



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:01 AM UTC

PDB ID : 4D6T / pdb_00004d6t
Title : Cytochrome bc1 bound to the 4(1H)-pyridone GW844520
Authors : Capper, M.J.; O'Neill, P.M.; Fisher, N.; Strange, R.W.; Moss, D.; Ward, S.A.;
Berry, N.G.; Lawrenson, A.S.; Hasnain, S.S.; Biagini, G.A.; Antonyuk, S.V.
Deposited on : 2014-11-14
Resolution : 3.57 Å(reported)

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

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

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

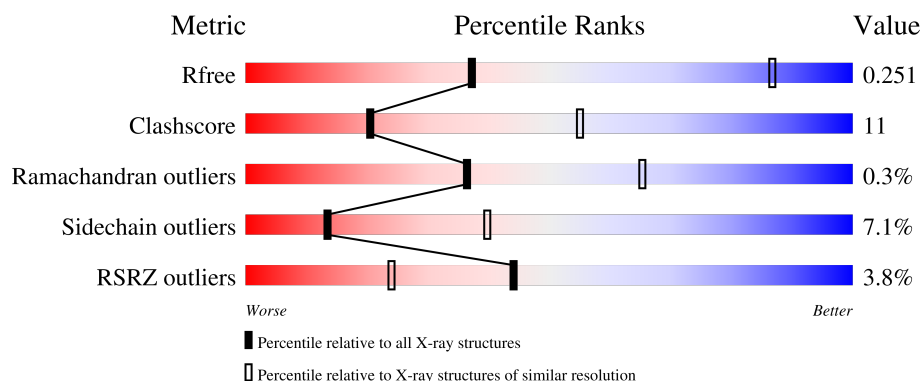
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.57 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1521 (3.66-3.50)
Clashscore	190562	1595 (3.66-3.50)
Ramachandran outliers	187476	1551 (3.66-3.50)
Sidechain outliers	187428	1551 (3.66-3.50)
RSRZ outliers	180081	1520 (3.66-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	5% 74% 17% .. 8%
1	N	480	5% 75% 16% • 8%
2	B	453	3% 71% 19% .. 7%
3	C	379	2% 73% 21% • •
3	P	379	0% 75% 19% • •

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	PEE	C	505	X	-	-	-
15	PEE	D	506	X	-	-	-
15	PEE	P	505	X	-	-	-
15	PEE	Q	506	X	-	-	-
18	FES	R	501	-	-	X	-

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 31051 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

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

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

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

- Molecule 3 is a protein called CYTOCHROME B.

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

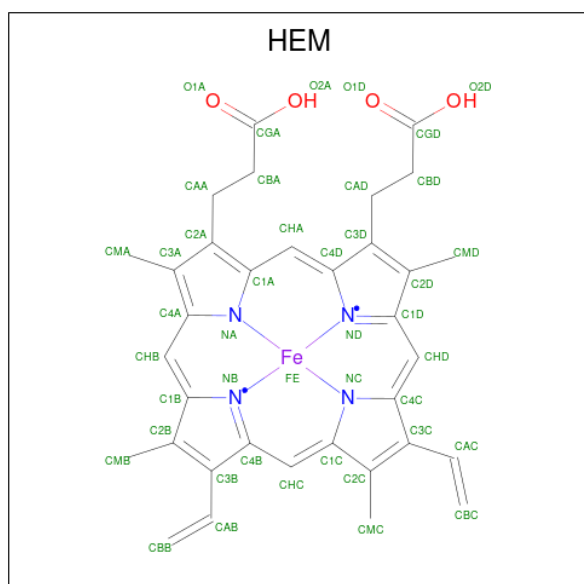
There is a discrepancy between the modelled and reference sequences:

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

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

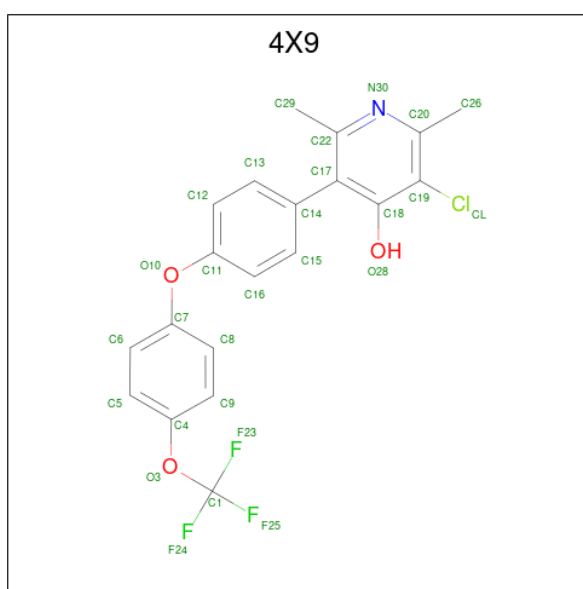
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	V	17	Total	C	N	O	0	0	0
			127	81	24	22			

