN	C-N	7.20	1.41	1.33
7	G	41	THR	CB-OG1	7.19	1.55	1.43
11	O	108	THR	CB-CG2	-6.93	1.29	1.52
11	O	99	THR	CB-OG1	6.76	1.54	1.43
8	U	39	LEU	CG-CD2	6.68	1.74	1.52
2	B	301	LYS	CE-NZ	6.64	1.69	1.49
4	Q	93	LYS	CB-CG	-6.56	1.32	1.52
1	A	146	ARG	CZ-NH1	-6.55	1.23	1.32
5	R	27	GLU	CG-CD	-6.53	1.35	1.52
1	A	302	LYS	CG-CD	-6.09	1.34	1.52
4	D	93	LYS	CB-CG	-6.02	1.34	1.52
6	F	20	TYR	CE2-CZ	-5.99	1.23	1.38
4	D	95	TYR	CE1-CZ	-5.88	1.24	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	49	TYR	CE1-CZ	-5.86	1.24	1.38
2	B	304	HIS	CE1-NE2	5.85	1.38	1.32
2	B	296	TYR	CE1-CZ	-5.76	1.24	1.38
7	T	30	PHE	CG-CD1	-5.69	1.26	1.38
11	O	169	ARG	NE-CZ	5.68	1.39	1.33
10	N	388	ARG	CZ-NH1	-5.66	1.24	1.32
11	O	322	PHE	CG-CD2	-5.66	1.26	1.38
4	D	95	TYR	CG-CD1	-5.65	1.27	1.39
4	Q	95	TYR	CG-CD1	-5.62	1.27	1.39
7	G	30	PHE	CG-CD1	-5.57	1.27	1.38
6	F	20	TYR	CG-CD2	-5.51	1.27	1.39
6	F	20	TYR	CG-CD1	-5.50	1.27	1.39
4	D	95	TYR	CG-CD2	-5.50	1.27	1.39
11	O	296	TYR	CE1-CZ	-5.47	1.25	1.38
6	S	20	TYR	CG-CD2	-5.47	1.27	1.39
4	Q	95	TYR	CG-CD2	-5.46	1.27	1.39
5	E	49	TYR	CG-CD2	-5.44	1.27	1.39
3	C	359	PHE	CG-CD1	-5.43	1.27	1.38
4	Q	95	TYR	CE1-CZ	-5.43	1.25	1.38
3	C	91	PHE	CG-CD2	-5.42	1.27	1.38
6	S	20	TYR	CG-CD1	-5.42	1.27	1.39
2	B	26	PHE	CG-CD1	-5.40	1.27	1.38
5	R	49	TYR	CG-CD2	-5.36	1.28	1.39
6	S	20	TYR	CE1-CZ	-5.36	1.25	1.38
5	E	27	GLU	CG-CD	-5.35	1.38	1.52
3	P	359	PHE	CG-CD2	-5.34	1.27	1.38
5	R	27	GLU	CD-OE1	5.33	1.35	1.25
3	P	91	PHE	CG-CD1	-5.29	1.27	1.38
2	B	322	PHE	CG-CD2	-5.29	1.27	1.38
11	O	26	PHE	CG-CD1	-5.25	1.27	1.38
3	C	359	PHE	CG-CD2	-5.25	1.27	1.38
11	O	296	TYR	CG-CD2	-5.25	1.28	1.39
11	O	296	TYR	CG-CD1	-5.19	1.28	1.39
7	G	30	PHE	CG-CD2	-5.18	1.27	1.38
12	V	62	ARG	C-N	5.18	1.40	1.33
2	B	99	THR	CB-CG2	-5.18	1.35	1.52
7	T	30	PHE	CG-CD2	-5.17	1.27	1.38
2	B	296	TYR	CG-CD1	-5.16	1.28	1.39
5	R	49	TYR	CE1-CZ	-5.13	1.25	1.38
3	P	91	PHE	CG-CD2	-5.13	1.28	1.38
5	R	175	PRO	N-CD	5.13	1.55	1.47
3	C	91	PHE	CG-CD1	-5.12	1.28	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	296	TYR	CG-CD2	-5.05	1.28	1.39
6	F	21	TYR	CE1-CZ	-5.04	1.26	1.38
3	P	359	PHE	CG-CD1	-5.02	1.28	1.38

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	75	ALA	N-CA-C	31.03	145.86	112.97
7	G	75	ALA	CB-CA-C	-21.88	77.69	111.17
7	G	76	ALA	N-CA-CB	-16.55	85.61	110.60
2	B	300	ALA	CB-CA-C	-15.16	87.56	111.06
5	R	72	SER	N-CA-C	14.55	126.83	110.97
8	H	50	THR	CA-CB-OG1	14.35	131.12	109.60
8	H	50	THR	OG1-CB-CG2	-14.02	81.27	109.30
10	N	302	LYS	CG-CD-CE	-12.70	82.09	111.30
5	I	53	GLU	N-CA-C	12.17	124.09	111.07
1	A	302	LYS	CB-CG-CD	-11.18	85.60	111.30
1	A	146	ARG	NH1-CZ-NH2	-11.04	104.94	119.30
7	G	78	GLU	N-CA-C	10.66	124.19	111.82
5	E	27	GLU	CB-CG-CD	-10.53	94.71	112.60
8	U	52	GLU	N-CA-C	-10.47	92.21	108.76
8	U	52	GLU	N-CA-CB	9.98	128.85	111.39
2	B	301	LYS	CD-CE-NZ	-9.66	80.99	111.90
8	U	50	THR	OG1-CB-CG2	-9.54	90.21	109.30
5	R	27	GLU	CB-CG-CD	-9.46	96.51	112.60
5	R	73	LYS	N-CA-C	-9.16	100.90	112.90
2	B	301	LYS	CG-CD-CE	-9.05	90.48	111.30
4	D	97	ASN	N-CA-C	8.79	116.04	108.13
2	B	301	LYS	N-CA-CB	8.44	124.76	110.49
2	B	303	VAL	N-CA-C	8.43	119.84	107.37
5	R	174	GLY	C-N-CD	8.42	139.12	120.60
3	P	10	LEU	CD1-CG-CD2	-8.34	92.44	110.80
1	A	302	LYS	CB-CA-C	-8.19	100.26	111.89
4	Q	97	ASN	N-CA-C	8.09	115.50	108.22
2	B	303	VAL	CB-CA-C	-7.91	100.20	111.19
8	H	48	SER	N-CA-C	7.81	121.31	111.24
8	U	50	THR	CA-CB-CG2	-7.78	97.27	110.50
11	O	116	VAL	CG1-CB-CG2	-7.62	94.03	110.80
4	D	93	LYS	CB-CA-C	-7.51	98.05	108.86
2	B	224	LEU	CB-CG-CD1	-7.49	88.23	110.70
1	A	146	ARG	NE-CZ-NH1	7.48	128.98	121.50
2	B	302	GLY	N-CA-C	-7.37	95.73	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	76	ILE	N-CA-C	-7.33	97.85	108.11
2	B	20	HIS	CA-C-N	7.19	128.83	119.84
2	B	20	HIS	C-N-CA	7.19	128.83	119.84
2	B	116	VAL	CG1-CB-CG2	-7.17	95.02	110.80
7	G	74	PRO	CA-N-CD	-7.07	102.10	112.00
4	Q	93	LYS	CG-CD-CE	-7.06	95.06	111.30
12	V	62	ARG	CB-CG-CD	7.05	127.52	111.30
7	T	72	LYS	N-CA-C	7.03	119.39	110.33
2	B	301	LYS	N-CA-C	7.02	125.76	110.80
4	Q	93	LYS	N-CA-CB	-6.99	99.14	109.90
5	I	52	ARG	N-CA-C	6.85	122.06	113.43
5	R	75	GLU	N-CA-C	-6.81	96.29	110.80
5	I	65	VAL	CB-CA-C	-6.78	101.77	111.19
8	H	40	CYS	CA-CB-SG	6.72	129.86	114.40
4	D	93	LYS	N-CA-CB	6.71	118.14	110.03
7	G	74	PRO	N-CA-C	6.68	120.98	110.50
10	N	444	LEU	CA-C-N	6.64	133.66	121.70
10	N	444	LEU	C-N-CA	6.64	133.66	121.70
1	A	248	LEU	CA-C-N	6.63	126.14	119.24
1	A	248	LEU	C-N-CA	6.63	126.14	119.24
12	V	64	VAL	N-CA-C	6.61	117.39	107.80
11	O	224	LEU	CD1-CG-CD2	-6.58	96.33	110.80
5	R	144	CYS	N-CA-CB	6.57	121.68	110.77
7	G	80	ASP	N-CA-C	-6.54	99.21	108.96
3	P	318	ARG	CA-C-N	6.33	127.75	119.84
3	P	318	ARG	C-N-CA	6.33	127.75	119.84
12	V	62	ARG	CA-CB-CG	-6.31	101.48	114.10
8	H	50	THR	N-CA-C	6.28	122.00	113.97
8	H	55	THR	CB-CA-C	-6.25	100.47	110.84
8	H	37	LEU	CD1-CG-CD2	-6.17	97.22	110.80
3	C	7	SER	CB-CA-C	6.09	117.38	109.28
11	O	224	LEU	CB-CG-CD1	-6.01	92.68	110.70
8	U	37	LEU	CD1-CG-CD2	-5.99	97.62	110.80
5	E	27	GLU	CB-CA-C	-5.97	101.70	110.95
3	C	318	ARG	CA-C-N	5.95	127.28	119.84
3	C	318	ARG	C-N-CA	5.95	127.28	119.84
10	N	302	LYS	N-CA-C	5.87	123.30	110.80
4	Q	97	ASN	CA-C-N	5.82	125.96	119.32
4	Q	97	ASN	C-N-CA	5.82	125.96	119.32
8	U	42	GLU	OE1-CD-OE2	5.79	136.79	122.90
6	S	95	LYS	CD-CE-NZ	5.72	130.21	111.90
5	I	60	ALA	N-CA-C	5.67	118.86	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	116	VAL	N-CA-CB	5.65	117.53	110.47
7	G	73	ASN	CA-C-N	-5.65	113.28	120.23
7	G	73	ASN	C-N-CA	-5.65	113.28	120.23
3	P	10	LEU	CB-CA-C	-5.61	99.44	110.10
10	N	326	CYS	N-CA-C	5.60	116.78	108.60
2	B	224	LEU	CD1-CG-CD2	-5.56	98.58	110.80
10	N	305	GLN	CB-CA-C	5.54	119.37	109.29
5	R	129	LYS	CA-C-N	5.52	126.74	119.84
5	R	129	LYS	C-N-CA	5.52	126.74	119.84
10	N	388	ARG	NE-CZ-NH2	5.51	124.16	119.20
11	O	104	ASN	N-CA-C	5.49	117.86	108.90
2	B	300	ALA	N-CA-C	-5.40	106.46	112.57
11	O	29	LEU	CA-C-N	5.40	126.59	119.84
11	O	29	LEU	C-N-CA	5.40	126.59	119.84
8	U	42	GLU	CG-CD-OE1	-5.39	106.01	118.40
10	N	248	LEU	CA-C-N	5.38	124.83	119.24
10	N	248	LEU	C-N-CA	5.38	124.83	119.24
2	B	104	ASN	N-CA-C	5.36	117.64	108.90
4	Q	6	HIS	CA-C-N	5.35	123.56	119.66
4	Q	6	HIS	C-N-CA	5.35	123.56	119.66
8	H	50	THR	CA-CB-CG2	-5.32	101.45	110.50
1	A	365	LEU	CA-CB-CG	5.32	134.92	116.30
3	P	191	ALA	N-CA-C	-5.30	105.15	111.03
5	R	77	LYS	N-CA-C	5.26	116.65	109.18
1	A	305	GLN	CB-CA-C	5.26	118.86	109.29
8	U	48	SER	N-CA-C	5.25	119.19	111.04
7	T	45	ILE	N-CA-C	5.25	115.97	110.62
7	G	74	PRO	N-CA-CB	-5.22	99.12	103.30
10	N	388	ARG	NH1-CZ-NH2	-5.21	112.53	119.30
8	H	50	THR	CB-CA-C	5.16	117.74	109.07
1	A	32	GLN	CA-C-N	5.15	124.94	119.28
1	A	32	GLN	C-N-CA	5.15	124.94	119.28
10	N	146	ARG	NE-CZ-NH1	5.13	126.63	121.50
9	W	2	ALA	CA-C-N	5.07	126.18	119.84
9	W	2	ALA	C-N-CA	5.07	126.18	119.84
5	R	143	GLY	N-CA-C	-5.06	101.19	113.18
10	N	32	GLN	CA-C-N	5.04	124.53	119.19
10	N	32	GLN	C-N-CA	5.04	124.53	119.19
3	C	16	ASN	N-CA-C	-5.02	107.32	113.50