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



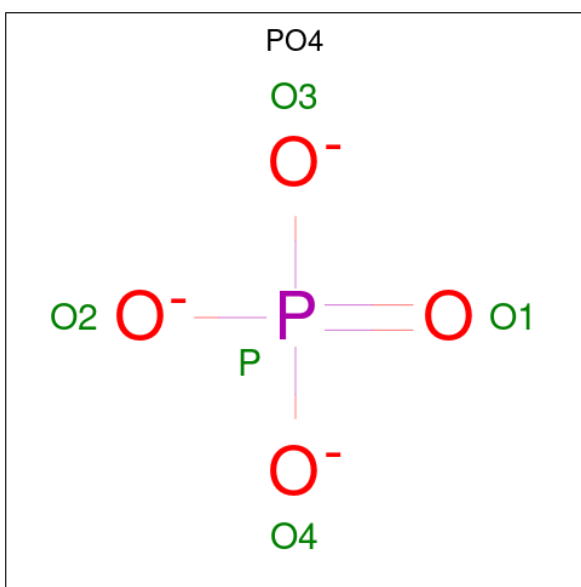
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
12	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 13 is 3-chloro-2,6-dimethyl-5-{4-[4-(trifluoromethoxy)phenoxy]phenyl}pyridin-4-ol (CCD ID: 4X9) (formula: C₂₀H₁₅ClF₃NO₃).



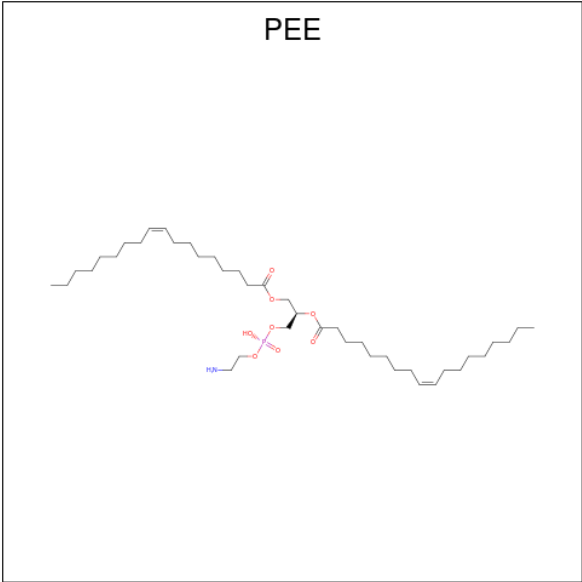
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total	C	Cl	F	N	O	0
			28	20	1	3	1	3	0
13	P	1	Total	C	Cl	F	N	O	0
			28	20	1	3	1	3	0

- Molecule 14 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



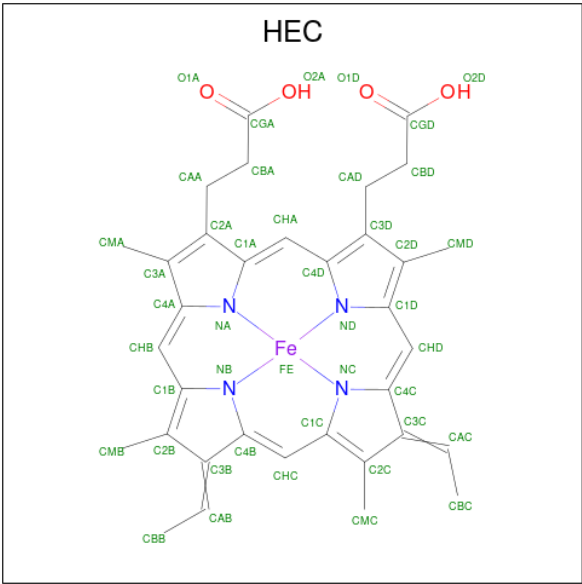
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total	O	P	0	0
			5	4	1		
14	D	1	Total	O	P	0	0
			5	4	1		
14	D	1	Total	O	P	0	0
			5	4	1		
14	D	1	Total	O	P	0	0
			5	4	1		
14	E	1	Total	O	P	0	0
			5	4	1		
14	F	1	Total	O	P	0	0
			5	4	1		
14	N	1	Total	O	P	0	0
			5	4	1		
14	N	1	Total	O	P	0	0
			5	4	1		
14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

- Molecule 15 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).



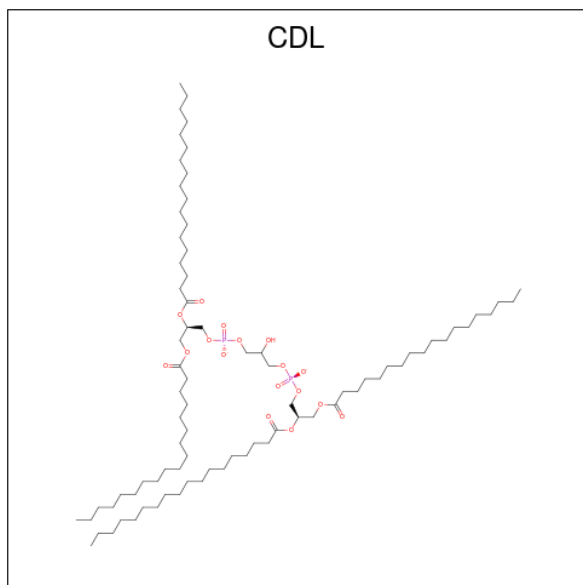
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
15	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
15	D	1	Total	C	N	O	P	0	0
			26	16	1	8	1		
15	P	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
15	Q	1	Total	C	N	O	P	0	0
			51	41	1	8	1		

- Molecule 16 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄).



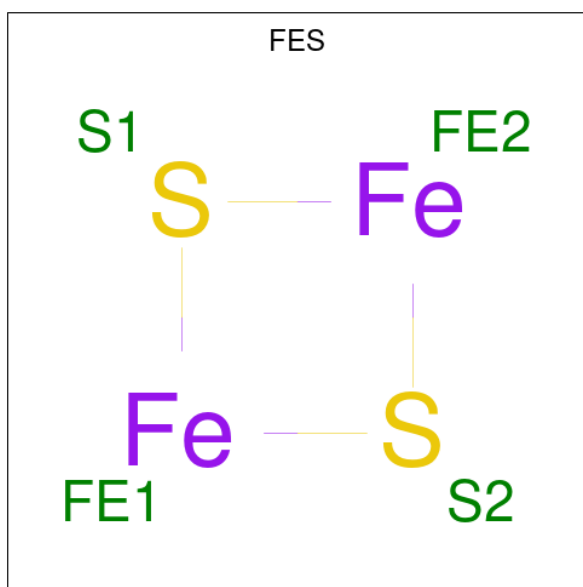
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	
16	Q	1	Total	C	Fe	N	O	
			43	34	1	4	4	

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



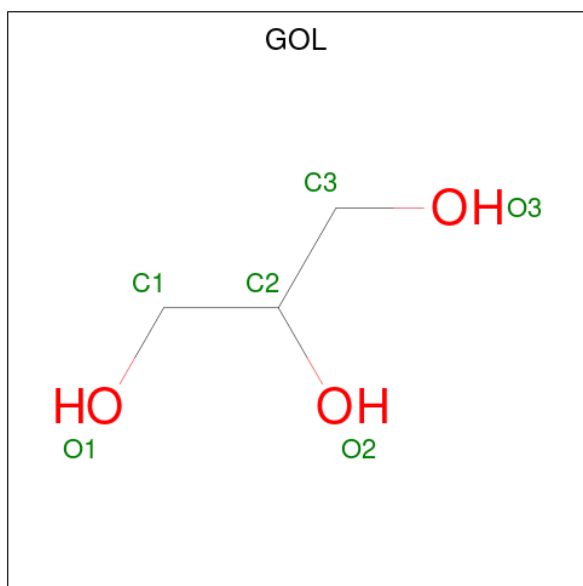
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	D	1	Total	C	O	P		
			39	24	13	2	0	0
17	G	1	Total	C	O	P		
			44	25	17	2	0	0
17	Q	1	Total	C	O	P		
			39	24	13	2	0	0
17	T	1	Total	C	O	P		
			49	30	17	2	0	0

- Molecule 18 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 19 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