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	85	0
2	B	3164	0	3144	85	0
3	C	2968	0	3028	133	0
3	P	2936	0	2996	110	0
4	D	1912	0	1862	49	0
4	Q	1918	0	1870	55	0
5	E	549	0	547	20	0
5	I	196	0	204	32	0
5	R	1518	0	1504	60	0
6	F	860	0	849	25	0
6	S	869	0	862	23	0
7	G	677	0	673	57	0
7	T	624	0	630	19	0
8	H	529	0	511	38	0
8	U	538	0	524	30	0
9	J	482	0	483	6	0
9	W	487	0	487	13	0
10	N	3430	0	3329	83	0
11	O	3140	0	3121	75	0
12	V	127	0	135	10	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	2	0
16	P	49	0	72	4	0
16	Q	51	0	82	4	0
17	D	43	0	32	6	0
17	Q	43	0	32	5	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	897	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (897) 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:CD2	8:U:39:LEU:CG	1.74	1.56
2:B:301:LYS:CE	2:B:301:LYS:NZ	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:C	10:N:445:LYS:CA	2.15	1.19
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:444:LEU:O	10:N:445:LYS:N	1.81	1.14
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
14:P:503:G8U:H16	14:P:503:G8U:H5	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:H12	14:C:503:G8U:C5	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:H12	14:C:503:G8U:H5	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
10:N:444:LEU:C	10:N:445:LYS:N	0.87	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:HG23	2:B:303:VAL:O	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
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
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
8:U:39:LEU:CD2	8:U:39:LEU:CD1	2.52	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
11:O:224:LEU:HD12	11:O:224:LEU:C	1.99	0.87
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:HMC1	13:P:501:HEM:HBC2	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:HD12	11:O:224:LEU:O	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:HA	10:N:443:TRP:CE3	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
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:HA	10:N:443:TRP:HE3	1.45	0.81
8:U:50:THR:HG22	8:U:50:THR:O	1.73	0.81
1:A:444:LEU:HD23	1:A:444:LEU:O	1.81	0.81
7:G:72:LYS:CE	7:G:72:LYS:H	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
7:G:74:PRO:HD2	7:G:78:GLU:CD	2.12	0.73
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
3:C:138:MET:HE2	3:C:138:MET:HA	1.71	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
3:P:138:MET:HA	3:P:138:MET:HE2	1.73	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
3:C:168:PHE:HE2	5:R:72:SER:HB2	1.56	0.70
4:D:40:CYS:SG	17:D:501:HEC:HBC3	2.31	0.70
14:P:503:G8U:H5	14:P:503:G8U:C16	2.07	0.69
4:Q:31:GLN:O	4:Q:35:GLN:HG2	1.91	0.69
10:N:58:PHE:CE2	10:N:182:LEU:HD11	2.26	0.69
10:N:146:ARG:HG2	10:N:146:ARG:HH11	1.58	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:77:TYR:O	7:G:80:ASP:O	2.09	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:71:LEU:HD23	5:I:68:VAL:HG11	1.75	0.68
3:C:185:LEU:HA	3:C:188:ILE:HD12	1.75	0.68
11:O:168:TYR:CD2	11:O:172:LEU:HB2	2.22	0.68
7:G:72:LYS:H	7:G:72:LYS:CD	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
5:R:142:LEU:O	5:R:143:GLY:C	2.38	0.67
3:C:78:ILE:HD13	4:D:204:MET:HE1	1.75	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:CD2	10:N:328:HIS:O	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:O	10:N:328:HIS:HD2	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
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
4:D:204:MET:HE3	16:D:506:PEE:H7	1.78	0.64
4:Q:211:MET:HE3	5:R:49:TYR:CD2	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:194:MET:CE	3:C:194:MET:CG	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
3:C:205:SER:OG	14:C:503:G8U:H272	1.99	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:77:TRP:CH2	3:C:78:ILE:HD11	2.34	0.63
3:C:200:LEU:CD2	3:C:201:HIS:HD2	2.12	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
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
7:G:76:ALA:O	7:G:77:TYR:CD2	2.52	0.62
1:A:443:TRP:CG	1:A:444:LEU:H	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:P:191:ALA:HA	3:P:194:MET:HE3	1.82	0.61
5:I:55:LEU:HD23	5:I:58:GLN:HG2	1.82	0.60
11:O:303:VAL:HG23	11:O:303:VAL:O	2.01	0.60
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
7:G:59:TYR:CD1	7:G:59:TYR:C	2.77	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:38:GLY:O	3:C:39:ILE:C	2.44	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
7:G:79:ASN:CG	8:H:52:GLU:HB2	2.27	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:C5	14:C:503:G8U:C12	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
5:I:64:LEU:HA	5:I:78:TYR:C	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:D:204:MET:HE3	16:D:506:PEE:C3	2.32	0.58
11:O:141:GLN:HB2	11:O:142:PRO:HD3	1.86	0.58
1:A:379:ILE:HG12	1:A:389:ARG:HD2	1.84	0.58
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
6:F:21:TYR:CD1	6:F:21:TYR:C	2.81	0.58
7:G:59:TYR:C	7:G:59:TYR:HD1	2.10	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
6:F:40:ASN:OD1	6:F:40:ASN:C	2.45	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
11:O:305:GLU:O	11:O:306:PRO:C	2.46	0.57
3:P:277:ALA:HB1	3:P:294:LEU:CD1	2.33	0.57
14:P:503:G8U:C5	14:P:503:G8U:C16	2.62	0.57
2:B:169:ARG:HE	2:B:240:HIS:CB	2.12	0.57
4:D:139:THR:OG1	8:H:41:ASP:OD1	2.22	0.57
4:D:149:PHE:HE1	4:D:156:GLN:HB3	1.70	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
7:T:59:TYR:CD1	7:T:59:TYR:C	2.80	0.57
1:A:442:PHE:C	1:A:443:TRP:O	2.46	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
4:Q:211:MET:HE3	5:R:49:TYR:HD2	1.69	0.57
2:B:170:ASN:OD1	2:B:171:ALA:N	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:254:HIS:ND1	2:B:325:TYR:OH	2.28	0.56
3:C:200:LEU:CD2	3:C:201:HIS:CD2	2.88	0.56
1:A:159:GLN:HB3	5:E:7:VAL:HG21	1.87	0.56
3:C:29:SER:O	3:C:32:ASN:HB2	2.05	0.56
10:N:382:SER:HB3	10:N:389:ARG:HA	1.87	0.56
11:O:24:LEU:HD12	11:O:38:LEU:HB2	1.87	0.56
13:P:501:HEM:HHA	13:P:501:HEM:HBA1	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
10:N:117:VAL:HG11	10:N:195:MET:HE1	1.88	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
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
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
1:A:443:TRP:CD1	1:A:444:LEU:H	2.23	0.55
3:C:75:TYR:CD2	5:E:57:GLN:HG2	2.40	0.55
3:C:220:PHE:CD1	3:C:224:TYR:HB2	2.41	0.55
3:P:78:ILE:HD12	4:Q:204:MET:HE1	1.89	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: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:OE1	5:R:75:GLU:HA	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:CD1	4:Q:165:TYR:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:O:124:LEU:HD11	11:O:219:VAL:HG13	1.89	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
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
10:N:21:ASN:HB2	10:N:221:GLY:CA	2.38	0.54
5:R:95:PRO:HB2	5:R:137:GLY:HA3	1.88	0.54
5:R:156:TYR:HB2	5:R:165:TYR:HB2	1.87	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
3:P:124:MET:HE1	3:P:298:ILE:HD12	1.88	0.54
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
2:B:87:ARG:HB3	6:S:107:TRP:CZ2	2.43	0.53
10:N:58:PHE:CZ	10:N:127:ILE:HG12	2.42	0.53
12:V:62:ARG:HB2	12:V:78:TYR:HD1	1.67	0.53
3:P:120:LEU:HG	3:P:124:MET:HE3	1.90	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
10:N:328:HIS:CD2	10:N:328:HIS:C	2.85	0.53
5:R:171:ILE:CD1	5:R:176:ALA:HB3	2.38	0.53
3:C:120:LEU:HG	3:C:124:MET:HE3	1.91	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
3:P:138:MET:HE1	3:P:268:ILE:HG22	1.91	0.53
2:B:243:GLU:HA	2:B:424:MET:O	2.09	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
1:A:442:PHE:C	1:A:442:PHE:HD1	2.16	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
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
1:A:117:VAL:HG11	1:A:195:MET:HE1	1.92	0.52
10:N:444:LEU:N	10:N:445:LYS:N	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:179:PHE:HE2	3:P:179:PHE:HE2	1.58	0.52
7:G:75:ALA:HB1	8:H:43:ARG:HH11	1.75	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
1:A:442:PHE:C	1:A:442:PHE:CD1	2.88	0.51
2:B:87:ARG:HB3	6:S:107:TRP:CE2	2.46	0.51
2:B:329:GLN:HB2	2:B:332:SER:HB2	1.93	0.51
3:P:104:TYR:CD1	3:P:208:PRO:HA	2.46	0.51
3:C:31:TRP:NE1	13:C:502:HEM:O1D	2.43	0.51
1:A:88:ALA:O	2:B:286:LYS:NZ	2.42	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
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
4:Q:11:PRO:HA	4:Q:15:ARG:HD2	1.92	0.51
5:R:41:ALA:HB2	9:W:20:PHE:HE1	1.75	0.51
8:U:44:VAL:HG12	8:U:45:SER:N	2.26	0.51
1:A:444:LEU:HD23	1:A:444:LEU:C	2.36	0.51
5:R:139:CYS:HG	5:R:165:TYR:HH	1.57	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
8:U:24:CYS:C	8:U:26:GLN:H	2.19	0.51
3:C:124:MET:HE1	3:C:298:ILE:HD12	1.92	0.50
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:S:40:ASN:OD1	6:S:40:ASN:C	2.55	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
8:H:24:CYS:C	8:H:26:GLN:H	2.20	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:11:MET:SD	3:P:198:LEU:HD12	2.52	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
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
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:97:ASN:HB2	4:Q:98:PRO:HD2	1.94	0.49
4:Q:164:ILE:HG22	4:Q:168:VAL:HG11	1.93	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
2:B:325:TYR:CD2	5:I:59:ALA:CB	2.96	0.49
3:C:138:MET:HE1	3:C:268:ILE:HG22	1.93	0.49
2:B:87:ARG:HD2	6:S:107:TRP:HE1	1.78	0.49
4:D:165:TYR:N	4:D:165:TYR:CD1	2.80	0.49
7:G:38:LEU:HA	7:G:41:THR:OG1	2.13	0.49
11:O:71:LEU:CD2	12:V:68:VAL:HG21	2.40	0.49
16:P:505:PEE:O5	18:T:501:CDL:HA32	2.13	0.49
8:U:40:CYS:SG	8:U:43:ARG:NH2	2.86	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:106:SER:CB	13:C:502:HEM:HBD2	2.34	0.48
3:C:277:ALA:HB1	3:C:294:LEU:HD12	1.95	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
3:C:324:LEU:O	3:C:327:ALA:HB3	2.13	0.48
11:O:227:ARG:HE	11:O:227:ARG:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:50:PHE:HE2	5:R:58:PHE:O	1.98	0.47
3:P:131:TYR:HA	13:P:501:HEM:HAA1	1.96	0.47
7:T:59:TYR:C	7:T:59:TYR:HD1	2.22	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
1:A:21:ASN:O	1:A:221:GLY:O	2.33	0.47
3:C:78:ILE:CD1	4:D:204:MET:HE1	2.42	0.47
11:O:141:GLN:HE22	11:O:186:VAL:HB	1.79	0.47
3:P:310:SER:HA	3:P:374:ASN:HD21	1.80	0.47
5:R:135:LEU:HD13	5:R:180:LEU:HD12	1.96	0.47
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:40:TRP:C	10:N:41:ILE:HG13	2.40	0.47
10:N:148:VAL:HG12	10:N:152:TYR:CE2	2.50	0.47
10:N:444:LEU:C	10:N:445:LYS:C	2.82	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
3:P:140:PHE:CD1	3:P:140:PHE:C	2.93	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
10:N:46:ARG:NH1	10:N:93:GLU:OE2	2.47	0.46
2:B:154:ASN:ND2	5:I:76:VAL:CG1	2.78	0.46
3:C:18:PHE:O	3:C:220:PHE:HD2	1.99	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
3:C:276:PHE:CD1	3:C:276:PHE:C	2.92	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:E:72:SER:HB2	3:P:168:PHE:CE2	2.50	0.46
11:O:261:SER:OG	11:O:262:ALA:N	2.48	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:34:GLY:CA	9:W:10:TYR:HB2	2.46	0.46
5:R:91:TRP:HZ3	5:R:136:ILE:HD11	1.81	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
2:B:301:LYS:HD2	2:B:301:LYS:HZ2	1.77	0.46
7:G:67:GLU:OE1	7:G:67:GLU:HA	2.15	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
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
4:D:37:CYS:C	4:D:39:SER:H	2.24	0.45
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:CMB	13:P:502:HEM:HBB2	2.45	0.45
4:D:97:ASN:HB2	4:D:98:PRO:HD2	1.98	0.45
10:N:159:GLN:CB	5:R:7:VAL:HG21	2.46	0.45
3:P:45:ILE:HA	13:P:501:HEM:HMC2	1.98	0.45
4:Q:126:TYR:CD1	4:Q:126:TYR:C	2.94	0.45
1:A:184:GLU:HG2	1:A:188:ARG:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:43:MET:HG2	4:D:46:VAL:HG23	1.98	0.45
4:D:164:ILE:HG22	4:D:168:VAL:HG11	1.96	0.45
3:P:284:ILE:HD12	3:P:293:ALA:HB2	1.97	0.45
3:C:150:LEU:HD13	3:C:160:LEU:HD22	1.98	0.45
5:E:72:SER:HB2	3:P:168:PHE:HE2	1.81	0.45
10:N:30:SER:OG	10:N:32:GLN:HG3	2.16	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:26:PHE:HZ	2:B:390:GLY:O	1.99	0.45
2:B:37:SER:HA	2:B:208:GLY:O	2.16	0.45
3:P:103:TYR:CD1	3:P:325:PHE:CD2	3.01	0.45
2:B:417:PHE:CD1	2:B:417:PHE:C	2.94	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:HBC2	13:P:502:HEM:HHD	1.98	0.45
6:S:83:TYR:C	6:S:83:TYR:CD1	2.94	0.45
11:O:76:THR:HG23	11:O:81:SER:HA	1.99	0.45
11:O:354:ASN:N	11:O:355:PRO:HD2	2.32	0.45
3:P:75:TYR:CD2	5:R:57:GLN:HG2	2.52	0.45
3:P:324:LEU:O	3:P:327:ALA:HB3	2.17	0.45
3:C:198:LEU:HD12	3:P:11:MET:SD	2.57	0.45
5:E:49:TYR:CD1	5:E:49:TYR:C	2.94	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:C:138:MET:HE3	3:C:265:PRO:HG2	1.99	0.45
3:P:94:LEU:O	3:P:98:VAL:HG23	2.16	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
4:Q:117:VAL:HG21	4:Q:190:LEU:C	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:212:MET:HE2	16:Q:506:PEE:C33	2.48	0.44
7:T:25:ALA:C	7:T:27:PRO:HD3	2.42	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
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
6:S:83:TYR:C	6:S:83:TYR:HD1	2.26	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:90:PHE:HE2	3:P:123:VAL:HG13	1.77	0.44
3:P:137:GLN:OE1	3:P:260:ASN:N	2.48	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
6:F:21:TYR:C	6:F:21:TYR:HD1	2.22	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
11:O:417:PHE:CD1	11:O:417:PHE:C	2.94	0.44
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
10:N:442:PHE:CD1	10:N:442:PHE:C	2.96	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:8:LEU:HB3	10:N:393:ALA:HB2	2.00	0.43
10:N:32:GLN:O	10:N:202:GLY:HA3	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:129:ALA:N	2:B:130:PRO:CD	2.81	0.43
2:B:305:GLN:HE21	2:B:305:GLN:HA	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:HD1	6:S:83:TYR:O	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
8:H:35:GLU:O	8:H:39:LEU:HD12	2.17	0.43
9:J:31:PHE:CD1	9:J:31:PHE:C	2.95	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: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
4:Q:37:CYS:C	4:Q:39:SER:H	2.25	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
2:B:87:ARG:HH11	6:S:107:TRP:CD1	2.37	0.43
3:C:102:LEU:HD21	3:C:304:ILE:HD12	2.00	0.43
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
2:B:87:ARG:HD2	6:S:107:TRP:NE1	2.33	0.43
3:C:111:GLU:O	3:C:112:THR:C	2.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:P:276:PHE:CD1	3:P:276:PHE:C	2.97	0.42
4:Q:43:MET:HE1	4:Q:189:PHE:CE2	2.54	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
7:G:79:ASN:HB2	8:H:50:THR:HG1	1.84	0.42
3:P:69:ILE:O	3:P:73:VAL:HB	2.19	0.42
2:B:283:PRO:HG3	5:I:56:ARG:O	2.19	0.42
8:H:73:LEU:O	8:H:73:LEU:HD23	2.19	0.42
10:N:185:TYR:HD1	10:N:185:TYR:C	2.28	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
1:A:185:TYR:CD1	1:A:185:TYR:C	2.98	0.42
3:C:35:SER:O	3:C:39:ILE:HD12	2.18	0.42
3:C:140:PHE:CD1	3:C:140:PHE:C	2.97	0.42
3:C:228:ASP:OD2	14:C:503:G8U:O23	2.37	0.42
8:H:72:LYS:O	8:H:73:LEU:C	2.63	0.42
11:O:37:SER:HB3	11:O:216:LEU:HD12	2.02	0.42
9:W:58:LYS:C	9:W:59:TYR:CD1	2.97	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
8:H:35:GLU:C	8:H:39:LEU:HD12	2.45	0.42
10:N:293:PRO:O	10:N:297:ILE:HG12	2.19	0.42
3:P:30:TRP:CH2	18:T:501:CDL:H711	2.55	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
1:A:98:TYR:HE2	1:A:373:THR:HG23	1.85	0.42
1:A:303:LEU:HB3	1:A:334:MET:HG2	2.02	0.42
2:B:134:ARG:NH2	6:S:49:ARG:O	2.53	0.42
3:C:120:LEU:CG	3:C:124:MET:HE3	2.50	0.42
3:C:200:LEU:HD23	3:C:200:LEU:C	2.45	0.42
3:C:304:ILE:HB	3:C:305:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:113:LEU:HA	10:N:116:ILE:HD12	2.02	0.42
10:N:185:TYR:C	10:N:185:TYR:CD1	2.97	0.42
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
3:P:29:SER:HB2	18:T:501:CDL:HB61	2.02	0.42
8:U:36:ARG:O	8:U:36:ARG:HG2	2.20	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:15:ARG:O	5:R:16:PRO:C	2.63	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: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
8:U:24:CYS:C	8:U:26:GLN:N	2.77	0.42
2:B:83:PHE:CE1	2:B:87:ARG:HG3	2.55	0.42
2:B:181:TYR:CZ	2:B:182:ARG:HG2	2.53	0.42
4:D:37:CYS:C	4:D:39:SER:N	2.78	0.42
4:D:47:ALA:O	4:D:50:HIS:HB2	2.20	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
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: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
2:B:290:ASN:ND2	5:I:56:ARG:HB3	2.35	0.41
3:C:12:LYS:C	3:C:14:VAL:H	2.28	0.41
7:G:37:VAL:O	7:G:41:THR:OG1	2.34	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
3:C:53:MET:HE2	3:P:181:PHE:CZ	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:O:272:PHE:CD1	11:O:413:ALA:HB1	2.55	0.41
3:P:138:MET:HE3	3:P:265:PRO:HG2	2.02	0.41
3:P:150:LEU:HD13	3:P:160:LEU:HD22	2.03	0.41
13:P:501:HEM:CMB	13:P:501:HEM:HBB2	2.50	0.41
4:Q:208:MET:HA	16:Q:506:PEE:H48	2.02	0.41
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:6:HIS:HA	4:Q:7:PRO:HD3	1.97	0.41
4:Q:178:THR:HG21	8:U:16:PRO:HD2	2.02	0.41
3:C:103:TYR:HD1	3:C:325:PHE:HD2	1.64	0.41
4:D:37:CYS:SG	17:D:501:HEC:CBB	3.08	0.41
4:D:162:PRO:HA	4:D:163:PRO:HD3	1.94	0.41
4:Q:37:CYS:C	4:Q:39:SER:N	2.78	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
11:O:378:PHE:CD1	11:O:378:PHE:C	2.98	0.41
3:P:120:LEU:CG	3:P:124:MET:HE3	2.50	0.41
4:Q:3:LEU:CD2	8:U:56:GLU:HG3	2.51	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
1:A:185:TYR:C	1:A:185:TYR:HD1	2.29	0.41
3:C:211:ILE:HD11	6:F:36:THR:HG22	2.03	0.41
5:I:76:VAL:O	5:I:76:VAL:CG1	2.67	0.41
10:N:204:GLU:O	10:N:205:HIS:C	2.63	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
9:W:31:PHE:CD1	9:W:31:PHE:C	2.99	0.41
1:A:70:ARG:HB3	1:A:74:ALA:HB3	2.03	0.41
1:A:294:LEU:HD11	1:A:334:MET:HE1	2.02	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
10:N:291:SER:HA	11:O:87:ARG:NE	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:O:393:THR:HG22	11:O:397:THR:HB	2.02	0.41
3:C:69:ILE:HA	3:C:73:VAL:CG2	2.51	0.41
3:C:366:MET:HB2	3:C:367:PRO:HD3	2.03	0.41
3:C:378:LYS:HG3	6:F:33:ARG:NH2	2.36	0.41
5:E:15:ARG:O	5:E:16:PRO:C	2.64	0.41
7:G:25:ALA:C	7:G:27:PRO:HD3	2.46	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
11:O:26:PHE:CZ	11:O:391:SER:HA	2.56	0.41
11:O:56:ARG:HB2	11:O:171:ALA:HB1	2.02	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
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
10:N:430:GLN:O	10:N:431:LEU:C	2.63	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:43:MET:HE1	4:Q:189:PHE:HE2	1.85	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:36:LEU:HB3	3:C:235:LEU:HD22	2.03	0.40
3:C:122:THR:HB	3:C:189:ILE:HG12	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
8:H:68:CYS:O	8:H:69:VAL:C	2.64	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
5:R:158:CYS:HB3	5:R:163:SER:HB2	2.03	0.40
12:V:76:VAL:O	12:V:77:ARG:C	2.63	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
4:D:138:PRO:O	4:D:139:THR:C	2.64	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
4:Q:140:GLY:HA3	8:U:53:ASP:HA	2.03	0.40
5:R:75:GLU:HB3	5:R:195:VAL:H	1.86	0.40
5:R:165:TYR:CE1	5:R:171:ILE:HD13	2.57	0.40
1:A:26:ALA:HB1	1:A:379:ILE:CG2	2.51	0.40
10:N:316:ASP:OD1	10:N:316:ASP:N	2.51	0.40
11:O:75:LEU:O	11:O:76:THR:C	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:42:THR:O	5:R:43:THR:C	2.65	0.40
5:R:121:GLN:NE2	5:R:126:ARG:HG2	2.37	0.40
6:S:96:GLU:HA	6:S:96:GLU:OE1	2.21	0.40
8:U:24:CYS:O	8:U:26:GLN:N	2.55	0.40
1:A:152:TYR:HB3	1:A:241:ILE:HG21	2.03	0.40
2:B:83:PHE:CE2	6:S:104:ARG:HA	2.56	0.40
3:C:220:PHE:CZ	14:C:503:G8U:H15	2.56	0.40
4:D:43:MET:HG2	4:D:46:VAL:CG2	2.52	0.40
4:D:149:PHE:CD1	4:D:156:GLN:HB3	2.56	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

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%)	18 55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	420/453 (93%)	377 (90%)	43 (10%)	0	100	100
3	C	372/379 (98%)	334 (90%)	37 (10%)	1 (0%)	36	70
3	P	368/379 (97%)	331 (90%)	36 (10%)	1 (0%)	36	70
4	D	238/325 (73%)	219 (92%)	18 (8%)	1 (0%)	30	65
4	Q	239/325 (74%)	221 (92%)	16 (7%)	2 (1%)	16	52
5	E	71/274 (26%)	62 (87%)	8 (11%)	1 (1%)	9	39
5	I	23/274 (8%)	20 (87%)	3 (13%)	0	100	100
5	R	194/274 (71%)	168 (87%)	25 (13%)	1 (0%)	24	61
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
8	H	63/91 (69%)	53 (84%)	9 (14%)	1 (2%)	7	37
8	U	64/91 (70%)	54 (84%)	9 (14%)	1 (2%)	7	37
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%)	24	61
11	O	417/453 (92%)	378 (91%)	38 (9%)	1 (0%)	43	76
12	V	15/274 (6%)	12 (80%)	3 (20%)	0	100	100
All	All	3824/5066 (76%)	3443 (90%)	366 (10%)	15 (0%)	30	65

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

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Mol	Chain	Res	Type
11	O	306	PRO
4	Q	176	PRO
4	D	176	PRO
4	Q	217	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	368/394 (93%)	354 (96%)	14 (4%)	29	51
2	B	331/355 (93%)	321 (97%)	10 (3%)	36	57
3	C	322/327 (98%)	313 (97%)	9 (3%)	38	59
3	P	318/327 (97%)	308 (97%)	10 (3%)	35	56
4	D	205/257 (80%)	197 (96%)	8 (4%)	28	51
4	Q	206/257 (80%)	198 (96%)	8 (4%)	28	51
5	E	63/228 (28%)	59 (94%)	4 (6%)	16	40
5	I	21/228 (9%)	19 (90%)	2 (10%)	8	27
5	R	168/228 (74%)	159 (95%)	9 (5%)	20	44
6	F	90/99 (91%)	85 (94%)	5 (6%)	19	43
6	S	91/99 (92%)	84 (92%)	7 (8%)	12	34
7	G	71/72 (99%)	62 (87%)	9 (13%)	4	19
7	T	66/72 (92%)	59 (89%)	7 (11%)	6	24
8	H	62/85 (73%)	55 (89%)	7 (11%)	5	22
8	U	63/85 (74%)	54 (86%)	9 (14%)	3	16
9	J	49/54 (91%)	47 (96%)	2 (4%)	27	50
9	W	49/54 (91%)	48 (98%)	1 (2%)	48	66
10	N	367/394 (93%)	355 (97%)	12 (3%)	33	55
11	O	328/355 (92%)	317 (97%)	11 (3%)	32	55
12	V	15/228 (7%)	14 (93%)	1 (7%)	15	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3253/4198 (78%)	3108 (96%)	145 (4%)	24	48

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	LEU
1	A	149	VAL
1	A	156	THR
1	A	185	TYR
1	A	230	THR
1	A	264	HIS
1	A	305	GLN
1	A	328	HIS
1	A	338	LEU
1	A	348	SER
1	A	365	LEU
1	A	388	ARG
1	A	442	PHE
1	A	444	LEU
2	B	24	LEU
2	B	99	THR
2	B	116	VAL
2	B	126	VAL
2	B	150	VAL
2	B	189	VAL
2	B	226	ILE
2	B	230	LEU
2	B	301	LYS
2	B	436	ILE
3	C	10	LEU
3	C	18	PHE
3	C	32	ASN
3	C	39	ILE
3	C	122	THR
3	C	156	ILE
3	C	161	VAL
3	C	233	LEU
3	C	257	THR
4	D	17	LEU
4	D	37	CYS
4	D	42	SER
4	D	46	VAL

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Mol	Chain	Res	Type
4	D	68	VAL
4	D	165	TYR
4	D	178	THR
4	D	182	VAL
5	E	7	VAL
5	E	27	GLU
5	E	54	VAL
5	E	72	SER
6	F	13	LEU
6	F	40	ASN
6	F	91	GLU
6	F	94	LEU
6	F	95	LYS
7	G	2	ARG
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	34	ARG
8	H	36	ARG
8	H	38	GLU
8	H	39	LEU
8	H	40	CYS
8	H	44	VAL
5	I	65	VAL
5	I	71	ASN
9	J	4	THR
9	J	9	LEU
10	N	112	LEU
10	N	146	ARG
10	N	149	VAL
10	N	156	THR
10	N	185	TYR
10	N	230	THR
10	N	305	GLN
10	N	328	HIS
10	N	348	SER

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Mol	Chain	Res	Type
10	N	365	LEU
10	N	388	ARG
10	N	443	TRP
11	O	24	LEU
11	O	99	THR
11	O	126	VAL
11	O	150	VAL
11	O	189	VAL
11	O	224	LEU
11	O	226	ILE
11	O	230	LEU
11	O	301	LYS
11	O	304	HIS
11	O	436	ILE
3	P	10	LEU
3	P	32	ASN
3	P	35	SER
3	P	39	ILE
3	P	122	THR
3	P	156	ILE
3	P	161	VAL
3	P	233	LEU
3	P	257	THR
3	P	378	LYS
4	Q	17	LEU
4	Q	37	CYS
4	Q	42	SER
4	Q	46	VAL
4	Q	68	VAL
4	Q	165	TYR
4	Q	178	THR
4	Q	182	VAL
5	R	7	VAL
5	R	47	VAL
5	R	54	VAL
5	R	72	SER
5	R	76	ILE
5	R	81	ILE
5	R	140	THR
5	R	173	LYS
5	R	182	VAL
6	S	13	LEU

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Mol	Chain	Res	Type
6	S	40	ASN
6	S	91	GLU
6	S	94	LEU
6	S	95	LYS
6	S	109	LYS
6	S	110	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	34	ARG
8	U	36	ARG
8	U	37	LEU
8	U	38	GLU
8	U	39	LEU
8	U	43	ARG
8	U	44	VAL
8	U	50	THR
12	V	71	ASN
9	W	9	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	118	GLN
1	A	240	GLN
1	A	267	ASN
1	A	271	GLN
1	A	311	ASN
1	A	328	HIS
2	B	20	HIS
2	B	22	GLN
2	B	31	ASN
2	B	104	ASN
2	B	154	ASN
2	B	156	GLN
2	B	240	HIS

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Mol	Chain	Res	Type
2	B	277	HIS
2	B	290	ASN
2	B	305	GLN
2	B	343	GLN
2	B	412	ASN
2	B	429	ASN
3	C	16	ASN
3	C	32	ASN
3	C	68	HIS
3	C	148	ASN
3	C	312	GLN
3	C	341	GLN
4	D	31	GLN
4	D	71	GLN
4	D	225	HIS
5	E	57	GLN
6	F	38	HIS
6	F	79	GLN
7	G	28	HIS
8	H	63	HIS
10	N	29	GLN
10	N	118	GLN
10	N	240	GLN
10	N	271	GLN
10	N	328	HIS
11	O	31	ASN
11	O	104	ASN
11	O	154	ASN
11	O	240	HIS
11	O	412	ASN
3	P	16	ASN
3	P	32	ASN
3	P	148	ASN
3	P	312	GLN
3	P	341	GLN
3	P	352	GLN
3	P	374	ASN
4	Q	31	GLN
4	Q	71	GLN
4	Q	225	HIS
5	R	57	GLN
5	R	141	HIS

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Mol	Chain	Res	Type
6	S	27	ASN
6	S	79	GLN
8	U	63	HIS

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 oligosaccharides 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	$\# Z > 2$
20	GOL	R	502	-	5,5,5	0.31	0	5,5,5	0.32	0
18	CDL	T	501	-	48,48,99	1.33	4 (8%)	54,60,111	1.28	4 (7%)
15	PO4	D	503	-	4,4,4	0.98	0	6,6,6	0.49	0
18	CDL	D	505	-	38,38,99	1.21	3 (7%)	42,47,111	1.08	4 (9%)
16	PEE	P	505	-	48,48,50	1.25	4 (8%)	51,53,55	1.00	2 (3%)
13	HEM	C	502	3	50,50,50	1.74	11 (22%)	67,82,82	1.60	14 (20%)
15	PO4	E	501	-	4,4,4	0.85	0	6,6,6	0.73	0
16	PEE	D	506	-	25,25,50	1.42	2 (8%)	28,30,55	1.24	3 (10%)
14	G8U	P	503	-	31,31,31	2.19	7 (22%)	42,45,45	1.57	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	HEM	C	501	3	50,50,50	1.64	7 (14%)	67,82,82	1.68	19 (28%)
14	G8U	C	503	-	31,31,31	2.29	7 (22%)	42,45,45	1.50	8 (19%)
15	PO4	C	504	-	4,4,4	1.07	0	6,6,6	0.23	0
18	CDL	G	501	-	43,43,99	1.51	4 (9%)	49,55,111	1.42	6 (12%)
17	HEC	D	501	4	46,50,50	2.64	25 (54%)	58,82,82	2.07	21 (36%)
15	PO4	F	501	-	4,4,4	0.96	0	6,6,6	0.54	0
13	HEM	P	502	3	50,50,50	1.65	8 (16%)	67,82,82	1.75	13 (19%)
15	PO4	D	502	-	4,4,4	0.88	0	6,6,6	0.47	0
16	PEE	Q	506	-	50,50,50	1.29	4 (8%)	53,55,55	1.00	3 (5%)
19	FES	R	501	5	0,4,4	-	-	-	-	-
18	CDL	Q	505	-	38,38,99	1.20	3 (7%)	42,47,111	1.12	3 (7%)
15	PO4	N	501	-	4,4,4	0.98	0	6,6,6	0.41	0
15	PO4	P	504	-	4,4,4	0.91	0	6,6,6	0.71	0
16	PEE	C	505	-	48,48,50	1.27	4 (8%)	51,53,55	0.96	2 (3%)
17	HEC	Q	501	4	46,50,50	2.69	23 (50%)	58,82,82	1.94	18 (31%)
13	HEM	P	501	3	50,50,50	1.63	9 (18%)	67,82,82	1.54	13 (19%)
15	PO4	S	501	-	4,4,4	0.93	0	6,6,6	0.39	0
15	PO4	D	504	-	4,4,4	0.97	0	6,6,6	0.44	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
13	HEM	C	502	3	-	4/14/54/54	-
16	PEE	Q	506	-	1/1/4/8	27/54/54/54	-
13	HEM	P	502	3	-	6/14/54/54	-
16	PEE	D	506	-	1/1/4/8	10/29/29/54	-
20	GOL	R	502	-	-	2/4/4/4	-
18	CDL	Q	505	-	-	11/43/43/110	-
16	PEE	C	505	-	1/1/4/8	24/52/52/54	-
17	HEC	Q	501	4	-	5/14/54/54	-
13	HEM	P	501	3	-	8/14/54/54	-
14	G8U	P	503	-	-	6/15/15/15	0/3/3/3
18	CDL	T	501	-	-	27/57/57/110	-
19	FES	R	501	5	-	-	0/1/1/1
13	HEM	C	501	3	-	6/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	G8U	C	503	-	-	5/15/15/15	0/3/3/3
18	CDL	G	501	-	-	30/52/52/110	-
18	CDL	D	505	-	-	24/43/43/110	-
17	HEC	D	501	4	-	4/14/54/54	-
16	PEE	P	505	-	1/1/4/8	28/52/52/54	-

All (125) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	503	G8U	C19-C20	7.16	1.48	1.38
14	P	503	G8U	C19-C20	6.51	1.47	1.38
14	C	503	G8U	C17-C18	5.78	1.47	1.40
18	G	501	CDL	OA6-CA5	5.55	1.47	1.35
13	C	501	HEM	FE-NB	5.52	2.11	1.94
13	P	502	HEM	FE-NB	5.47	2.11	1.94
14	P	503	G8U	C17-C18	5.46	1.46	1.40
14	P	503	G8U	O23-C18	-5.35	1.24	1.36
13	P	501	HEM	FE-NB	5.27	2.11	1.94
17	D	501	HEC	CHC-C4B	5.26	1.48	1.38
17	Q	501	HEC	C2A-C3A	5.21	1.48	1.36
17	Q	501	HEC	CHC-C4B	5.19	1.48	1.38
14	C	503	G8U	O23-C18	-5.18	1.25	1.36
13	C	502	HEM	FE-NB	5.06	2.10	1.94
18	T	501	CDL	OA6-CA5	5.06	1.46	1.35
17	Q	501	HEC	CHB-C4A	5.05	1.48	1.38
18	G	501	CDL	OB6-CB5	4.92	1.48	1.34
17	Q	501	HEC	CHA-C1A	4.91	1.48	1.38
16	Q	506	PEE	O2-C10	4.76	1.47	1.34
13	P	502	HEM	FE-NC	4.74	2.10	1.95
16	D	506	PEE	O3-C30	4.72	1.47	1.33
18	D	505	CDL	OA6-CA5	4.72	1.47	1.34
17	D	501	HEC	CHD-C4C	4.69	1.47	1.38
18	G	501	CDL	OB8-CB7	4.68	1.47	1.33
16	P	505	PEE	O2-C10	4.66	1.47	1.34
17	D	501	HEC	CHA-C1A	4.66	1.47	1.38
17	D	501	HEC	C2A-C3A	4.62	1.46	1.36
18	Q	505	CDL	OA6-CA5	4.59	1.47	1.34
17	D	501	HEC	CAC-C3C	4.58	1.49	1.35
17	D	501	HEC	CHB-C4A	4.53	1.47	1.38
18	T	501	CDL	OB6-CB5	4.51	1.47	1.34
17	Q	501	HEC	CHD-C4C	4.50	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	501	HEM	FE-NC	4.44	2.09	1.95
16	D	506	PEE	O2-C10	4.43	1.46	1.34
17	Q	501	HEC	CAB-C3B	4.40	1.49	1.35
16	C	505	PEE	O2-C10	4.39	1.46	1.34
17	Q	501	HEC	CAC-C3C	4.38	1.49	1.35
18	D	505	CDL	OA8-CA7	4.37	1.46	1.33
18	Q	505	CDL	OA8-CA7	4.36	1.46	1.33
17	D	501	HEC	CHC-C1C	4.31	1.49	1.39
16	Q	506	PEE	O3-C30	4.29	1.45	1.33
18	T	501	CDL	OB8-CB7	4.19	1.45	1.33
16	C	505	PEE	O3-C30	4.19	1.45	1.33
17	D	501	HEC	CAB-C3B	4.16	1.48	1.35
17	Q	501	HEC	CHB-C1B	4.15	1.48	1.39
16	P	505	PEE	O3-C30	4.08	1.45	1.33
13	P	501	HEM	FE-NC	4.05	2.08	1.95
17	Q	501	HEC	CHC-C1C	4.04	1.48	1.39
16	Q	506	PEE	C18-C19	3.96	1.54	1.31
14	P	503	G8U	C17-C22	3.94	1.49	1.40
13	C	502	HEM	FE-NC	3.92	2.08	1.95
16	C	505	PEE	C39-C38	3.91	1.53	1.31
14	C	503	G8U	C18-C19	3.89	1.45	1.39
16	C	505	PEE	C18-C19	3.85	1.53	1.31
16	Q	506	PEE	C39-C38	3.82	1.53	1.31
17	D	501	HEC	CHA-C4D	3.77	1.47	1.39
16	P	505	PEE	C39-C38	3.72	1.52	1.31
17	Q	501	HEC	CHD-C1D	3.69	1.47	1.39
16	P	505	PEE	C18-C19	3.69	1.52	1.31
14	P	503	G8U	C18-C19	3.68	1.45	1.39
13	C	502	HEM	C4D-ND	-3.63	1.34	1.40
13	C	502	HEM	C1B-NB	-3.62	1.34	1.40
13	P	502	HEM	C1B-NB	-3.58	1.34	1.40
17	D	501	HEC	CHB-C1B	3.58	1.47	1.39
17	Q	501	HEC	C3D-C2D	3.55	1.48	1.38
17	D	501	HEC	CHD-C1D	3.50	1.47	1.39
17	Q	501	HEC	CHA-C4D	3.49	1.47	1.39
13	P	501	HEM	C1B-NB	-3.47	1.34	1.40
14	C	503	G8U	C17-C22	3.44	1.48	1.40
17	D	501	HEC	C3D-C2D	3.33	1.47	1.38
13	C	501	HEM	C1B-NB	-3.26	1.34	1.40
13	P	501	HEM	C4D-ND	-3.11	1.34	1.40
13	P	502	HEM	C4D-ND	-2.96	1.35	1.40
17	D	501	HEC	C1C-C2C	2.92	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Q	501	HEC	C1C-C2C	2.91	1.49	1.43
17	D	501	HEC	C4A-NA	-2.89	1.34	1.39
13	C	501	HEM	C4D-ND	-2.88	1.35	1.40
18	G	501	CDL	OA8-CA7	2.84	1.47	1.33
13	P	501	HEM	C4B-NB	-2.79	1.33	1.38
13	C	502	HEM	C3B-C4B	2.79	1.50	1.44
13	P	502	HEM	C1D-ND	-2.77	1.33	1.38
17	Q	501	HEC	C4D-ND	-2.75	1.34	1.39
13	C	502	HEM	C1D-ND	-2.74	1.33	1.38
13	C	502	HEM	C3C-C4C	-2.73	1.41	1.46
13	C	502	HEM	C4B-NB	-2.67	1.33	1.38
13	C	502	HEM	C1C-C2C	-2.67	1.40	1.45
17	Q	501	HEC	C4A-NA	-2.60	1.34	1.39
17	D	501	HEC	C1B-C2B	2.59	1.49	1.43
13	C	501	HEM	C3B-C4B	2.56	1.49	1.44
13	C	501	HEM	C1D-ND	-2.56	1.33	1.38
13	C	502	HEM	FE-ND	-2.55	1.87	1.94
17	Q	501	HEC	C1B-C2B	2.54	1.49	1.43
17	D	501	HEC	C4C-NC	-2.54	1.34	1.39
17	Q	501	HEC	C1B-NB	-2.52	1.34	1.39
18	T	501	CDL	OA8-CA7	2.51	1.45	1.33
14	C	503	G8U	C19-CL	2.49	1.78	1.72
13	C	502	HEM	C1C-NC	-2.45	1.35	1.39
17	D	501	HEC	C1D-C2D	2.45	1.48	1.43
17	Q	501	HEC	C1C-NC	-2.44	1.35	1.39
17	D	501	HEC	C4B-NB	-2.42	1.35	1.39
13	P	502	HEM	C4B-NB	-2.41	1.34	1.38
13	P	502	HEM	C1C-C2C	-2.38	1.40	1.45
13	P	502	HEM	FE-ND	-2.38	1.87	1.94
17	Q	501	HEC	C1D-C2D	2.35	1.48	1.43
13	C	501	HEM	C4B-NB	-2.34	1.34	1.38
17	D	501	HEC	C1B-NB	-2.32	1.35	1.39
17	Q	501	HEC	C1A-NA	-2.30	1.35	1.39
17	Q	501	HEC	C4D-C3D	2.29	1.49	1.44
17	Q	501	HEC	C4B-NB	-2.28	1.35	1.39
17	D	501	HEC	C1A-NA	-2.26	1.35	1.39
13	P	501	HEM	C1C-C2C	-2.25	1.40	1.45
17	D	501	HEC	C1D-ND	-2.25	1.35	1.39
13	P	501	HEM	C3C-C4C	-2.24	1.42	1.46
13	P	501	HEM	C4C-NC	-2.21	1.35	1.39
17	Q	501	HEC	C4A-C3A	2.20	1.49	1.45
17	D	501	HEC	C3B-C4B	2.18	1.49	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P	501	HEM	C1D-C2D	2.18	1.49	1.44
17	D	501	HEC	C4D-ND	-2.18	1.35	1.39
14	P	503	G8U	C19-CL	2.17	1.77	1.72
17	D	501	HEC	C4D-C3D	2.16	1.48	1.44
17	D	501	HEC	C1C-NC	-2.11	1.35	1.39
18	Q	505	CDL	PB2-OB5	2.07	1.62	1.54
18	D	505	CDL	PB2-OB5	2.04	1.62	1.54
14	C	503	G8U	O29-C1	2.04	1.42	1.31
14	P	503	G8U	O29-C1	2.01	1.42	1.31