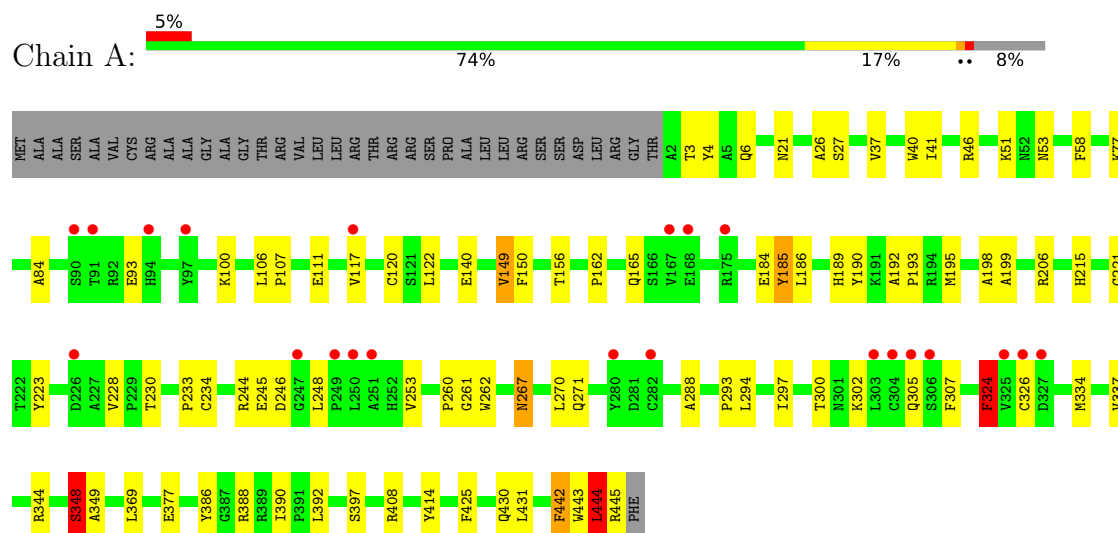


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	R	1	Total	C	O	0	0
			6	3	3		

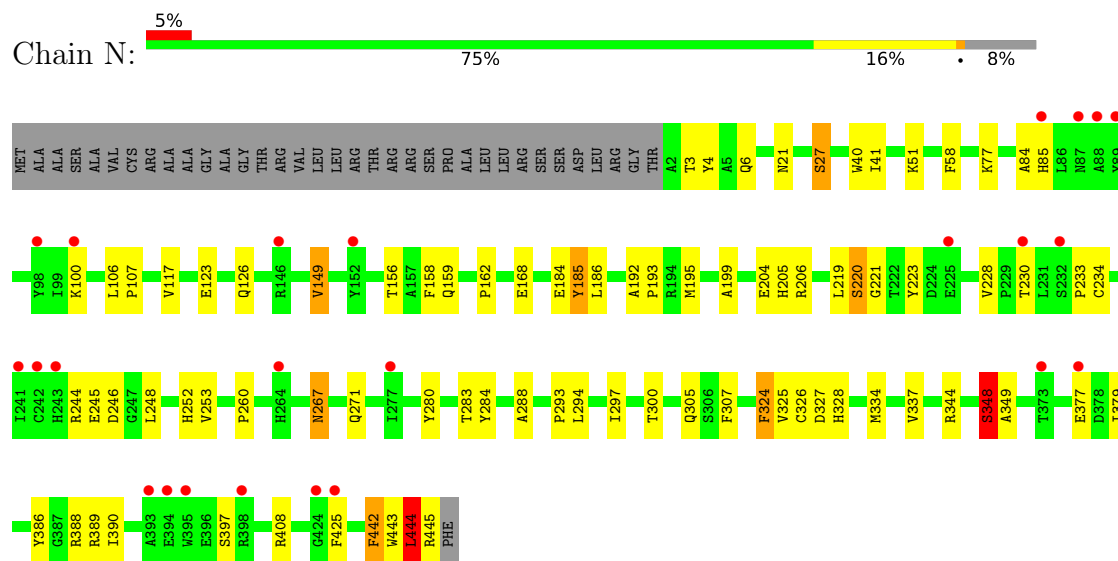
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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