All (138) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	G	501	CDL	OA6-CA5-C11	5.87	121.56	111.09
14	P	503	G8U	C27-C20-C19	-5.78	119.56	122.97
18	T	501	CDL	OA6-CA5-C11	5.75	121.34	111.09
13	P	502	HEM	CHD-C1D-ND	5.32	130.15	124.42
17	Q	501	HEC	C2A-C1A-NA	5.13	115.28	110.32
17	D	501	HEC	C2A-C1A-NA	5.04	115.19	110.32
17	D	501	HEC	C3D-C4D-ND	4.61	115.27	110.15
13	P	502	HEM	CAD-C3D-C4D	4.52	132.57	124.70
13	P	501	HEM	CHC-C4B-NB	4.39	129.15	124.42
17	Q	501	HEC	C1D-C2D-C3D	-4.30	101.89	106.82
13	P	501	HEM	C1B-NB-C4B	4.24	110.23	105.21
17	D	501	HEC	C2B-C1B-NB	4.24	116.94	110.14
18	Q	505	CDL	OA6-CA5-C11	4.15	120.45	111.48
13	P	502	HEM	CHC-C4B-NB	4.14	128.87	124.42
13	C	502	HEM	CHD-C1D-ND	4.13	128.86	124.42
14	C	503	G8U	C27-C20-C19	-4.12	120.54	122.97
13	C	502	HEM	CHA-C4D-ND	4.08	129.42	124.37
16	D	506	PEE	O2-C10-C11	4.06	120.27	111.48
17	Q	501	HEC	C3D-C4D-ND	3.94	114.53	110.15
14	P	503	G8U	C20-N28-C22	3.94	123.67	118.66
18	T	501	CDL	OB6-CB5-C51	3.93	119.98	111.48
18	D	505	CDL	OA6-CA5-C11	3.91	119.95	111.48
13	C	502	HEM	CHC-C4B-NB	3.87	128.58	124.42
14	C	503	G8U	C20-N28-C22	3.74	123.42	118.66
13	C	501	HEM	C1B-NB-C4B	3.58	109.44	105.21
17	Q	501	HEC	C1A-C2A-C3A	-3.46	102.55	107.11
17	D	501	HEC	CAA-CBA-CGA	-3.45	104.50	113.67
16	C	505	PEE	O2-C10-C11	3.45	118.95	111.48
16	P	505	PEE	O2-C10-C11	3.43	118.91	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	D	501	HEC	C1D-C2D-C3D	-3.35	102.98	106.82
17	Q	501	HEC	C2D-C1D-ND	3.33	115.48	110.14
13	C	501	HEM	CHC-C4B-NB	3.32	128.00	124.42
17	D	501	HEC	C1A-C2A-C3A	-3.30	102.76	107.11
14	P	503	G8U	C20-C19-C18	-3.27	119.16	122.65
18	G	501	CDL	OB6-CB5-C51	3.25	122.87	110.93
13	C	501	HEM	CHB-C1B-NB	3.22	128.35	124.37
13	P	502	HEM	C1B-NB-C4B	3.22	109.02	105.21
13	C	501	HEM	CBA-CAA-C2A	-3.15	103.82	112.53
17	D	501	HEC	C3A-C4A-NA	3.14	115.45	109.64
13	C	501	HEM	CHA-C4D-ND	3.09	128.19	124.37
18	D	505	CDL	OA8-CA7-C31	3.08	121.22	111.83
17	D	501	HEC	C2D-C1D-ND	3.07	115.07	110.14
17	D	501	HEC	C2C-C1C-NC	3.07	115.06	110.14
14	C	503	G8U	C20-C19-C18	-3.07	119.38	122.65
13	C	501	HEM	CHD-C4C-NC	3.05	127.78	124.45
13	C	502	HEM	C1B-NB-C4B	3.05	108.81	105.21
13	P	502	HEM	CAD-C3D-C2D	-3.02	122.20	127.87
13	P	501	HEM	CHA-C4D-ND	3.01	128.09	124.37
18	G	501	CDL	OB8-CB7-C71	3.00	120.98	111.83
16	Q	506	PEE	O2-C10-C11	3.00	117.97	111.48
13	P	501	HEM	CHD-C1D-ND	2.97	127.62	124.42
13	C	501	HEM	CHD-C1D-ND	2.97	127.62	124.42
13	P	501	HEM	C3B-C4B-NB	-2.96	107.34	109.47
13	C	502	HEM	CHD-C4C-NC	2.96	127.67	124.45
13	P	502	HEM	CHA-C4D-ND	2.94	128.01	124.37
17	Q	501	HEC	C2B-C1B-NB	2.94	114.85	110.14
13	C	502	HEM	CHD-C1D-C2D	-2.92	120.42	125.03
13	P	502	HEM	CHD-C1D-C2D	-2.89	120.46	125.03
17	D	501	HEC	C4A-C3A-C2A	-2.88	102.69	106.97
13	P	501	HEM	CHA-C4D-C3D	-2.88	119.92	125.23
18	Q	505	CDL	OA8-CA7-C31	2.87	120.58	111.83
17	Q	501	HEC	C2C-C1C-NC	2.86	114.73	110.14
17	Q	501	HEC	CHD-C4C-C3C	-2.85	120.40	125.21
13	P	502	HEM	CAC-C3C-C4C	2.80	131.51	124.82
17	Q	501	HEC	C4A-C3A-C2A	-2.78	102.85	106.97
17	D	501	HEC	C4D-C3D-C2D	-2.76	102.59	106.87
17	Q	501	HEC	CMA-C3A-C4A	2.76	129.59	124.73
17	D	501	HEC	CBB-CAB-C3B	-2.76	121.92	127.43
13	C	502	HEM	C4A-C3A-C2A	2.76	109.97	106.82
13	P	502	HEM	CAD-CBD-CGD	-2.75	106.38	113.67
17	D	501	HEC	CMA-C3A-C4A	2.74	129.56	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	D	506	PEE	O3-C30-C31	2.74	120.19	111.83
17	Q	501	HEC	C3A-C4A-NA	2.73	114.68	109.64
13	P	501	HEM	CMD-C2D-C1D	2.73	129.29	125.03
17	D	501	HEC	CAA-C2A-C1A	2.72	130.39	124.85
13	P	502	HEM	CHB-C1B-NB	2.71	127.72	124.37
13	C	502	HEM	CAA-C2A-C1A	2.68	130.18	124.94
17	D	501	HEC	CHB-C1B-C2B	-2.68	119.65	127.43
14	C	503	G8U	C24-C22-N28	2.66	119.22	115.75
14	C	503	G8U	C20-C19-CL	2.65	124.90	121.05
13	C	501	HEM	CBB-CAB-C3B	-2.65	114.31	127.53
13	P	501	HEM	CHD-C1D-C2D	-2.63	120.87	125.03
14	P	503	G8U	C17-C22-N28	-2.58	120.51	123.47
17	Q	501	HEC	CHA-C1A-C2A	-2.58	120.80	124.86
13	C	501	HEM	C3B-C4B-NB	-2.52	107.66	109.47
13	C	502	HEM	CHA-C4D-C3D	-2.52	120.58	125.23
17	Q	501	HEC	CHD-C1D-C2D	-2.51	120.14	127.43
13	P	501	HEM	CHB-C1B-NB	2.47	127.42	124.37
13	C	501	HEM	CMB-C2B-C1B	2.45	128.86	125.03
13	C	501	HEM	CHA-C4D-C3D	-2.45	120.72	125.23
13	C	501	HEM	C4C-NC-C1C	2.44	109.80	105.82
18	T	501	CDL	OB8-CB7-C71	2.44	119.27	111.83
18	T	501	CDL	OA6-CA5-OA7	-2.42	118.32	122.99
16	Q	506	PEE	C2-O2-C10	2.40	123.55	117.80
13	P	501	HEM	O2D-CGD-CBD	2.39	121.56	114.00
18	G	501	CDL	OB6-CB5-OB7	-2.38	118.14	123.70
16	C	505	PEE	O3-C30-C31	2.36	119.03	111.83
13	C	501	HEM	CHD-C1D-C2D	-2.35	121.32	125.03
13	C	502	HEM	O2D-CGD-CBD	2.34	121.40	114.00
13	P	502	HEM	C4D-ND-C1D	2.34	107.98	105.21
17	Q	501	HEC	CBB-CAB-C3B	-2.34	122.77	127.43
13	C	502	HEM	CBB-CAB-C3B	-2.33	115.90	127.53
17	D	501	HEC	CHA-C1A-C2A	-2.30	121.23	124.86
14	P	503	G8U	C14-C17-C18	-2.29	115.86	120.06
16	Q	506	PEE	O3-C30-C31	2.28	118.79	111.83
18	Q	505	CDL	OB4-PB2-OB3	2.28	119.72	110.83
13	C	502	HEM	C4C-CHD-C1D	-2.28	121.18	126.02
13	C	501	HEM	CMD-C2D-C1D	2.26	128.57	125.03
16	P	505	PEE	O3-C30-C31	2.25	118.71	111.83
17	D	501	HEC	CHB-C4A-C3A	-2.23	120.84	125.49
14	C	503	G8U	C15-C14-C17	-2.22	116.98	120.80
16	D	506	PEE	O3-C30-O5	-2.22	118.08	123.63
17	D	501	HEC	CMB-C2B-C3B	2.21	131.74	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	501	HEM	CHA-C1A-NA	2.21	127.86	123.86
14	C	503	G8U	C17-C18-C19	-2.20	116.52	119.23
17	Q	501	HEC	CBC-CAC-C3C	-2.20	123.03	127.43
18	D	505	CDL	OA8-CA7-OA9	-2.20	118.13	123.63
13	C	501	HEM	CAD-C3D-C4D	2.16	128.46	124.70
13	P	501	HEM	C4C-NC-C1C	2.16	109.34	105.82
13	P	501	HEM	CAD-C3D-C4D	2.15	128.45	124.70
13	C	501	HEM	CMB-C2B-C3B	-2.15	123.23	128.43
17	Q	501	HEC	C4D-C3D-C2D	-2.15	103.55	106.87
18	G	501	CDL	CA6-OA8-CA7	2.14	122.37	117.08
13	C	502	HEM	C1A-C2A-C3A	-2.13	103.57	106.87
13	C	501	HEM	C4B-C3B-C2B	-2.13	105.32	107.28
13	P	501	HEM	CHD-C4C-NC	2.12	126.76	124.45
17	D	501	HEC	CHD-C4C-C3C	-2.12	121.64	125.21
17	D	501	HEC	CHD-C1D-C2D	-2.11	121.29	127.43
13	C	501	HEM	CAB-C3B-C2B	-2.10	121.59	128.43
18	D	505	CDL	OB4-PB2-OB3	2.09	118.98	110.83
17	Q	501	HEC	CHB-C1B-C2B	-2.09	121.37	127.43
14	C	503	G8U	C17-C22-N28	-2.06	121.10	123.47
17	Q	501	HEC	CMD-C2D-C3D	2.06	130.00	125.62
18	G	501	CDL	OA8-CA7-C31	2.06	121.11	112.38
13	P	502	HEM	CBD-CAD-C3D	2.05	118.21	112.53
17	D	501	HEC	CAD-C3D-C4D	2.05	128.95	124.94
13	C	502	HEM	CMD-C2D-C1D	2.05	128.23	125.03
13	P	502	HEM	CAC-C3C-C2C	-2.00	121.92	128.43

All (4) chirality outliers are listed below:

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

All (227) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	P	501	HEM	C3A-C2A-CAA-CBA
13	P	502	HEM	C2D-C3D-CAD-CBD
16	D	506	PEE	C4-O4P-P-O3P
16	D	506	PEE	C4-O4P-P-O1P
16	D	506	PEE	O4P-C4-C5-N

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Mol	Chain	Res	Type	Atoms
16	P	505	PEE	C1-O3P-P-O4P
16	P	505	PEE	O4P-C4-C5-N
16	Q	506	PEE	C1-O3P-P-O2P
16	Q	506	PEE	C1-O3P-P-O1P
16	Q	506	PEE	C1-O3P-P-O4P
16	Q	506	PEE	C4-O4P-P-O3P
16	Q	506	PEE	O4P-C4-C5-N
18	D	505	CDL	CA2-C1-CB2-OB2
18	D	505	CDL	CB2-OB2-PB2-OB4
18	D	505	CDL	CB2-OB2-PB2-OB5
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	CA3-OA5-PA1-OA4
18	G	501	CDL	C11-CA5-OA6-CA4
18	G	501	CDL	CB3-OB5-PB2-OB4
18	G	501	CDL	OB7-CB5-OB6-CB4
18	G	501	CDL	C51-CB5-OB6-CB4
18	Q	505	CDL	CA2-OA2-PA1-OA3
18	T	501	CDL	CA2-OA2-PA1-OA3
18	T	501	CDL	C11-CA5-OA6-CA4
18	T	501	CDL	CB3-OB5-PB2-OB2
18	T	501	CDL	CB3-OB5-PB2-OB3
18	G	501	CDL	OA7-CA5-OA6-CA4
18	T	501	CDL	OA7-CA5-OA6-CA4
18	Q	505	CDL	OA9-CA7-OA8-CA6
18	T	501	CDL	C31-CA7-OA8-CA6
18	T	501	CDL	OA9-CA7-OA8-CA6
16	C	505	PEE	C37-C38-C39-C40
13	P	502	HEM	C4D-C3D-CAD-CBD
18	D	505	CDL	O1-C1-CB2-OB2
18	G	501	CDL	O1-C1-CA2-OA2
18	G	501	CDL	O1-C1-CB2-OB2
18	T	501	CDL	O1-C1-CA2-OA2
18	T	501	CDL	O1-C1-CB2-OB2
18	Q	505	CDL	C31-CA7-OA8-CA6
13	P	501	HEM	C1A-C2A-CAA-CBA
18	G	501	CDL	CA2-C1-CB2-OB2
18	G	501	CDL	C31-CA7-OA8-CA6
16	C	505	PEE	C30-C31-C32-C33
14	C	503	G8U	F3-C1-O29-C4
18	Q	505	CDL	CA7-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
13	P	501	HEM	C2A-CAA-CBA-CGA
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
16	Q	506	PEE	C17-C18-C19-C20
16	P	505	PEE	C11-C10-O2-C2
16	P	505	PEE	O4-C10-O2-C2
18	T	501	CDL	CA2-C1-CB2-OB2
18	D	505	CDL	C31-CA7-OA8-CA6
16	C	505	PEE	C11-C10-O2-C2
16	C	505	PEE	O4-C10-O2-C2
16	P	505	PEE	C37-C38-C39-C40
16	D	506	PEE	C31-C30-O3-C3
18	G	501	CDL	OA9-CA7-OA8-CA6
18	G	501	CDL	CB4-CB3-OB5-PB2
13	C	501	HEM	C3D-CAD-CBD-CGD
13	P	501	HEM	C3D-CAD-CBD-CGD
20	R	502	GOL	C1-C2-C3-O3
18	D	505	CDL	OA9-CA7-OA8-CA6
18	T	501	CDL	C71-C72-C73-C74
18	Q	505	CDL	C38-C39-C40-C41
16	Q	506	PEE	C31-C32-C33-C34
18	T	501	CDL	C74-C75-C76-C77
18	D	505	CDL	C11-CA5-OA6-CA4
16	P	505	PEE	C42-C43-C44-C45
18	D	505	CDL	C37-C38-C39-C40
18	G	501	CDL	C74-C75-C76-C77
16	D	506	PEE	O5-C30-O3-C3
16	C	505	PEE	C21-C22-C23-C24
13	C	502	HEM	C3D-CAD-CBD-CGD
16	P	505	PEE	C21-C22-C23-C24
16	Q	506	PEE	C32-C33-C34-C35
16	Q	506	PEE	C41-C42-C43-C44
18	Q	505	CDL	C37-C38-C39-C40
18	D	505	CDL	OA7-CA5-OA6-CA4
18	G	501	CDL	C71-CB7-OB8-CB6
16	P	505	PEE	C41-C42-C43-C44
16	Q	506	PEE	C11-C12-C13-C14
18	T	501	CDL	C52-C53-C54-C55
16	C	505	PEE	C31-C32-C33-C34
16	C	505	PEE	C42-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
18	T	501	CDL	C53-C54-C55-C56
18	T	501	CDL	C73-C74-C75-C76
16	D	506	PEE	C11-C10-O2-C2
16	C	505	PEE	C12-C13-C14-C15
16	D	506	PEE	O4-C10-O2-C2
14	C	503	G8U	F2-C1-O29-C4
16	Q	506	PEE	C34-C35-C36-C37
16	Q	506	PEE	C39-C40-C41-C42
16	C	505	PEE	C13-C14-C15-C16
16	P	505	PEE	C12-C13-C14-C15
16	Q	506	PEE	C21-C22-C23-C24
18	Q	505	CDL	C34-C35-C36-C37
13	C	501	HEM	C2B-C3B-CAB-CBB
18	T	501	CDL	C51-C52-C53-C54
16	C	505	PEE	C33-C34-C35-C36
16	C	505	PEE	C15-C16-C17-C18
16	P	505	PEE	O2-C2-C3-O3
18	D	505	CDL	C38-C39-C40-C41
17	Q	501	HEC	C3D-CAD-CBD-CGD
18	T	501	CDL	CB2-C1-CA2-OA2
16	D	506	PEE	C32-C33-C34-C35
18	G	501	CDL	OB9-CB7-OB8-CB6
18	T	501	CDL	C72-C73-C74-C75
16	P	505	PEE	C39-C40-C41-C42
16	Q	506	PEE	C19-C20-C21-C22
16	Q	506	PEE	O3P-C1-C2-C3
18	G	501	CDL	OB5-CB3-CB4-CB6
16	C	505	PEE	C40-C41-C42-C43
16	P	505	PEE	C1-C2-C3-O3
16	Q	506	PEE	C40-C41-C42-C43
16	C	505	PEE	C19-C20-C21-C22
16	Q	506	PEE	C22-C23-C24-C25
16	C	505	PEE	C20-C21-C22-C23
16	C	505	PEE	C1-C2-O2-C10
16	P	505	PEE	C1-C2-O2-C10
16	P	505	PEE	C19-C20-C21-C22
16	P	505	PEE	C34-C35-C36-C37
16	P	505	PEE	C33-C34-C35-C36
14	C	503	G8U	F1-C1-O29-C4
18	G	501	CDL	OA6-CA4-CA6-OA8
16	P	505	PEE	C23-C24-C25-C26
18	Q	505	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
18	D	505	CDL	CA4-CA3-OA5-PA1
16	C	505	PEE	O3P-C1-C2-C3
16	D	506	PEE	O3P-C1-C2-C3
14	P	503	G8U	C17-C22-C24-O25
16	P	505	PEE	C35-C36-C37-C38
16	P	505	PEE	C13-C14-C15-C16
16	Q	506	PEE	C1-C2-C3-O3
18	D	505	CDL	CA3-CA4-CA6-OA8
18	G	501	CDL	CA3-CA4-CA6-OA8
18	D	505	CDL	C36-C37-C38-C39
18	D	505	CDL	OA5-CA3-CA4-OA6
18	G	501	CDL	OB5-CB3-CB4-OB6
16	Q	506	PEE	O2-C2-C3-O3
18	G	501	CDL	C73-C74-C75-C76
16	P	505	PEE	C20-C21-C22-C23
20	R	502	GOL	O2-C2-C3-O3
18	D	505	CDL	C33-C34-C35-C36
16	C	505	PEE	C35-C36-C37-C38
16	Q	506	PEE	C35-C36-C37-C38
16	Q	506	PEE	C42-C43-C44-C45
16	C	505	PEE	O3P-C1-C2-O2
16	D	506	PEE	O3P-C1-C2-O2
16	Q	506	PEE	O3P-C1-C2-O2
16	P	505	PEE	C5-C4-O4P-P
18	T	501	CDL	C54-C55-C56-C57
18	D	505	CDL	OA5-CA3-CA4-CA6
18	T	501	CDL	OA5-CA3-CA4-CA6
18	T	501	CDL	OB5-CB3-CB4-CB6
16	Q	506	PEE	C13-C14-C15-C16
18	T	501	CDL	OA5-CA3-CA4-OA6
18	T	501	CDL	OB5-CB3-CB4-OB6
16	C	505	PEE	C4-O4P-P-O1P
16	P	505	PEE	C1-O3P-P-O1P
18	G	501	CDL	CA2-OA2-PA1-OA5
18	G	501	CDL	CB2-OB2-PB2-OB3
18	G	501	CDL	CB3-OB5-PB2-OB2
18	G	501	CDL	CB3-OB5-PB2-OB3
18	Q	505	CDL	CA2-OA2-PA1-OA5
18	Q	505	CDL	CA3-OA5-PA1-OA3
18	T	501	CDL	CB2-OB2-PB2-OB3
18	T	501	CDL	CB3-OB5-PB2-OB4
18	T	501	CDL	CB4-CB3-OB5-PB2

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Mol	Chain	Res	Type	Atoms
18	D	505	CDL	CB2-OB2-PB2-OB3
17	Q	501	HEC	C1A-C2A-CAA-CBA
14	P	503	G8U	F2-C1-O29-C4
18	D	505	CDL	C34-C35-C36-C37
16	C	505	PEE	O2-C2-C3-O3
18	D	505	CDL	OA6-CA4-CA6-OA8
17	Q	501	HEC	CAD-CBD-CGD-O2D
16	P	505	PEE	C31-C32-C33-C34
13	C	502	HEM	C4B-C3B-CAB-CBB
17	Q	501	HEC	CAD-CBD-CGD-O1D
18	G	501	CDL	C71-C72-C73-C74
16	C	505	PEE	C36-C37-C38-C39
18	T	501	CDL	C75-C76-C77-C78
13	C	502	HEM	CAA-CBA-CGA-O1A
13	C	502	HEM	CAA-CBA-CGA-O2A
13	P	501	HEM	CAA-CBA-CGA-O2A
13	P	502	HEM	CAA-CBA-CGA-O1A
16	P	505	PEE	C14-C15-C16-C17
13	P	501	HEM	CAA-CBA-CGA-O1A
13	P	502	HEM	CAA-CBA-CGA-O2A
14	C	503	G8U	C5-C4-O29-C1
17	Q	501	HEC	C3A-C2A-CAA-CBA
13	P	502	HEM	CAD-CBD-CGD-O2D
16	P	505	PEE	C43-C44-C45-C46
17	D	501	HEC	CAA-CBA-CGA-O2A
17	D	501	HEC	CAD-CBD-CGD-O2D
16	Q	506	PEE	C38-C39-C40-C41
13	C	501	HEM	CAD-CBD-CGD-O2D
13	P	501	HEM	CAD-CBD-CGD-O2D
13	P	502	HEM	CAD-CBD-CGD-O1D
17	D	501	HEC	CAD-CBD-CGD-O1D
18	D	505	CDL	CA5-C11-C12-C13
16	Q	506	PEE	C1-C2-O2-C10
18	D	505	CDL	C35-C36-C37-C38
14	C	503	G8U	C9-C4-O29-C1
13	C	501	HEM	CAA-CBA-CGA-O2A
18	G	501	CDL	OA5-CA3-CA4-OA6
16	P	505	PEE	C36-C37-C38-C39
16	Q	506	PEE	C16-C17-C18-C19
13	C	501	HEM	CAA-CBA-CGA-O1A
16	C	505	PEE	C14-C15-C16-C17
17	D	501	HEC	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
18	G	501	CDL	OA5-CA3-CA4-CA6
13	P	501	HEM	CAD-CBD-CGD-O1D
13	C	501	HEM	CAD-CBD-CGD-O1D
18	D	505	CDL	C12-C11-CA5-OA6
18	D	505	CDL	CA7-C31-C32-C33
14	P	503	G8U	C5-C4-O29-C1
14	P	503	G8U	F1-C1-O29-C4
14	P	503	G8U	C9-C4-O29-C1
16	C	505	PEE	C22-C23-C24-C25
14	P	503	G8U	F3-C1-O29-C4
18	D	505	CDL	C12-C11-CA5-OA7
18	Q	505	CDL	C35-C36-C37-C38

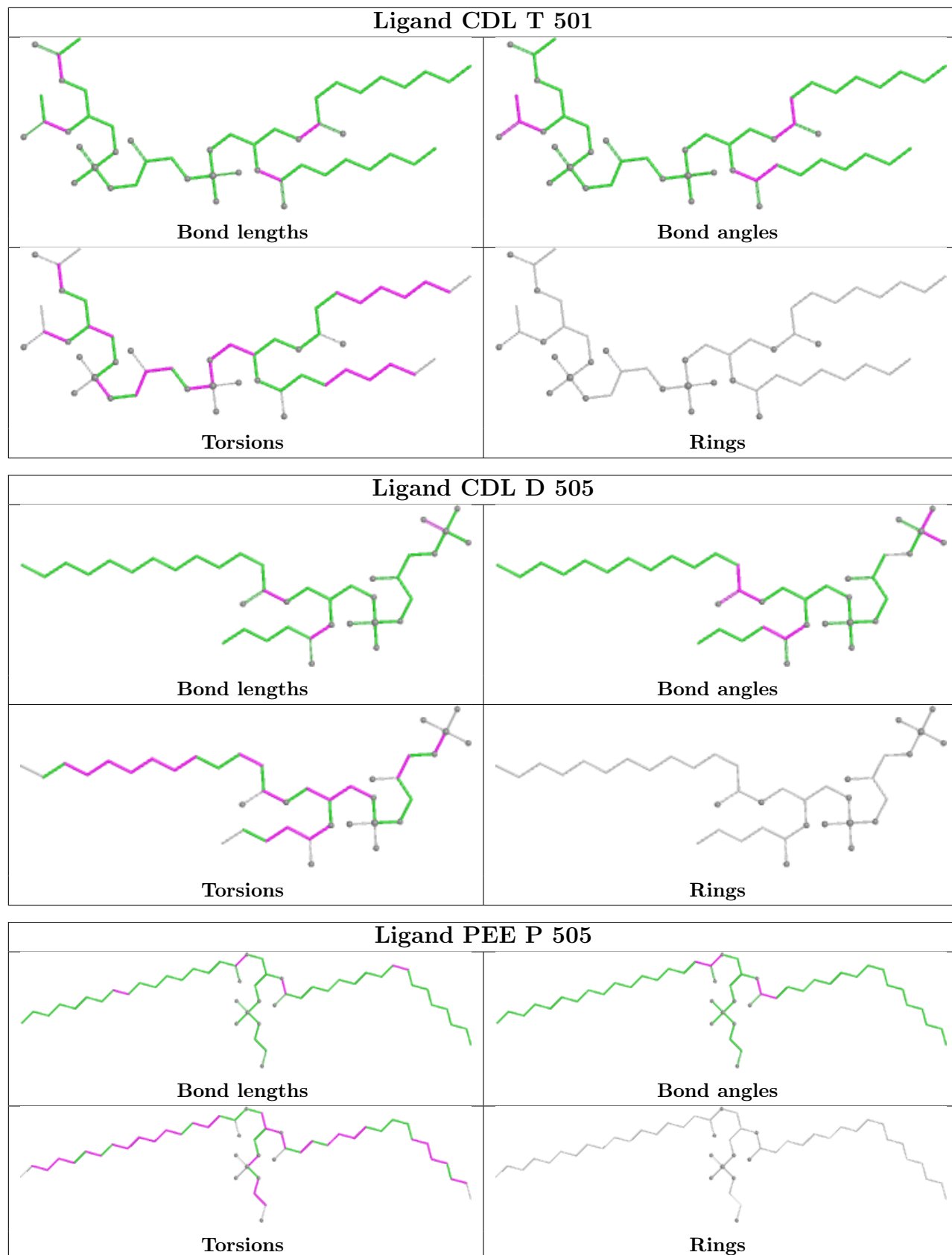
There are no ring outliers.

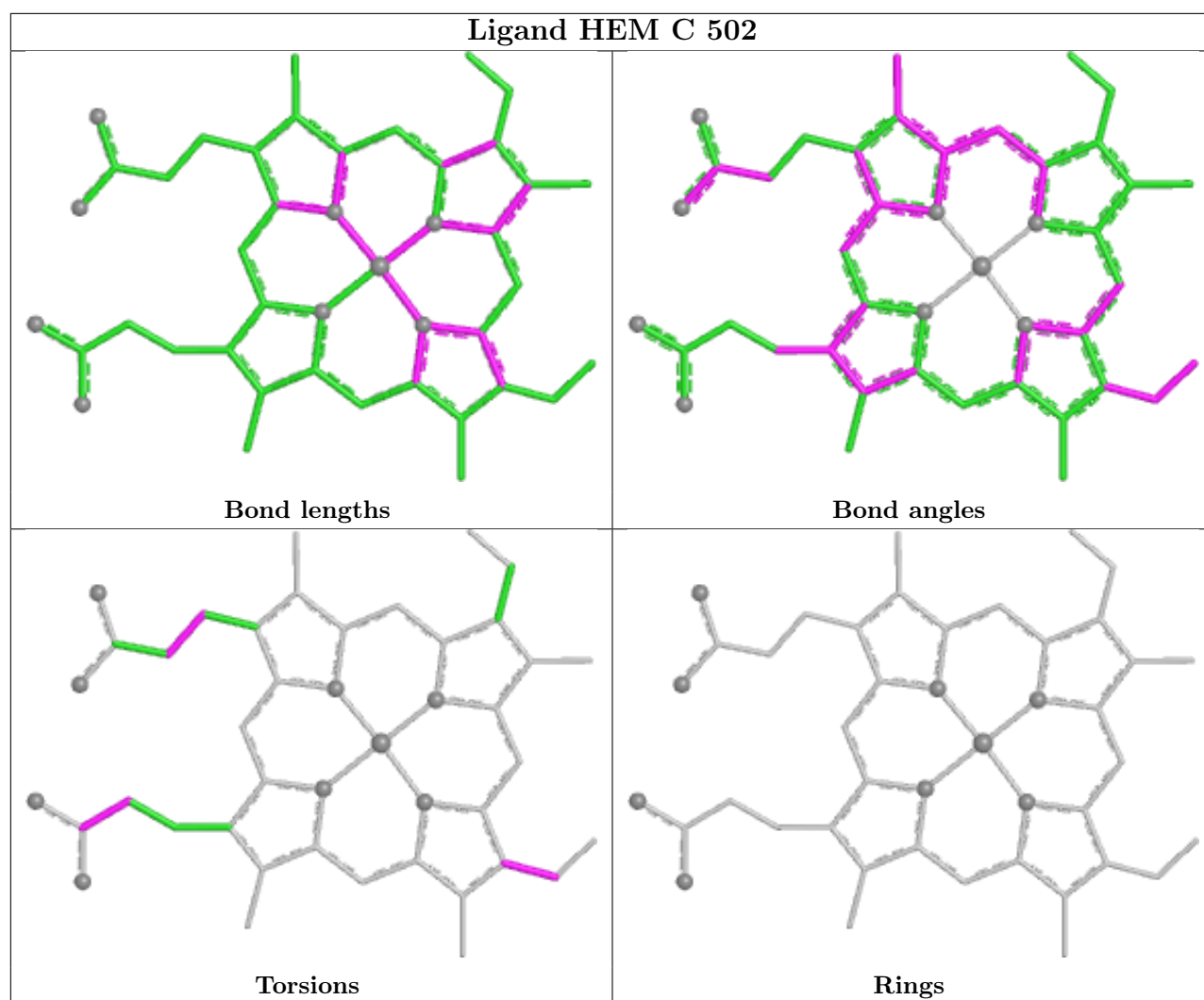
13 monomers are involved in 69 short contacts:

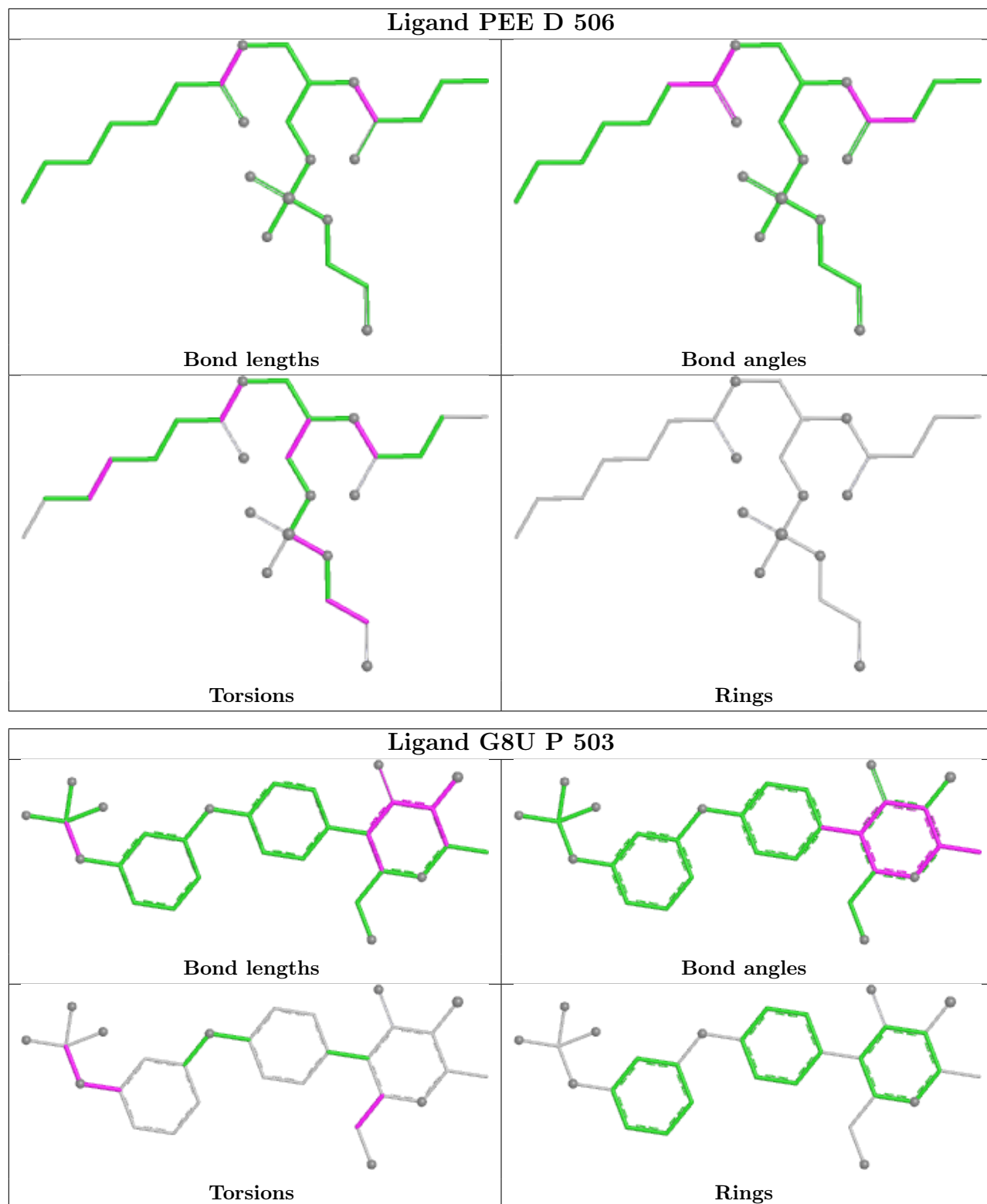
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	T	501	CDL	5	0
16	P	505	PEE	4	0
13	C	502	HEM	3	0
16	D	506	PEE	2	0
14	P	503	G8U	9	0
13	C	501	HEM	5	0
14	C	503	G8U	13	0
17	D	501	HEC	6	0
13	P	502	HEM	2	0
16	Q	506	PEE	4	0
19	R	501	FES	3	0
17	Q	501	HEC	5	0
13	P	501	HEM	10	0

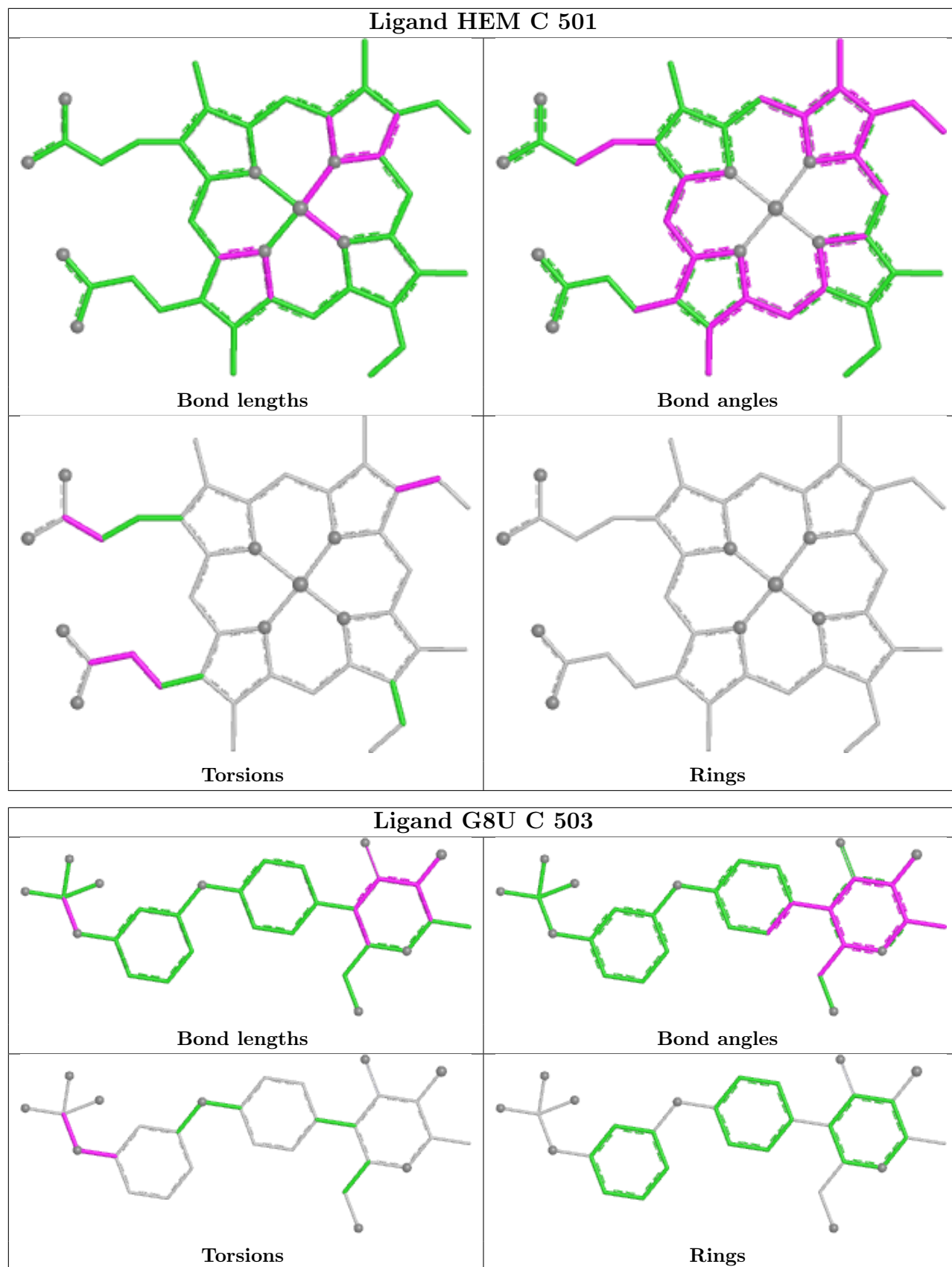
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

equivalents in the CSD to analyse the geometry.