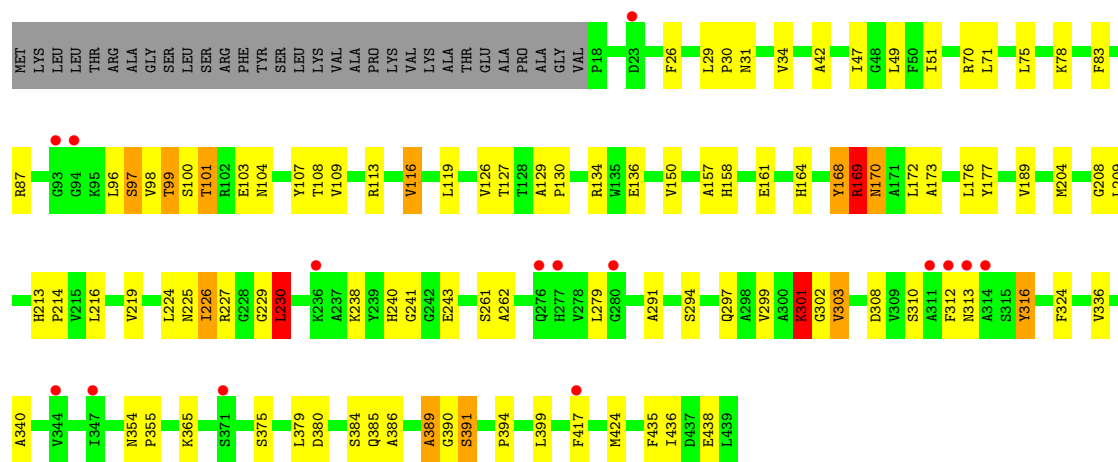


• Molecule 1: CYTOCHROME B-C1 COMPLEX SUBUNIT 1, MITOCHONDRIAL

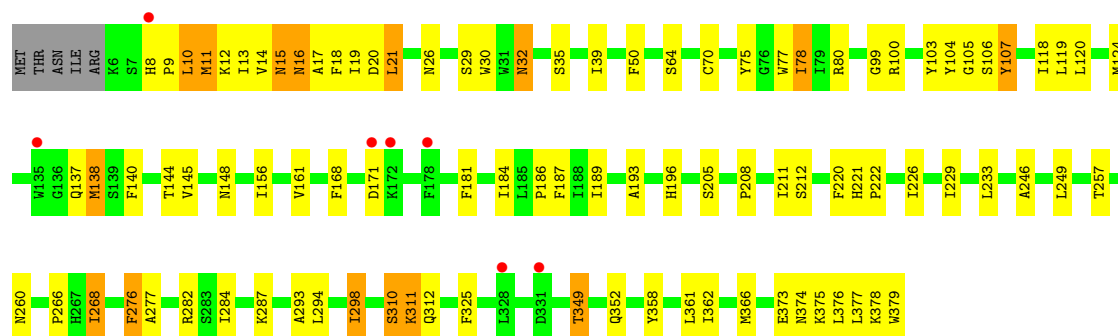
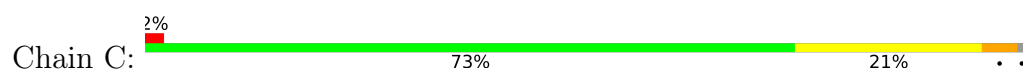


• Molecule 2: CYTOCHROME B-C1 COMPLEX SUBUNIT 2, MITOCHONDRIAL

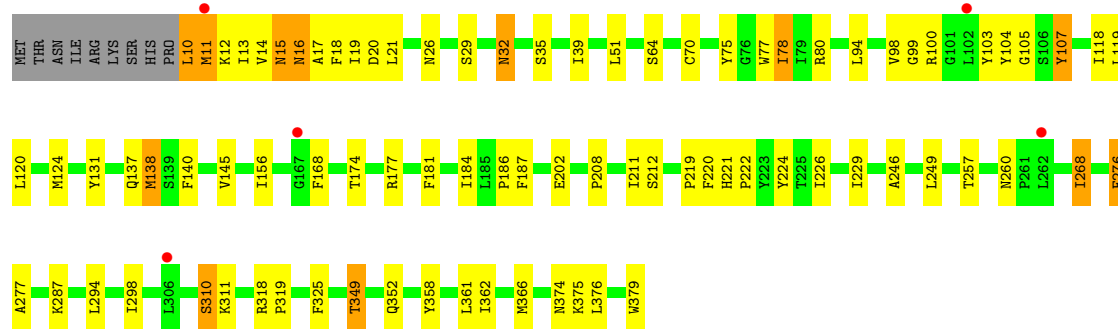
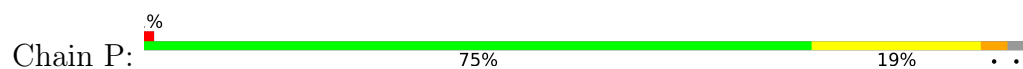