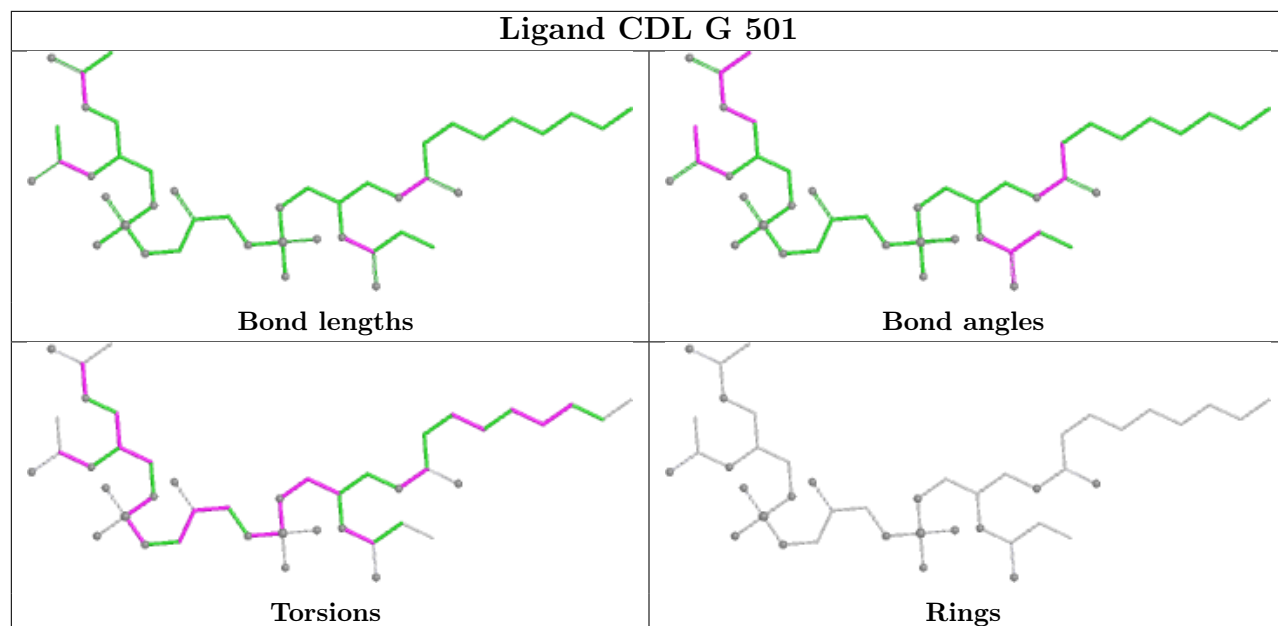




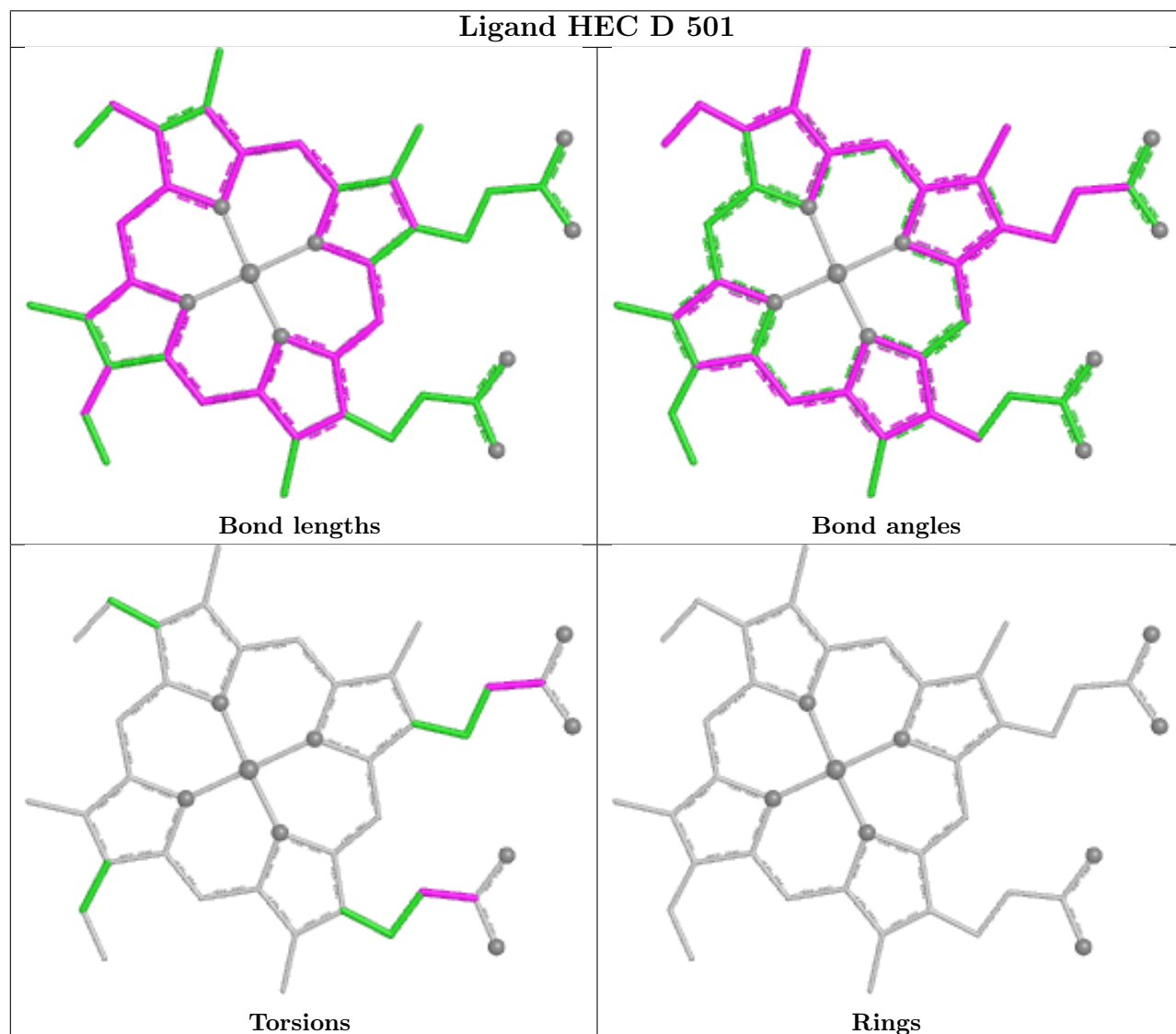


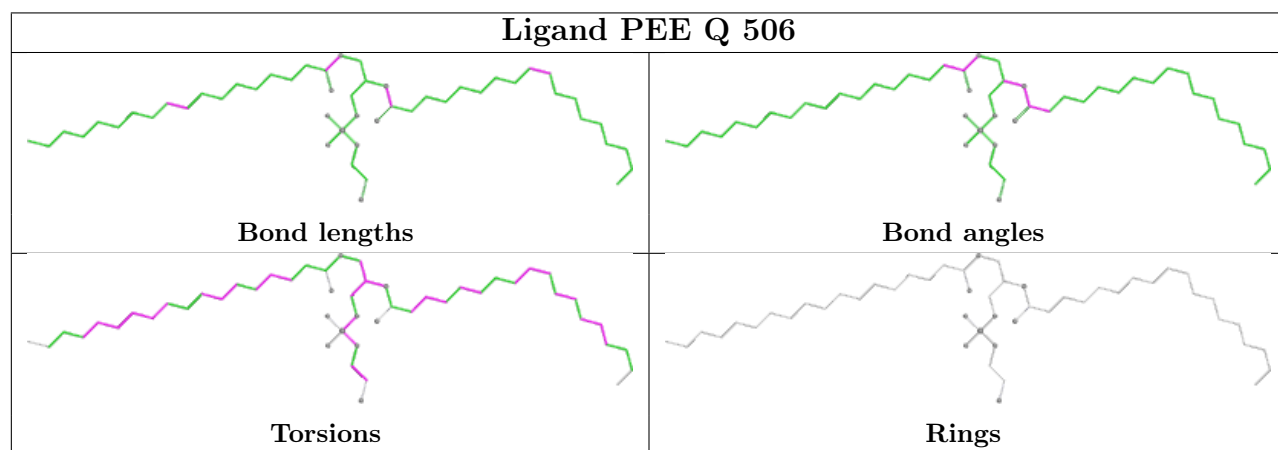
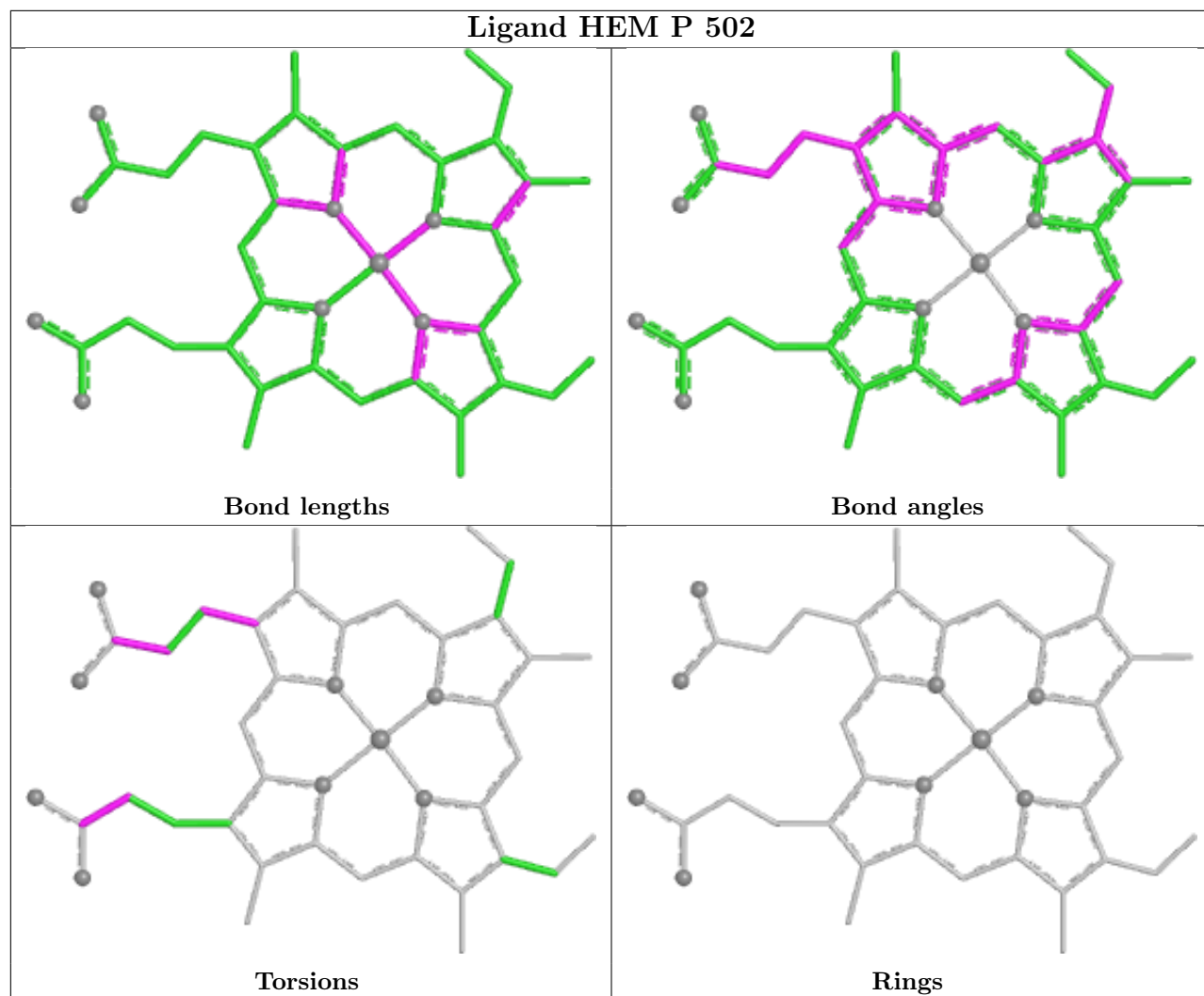


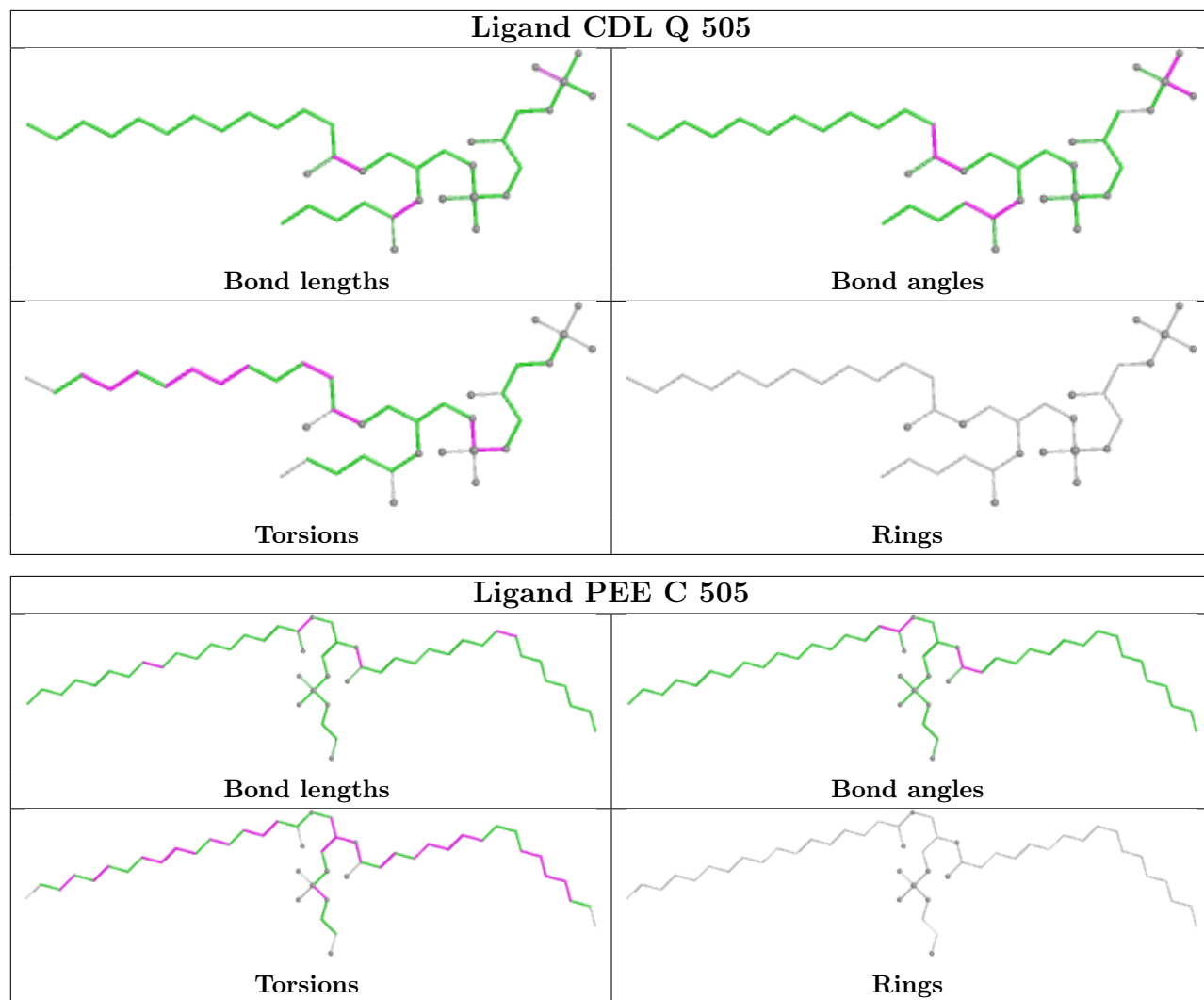
Ligand CDL G 501

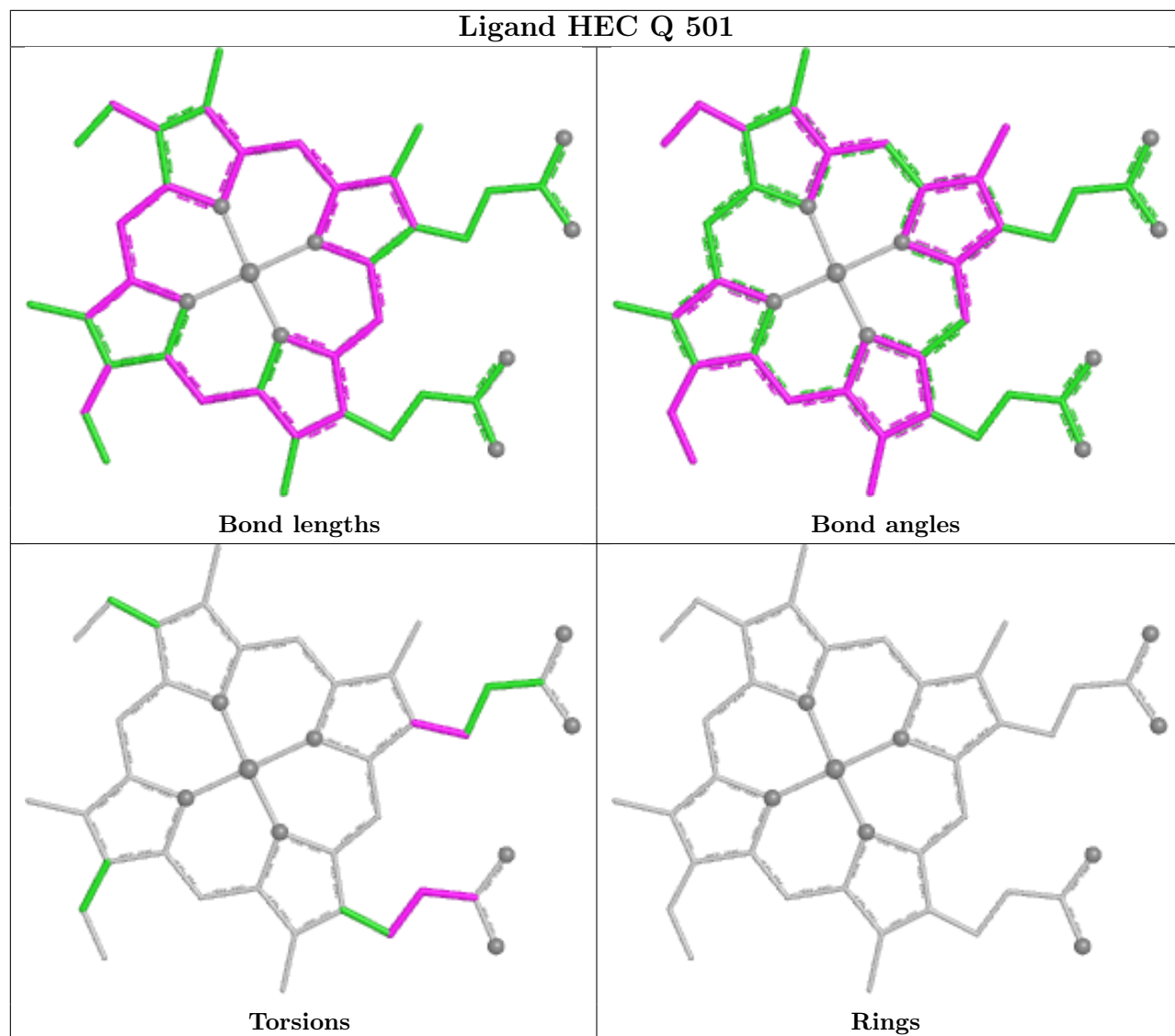


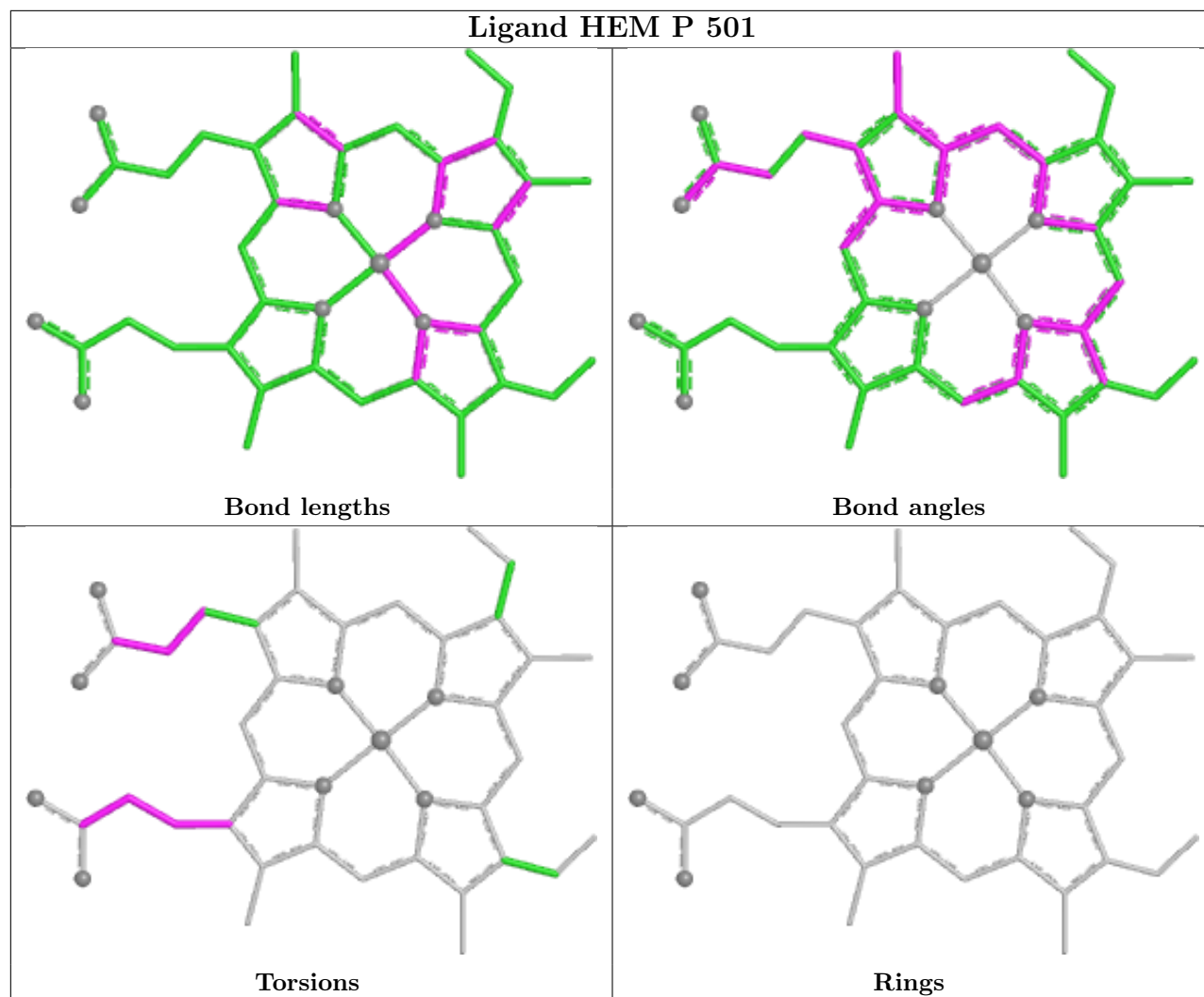
Ligand HEC D 501











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	444/480 (92%)	-0.46	0 100 100	24, 182, 228, 270	0
2	B	422/453 (93%)	-0.27	10 (2%) 59 45	126, 187, 223, 271	0
3	C	374/379 (98%)	-0.47	2 (0%) 87 74	23, 131, 164, 249	0
3	P	370/379 (97%)	-0.34	10 (2%) 56 42	99, 138, 177, 195	0
4	D	240/325 (73%)	-0.50	1 (0%) 88 76	119, 149, 186, 210	0
4	Q	241/325 (74%)	-0.48	0 100 100	115, 162, 198, 232	0
5	E	73/274 (26%)	-0.33	0 100 100	123, 155, 194, 211	0
5	I	27/274 (9%)	0.19	2 (7%) 20 20	168, 214, 255, 306	0
5	R	196/274 (71%)	-0.41	2 (1%) 79 62	30, 190, 238, 288	0
6	F	98/111 (88%)	-0.39	0 100 100	121, 153, 190, 200	0
6	S	99/111 (89%)	-0.40	1 (1%) 79 62	117, 148, 182, 208	0
7	G	80/82 (97%)	-0.38	1 (1%) 75 58	30, 149, 204, 273	0
7	T	74/82 (90%)	-0.38	1 (1%) 73 56	114, 156, 198, 212	0
8	H	65/91 (71%)	-0.35	0 100 100	130, 160, 190, 202	0
8	U	66/91 (72%)	-0.59	0 100 100	161, 190, 238, 284	0
9	J	58/64 (90%)	-0.43	0 100 100	131, 158, 191, 222	0
9	W	59/64 (92%)	-0.73	0 100 100	115, 150, 186, 198	0
10	N	444/480 (92%)	-0.40	3 (0%) 84 69	24, 162, 208, 261	0
11	O	419/453 (92%)	-0.33	2 (0%) 87 74	30, 176, 212, 247	0
12	V	17/274 (6%)	-0.06	1 (5%) 28 25	174, 195, 225, 228	0
All	All	3866/5066 (76%)	-0.40	36 (0%) 81 65	23, 162, 216, 306	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	75	ALA	5.0
6	S	38	HIS	3.9
3	P	104	TYR	3.7
11	O	302	GLY	3.7
10	N	424	GLY	3.5
3	P	206	ASN	3.5
3	P	106	SER	3.4
2	B	313	ASN	3.4
5	R	174	GLY	3.4
5	I	73	PRO	3.2
3	C	379	TRP	3.0
10	N	242	CYS	3.0
3	C	201	HIS	2.9
3	P	14	VAL	2.9
2	B	397	THR	2.7
3	P	313	ARG	2.5
3	P	210	GLY	2.5
2	B	276	GLN	2.4
3	P	102	LEU	2.4
2	B	21	PRO	2.4
3	P	105	GLY	2.4
2	B	391	SER	2.3
10	N	393	ALA	2.3
11	O	368	TYR	2.2
2	B	396	SER	2.2
5	R	13	TYR	2.2
2	B	138	ALA	2.1
2	B	280	GLY	2.1
3	P	11	MET	2.1
4	D	180	SER	2.1
2	B	312	PHE	2.1
2	B	126	VAL	2.1
12	V	71	ASN	2.1
5	I	74	ALA	2.1
3	P	205	SER	2.1
7	T	32	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

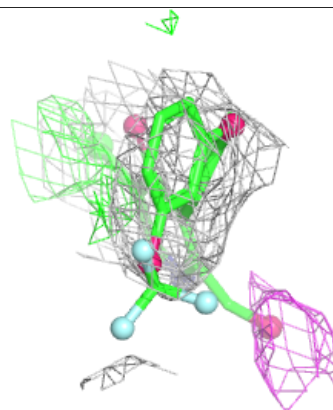
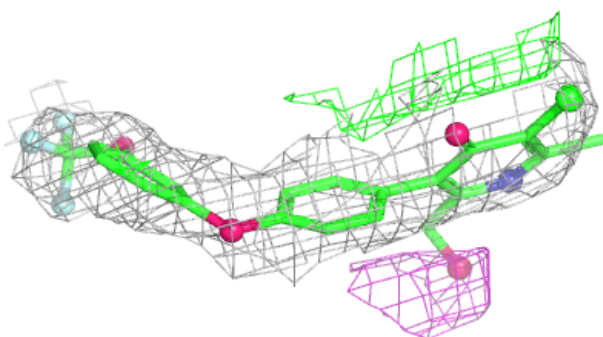
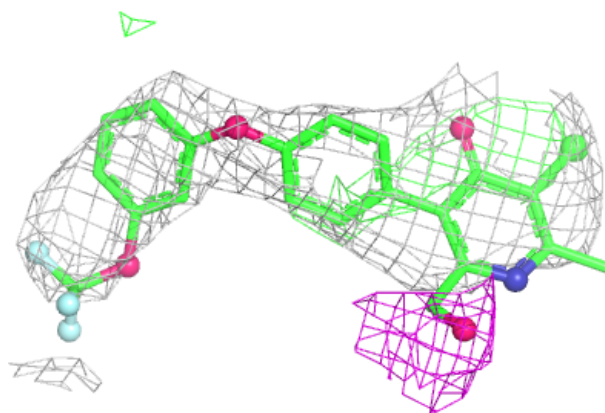
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	PO4	P	504	5/5	0.60	0.09	159,166,173,174	0
15	PO4	N	501	5/5	0.63	0.12	155,167,169,176	0
15	PO4	F	501	5/5	0.64	0.09	251,252,258,259	0
15	PO4	D	503	5/5	0.73	0.08	212,225,230,231	0
15	PO4	E	501	5/5	0.74	0.08	142,147,152,152	0
15	PO4	C	504	5/5	0.77	0.10	156,159,161,168	0
15	PO4	D	504	5/5	0.78	0.07	246,252,254,257	0
15	PO4	D	502	5/5	0.80	0.06	234,240,241,242	0
15	PO4	S	501	5/5	0.86	0.05	268,268,275,278	0
14	G8U	P	503	29/29	0.87	0.17	125,164,212,219	0
14	G8U	C	503	29/29	0.87	0.19	128,171,211,230	0
16	PEE	Q	506	51/51	0.94	0.15	125,148,166,171	0
18	CDL	D	505	39/100	0.94	0.09	112,152,165,174	0
18	CDL	Q	505	39/100	0.94	0.08	116,140,173,174	0
18	CDL	T	501	49/100	0.94	0.09	111,152,190,204	0
20	GOL	R	502	6/6	0.94	0.16	215,221,224,225	0
16	PEE	D	506	26/51	0.95	0.11	124,151,176,178	0
18	CDL	G	501	44/100	0.96	0.08	111,137,175,179	0
19	FES	R	501	4/4	0.97	0.03	200,213,218,224	0
16	PEE	C	505	49/51	0.98	0.10	113,144,173,183	0
17	HEC	D	501	43/43	0.98	0.10	125,134,153,161	0
13	HEM	P	502	43/43	0.98	0.09	100,107,130,132	0
16	PEE	P	505	49/51	0.98	0.11	129,146,172,180	0
13	HEM	C	502	43/43	0.99	0.06	96,108,120,147	0
17	HEC	Q	501	43/43	0.99	0.06	119,145,161,164	0
13	HEM	P	501	43/43	0.99	0.07	113,130,145,151	0
13	HEM	C	501	43/43	0.99	0.09	110,118,132,142	0

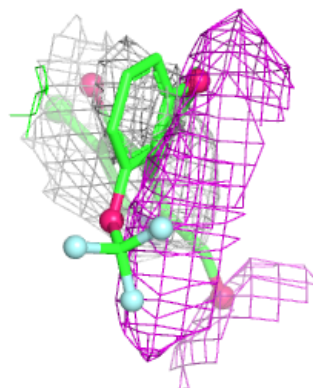
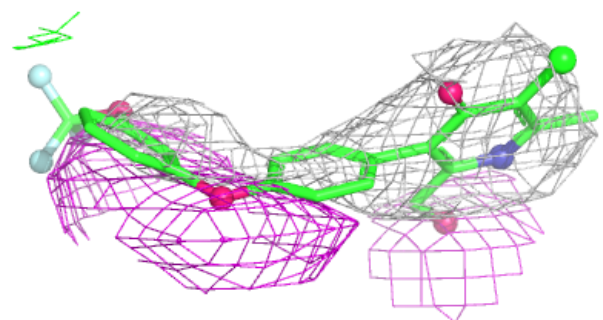
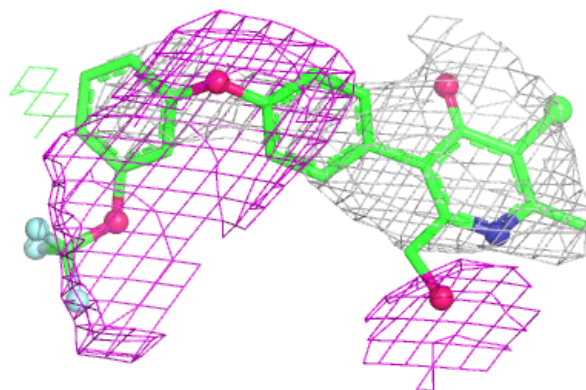
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around G8U P 503:

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

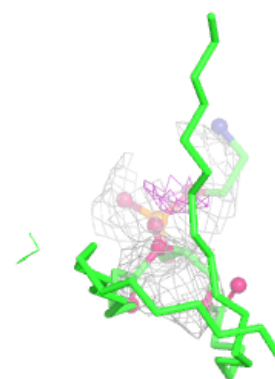
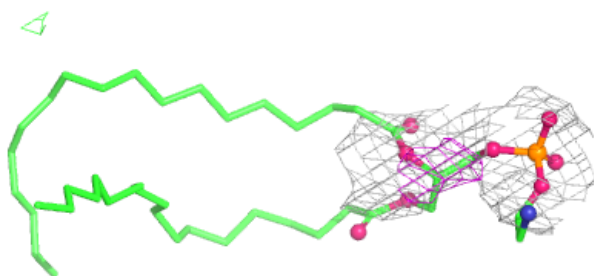
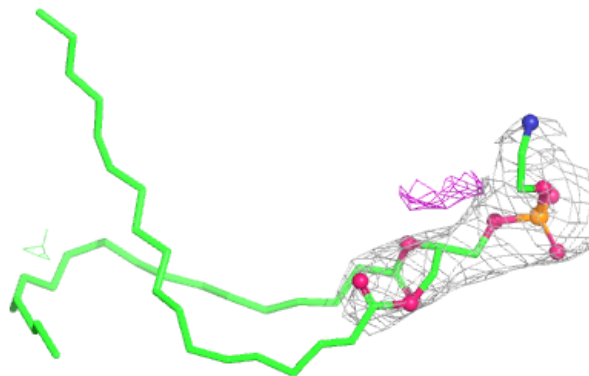
**Electron density around G8U C 503:**

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

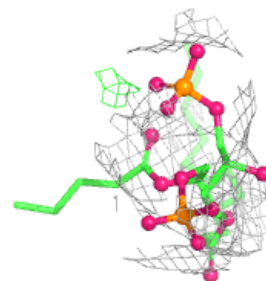
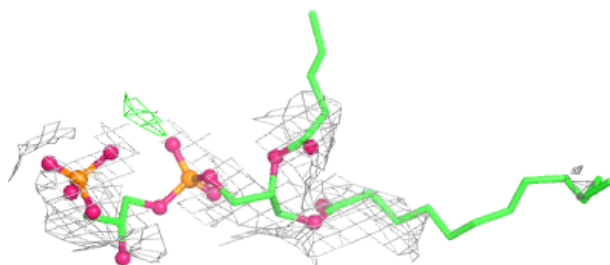
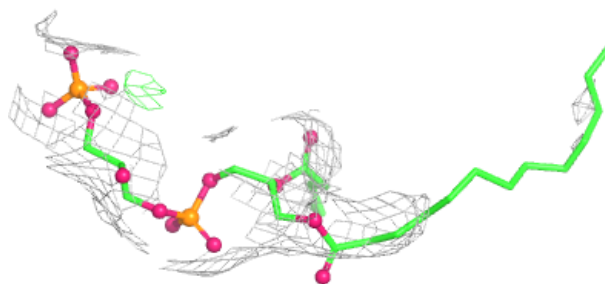


Electron density around PEE Q 506:

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

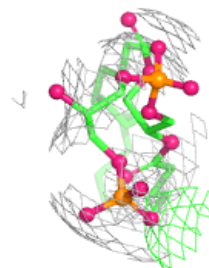
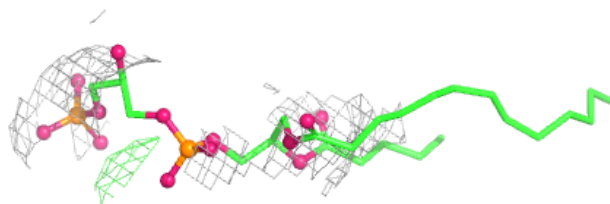
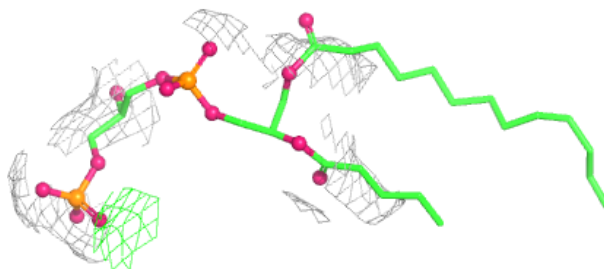
**Electron density around CDL D 505:**

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and green (positive)

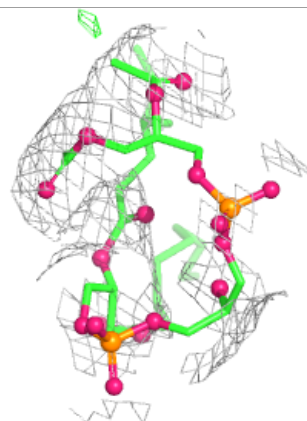
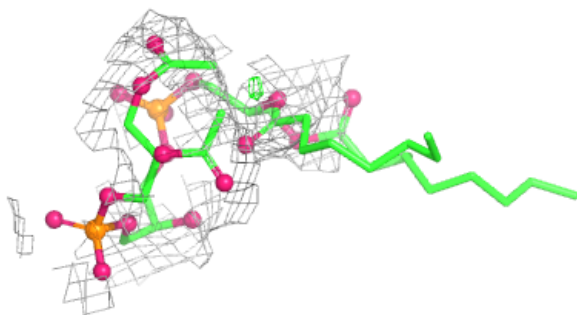
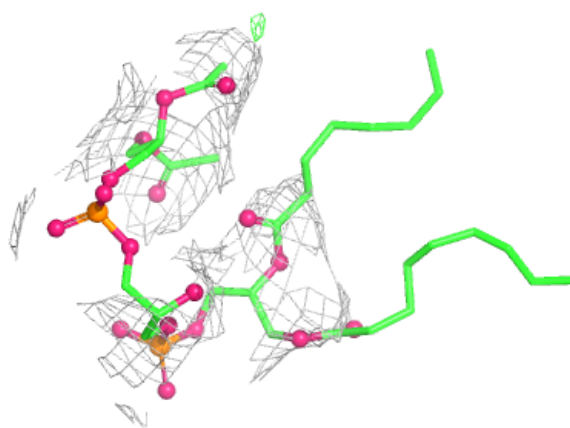


Electron density around CDL Q 505:

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and green (positive)

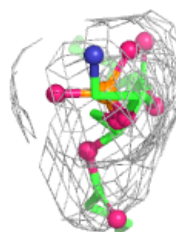
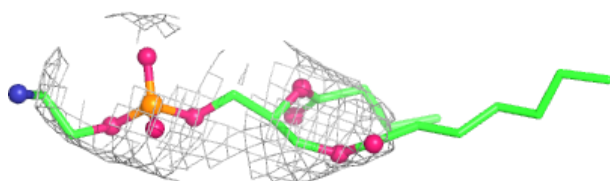
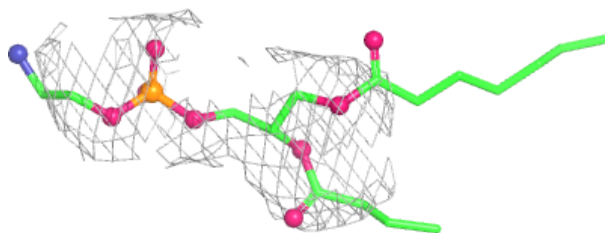
**Electron density around CDL T 501:**

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

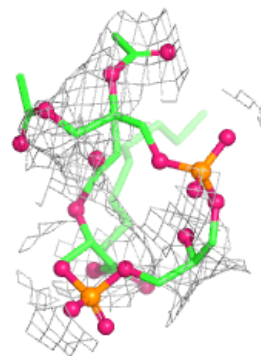
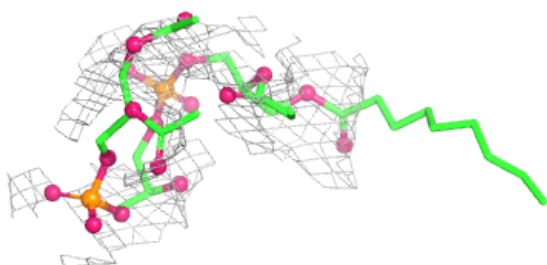
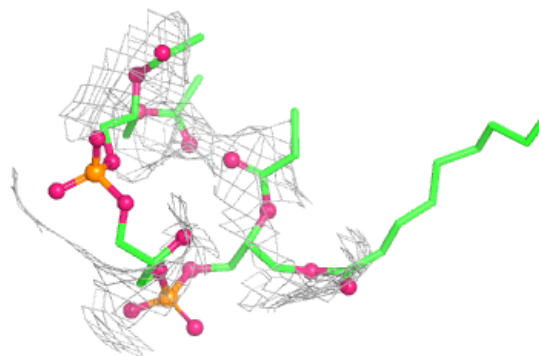


Electron density around PEE D 506:

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

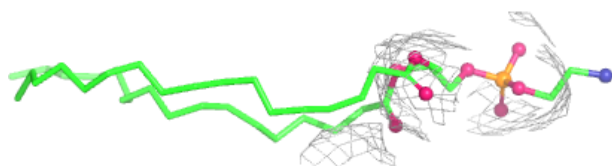
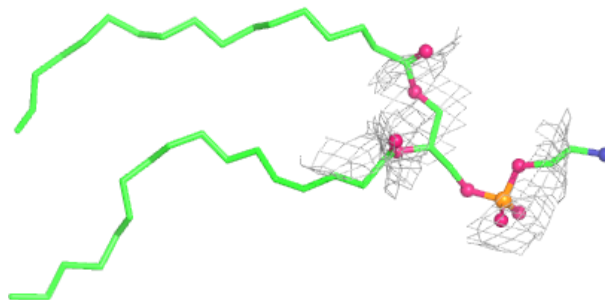
**Electron density around CDL G 501:**

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and green (positive)

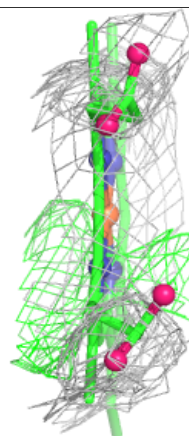
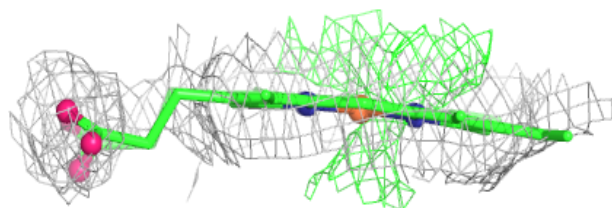
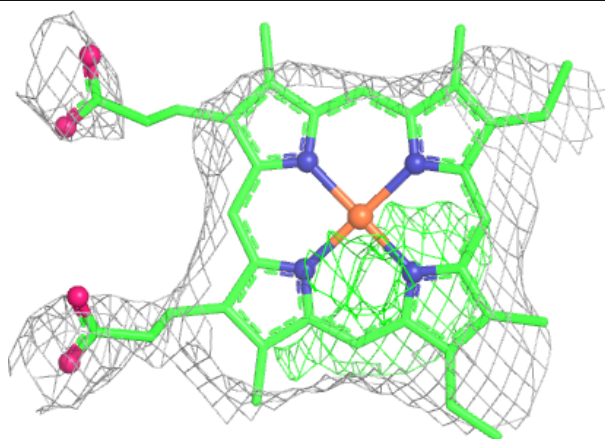


Electron density around PEE C 505:

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and green (positive)

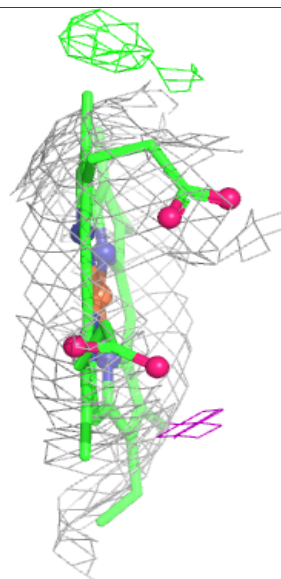
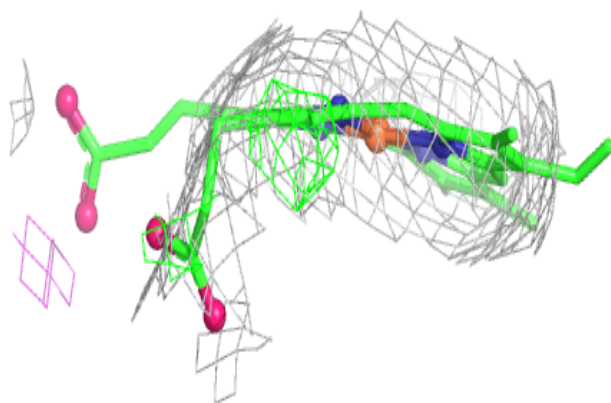
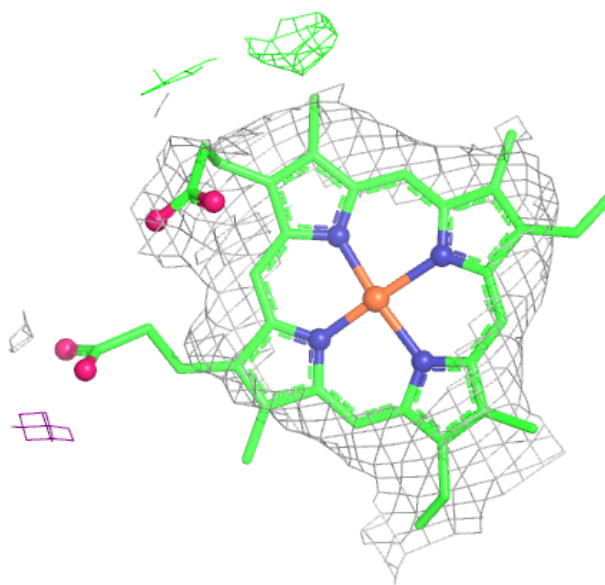
**Electron density around HEC D 501:**

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



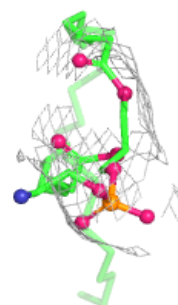
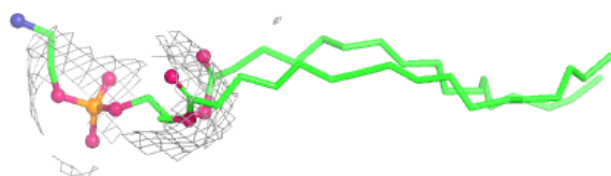
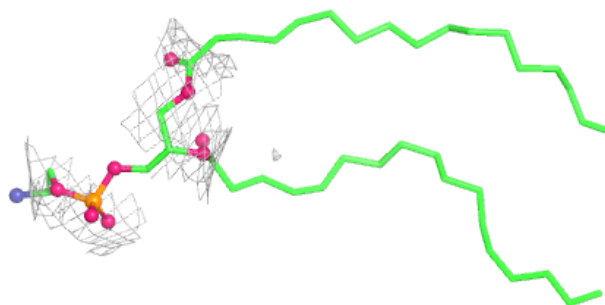
Electron density around HEM P 502:

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



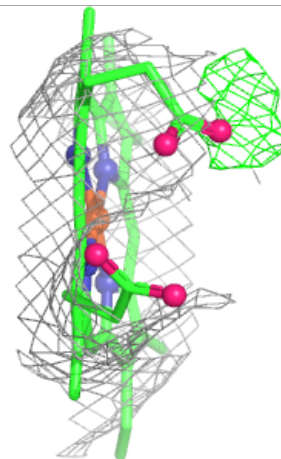
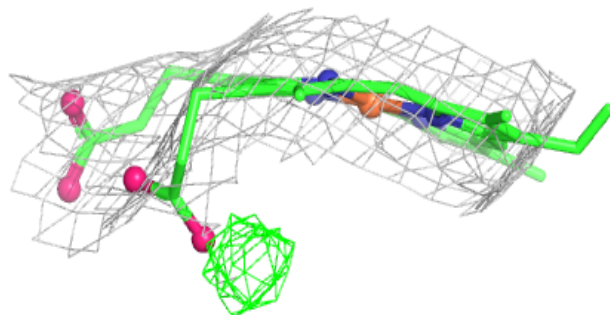
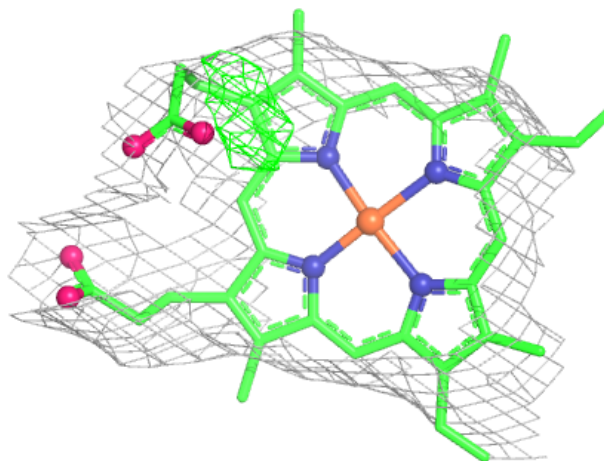
Electron density around PEE P 505:

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



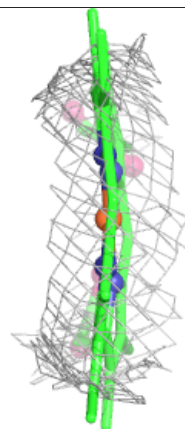
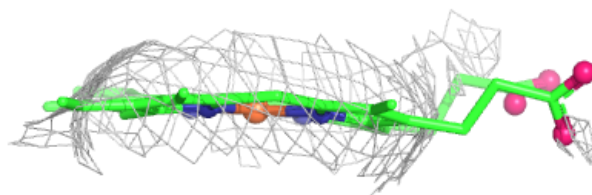
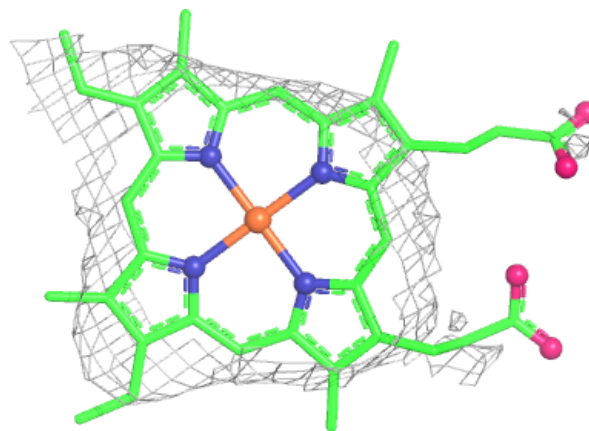
Electron density around HEM C 502:

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



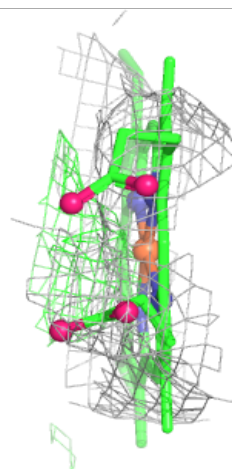
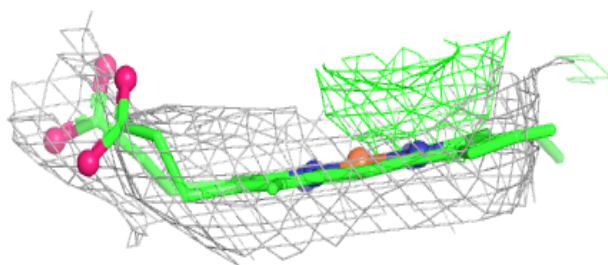
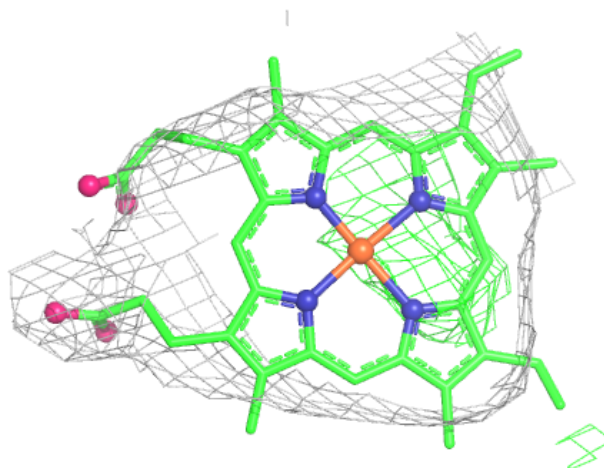
Electron density around HEC Q 501:

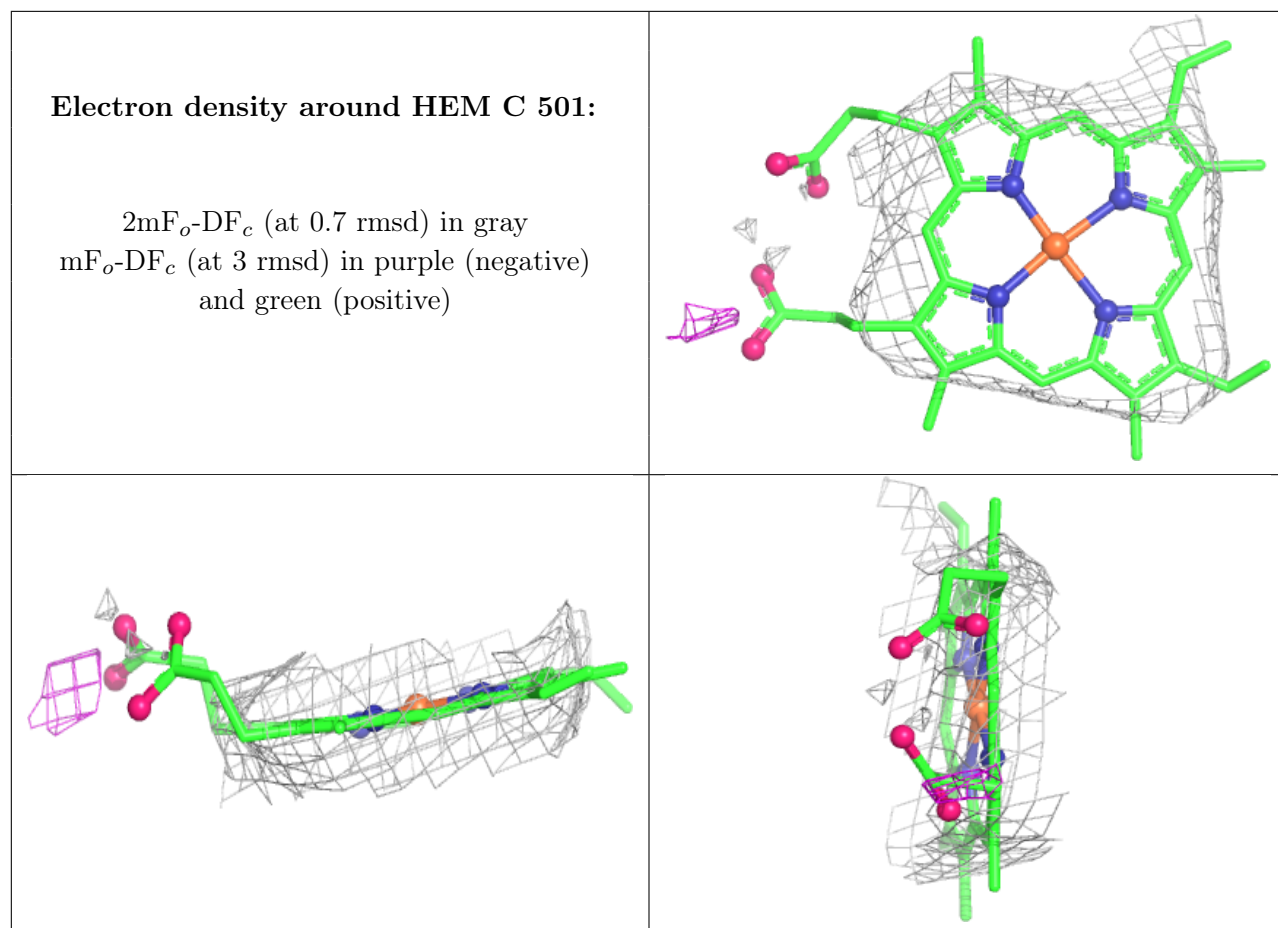
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM P 501:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.