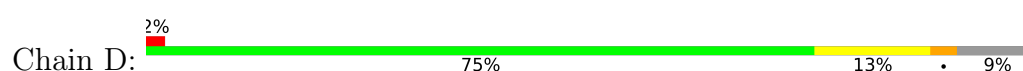
• Molecule 3: CYTOCHROME B



• Molecule 3: CYTOCHROME B

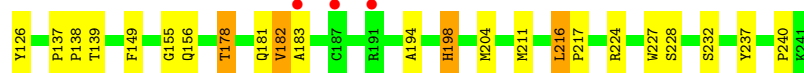
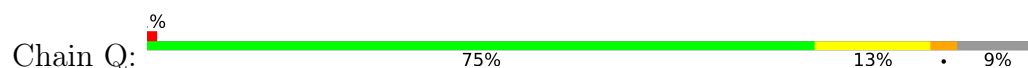


• Molecule 4: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL

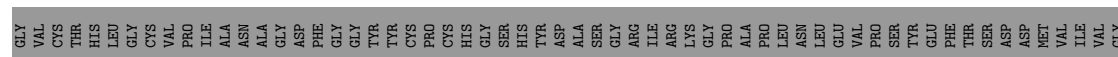
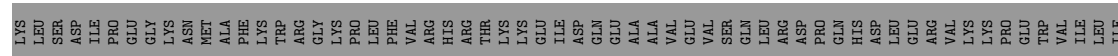
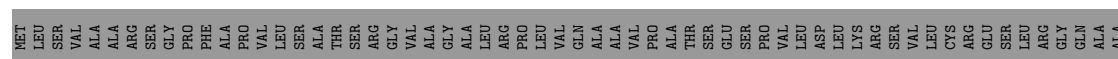




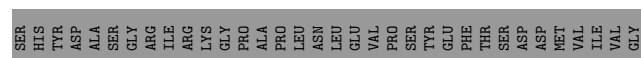
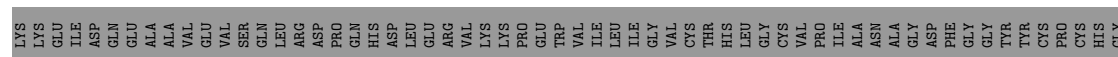
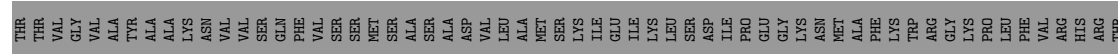
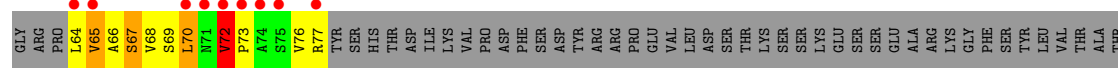
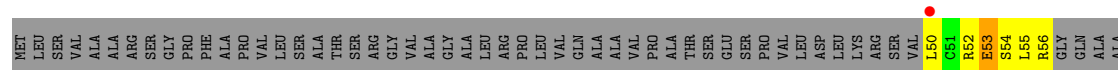
• Molecule 4: CYTOCHROME C1, HEME PROTEIN, MITOCHONDRIAL



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

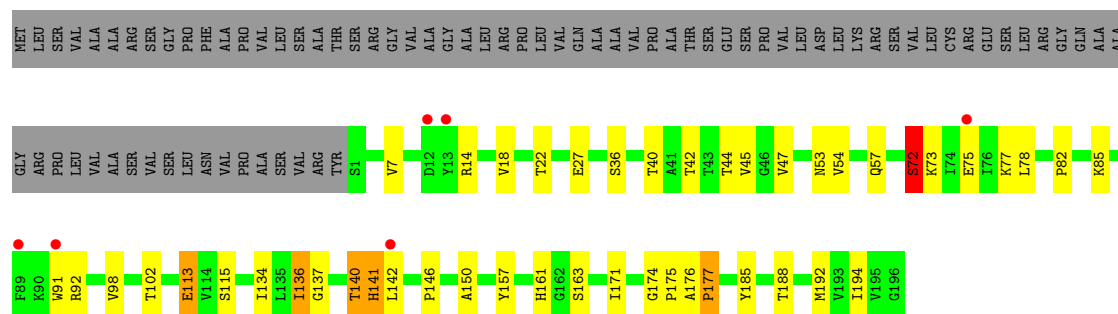


• Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL

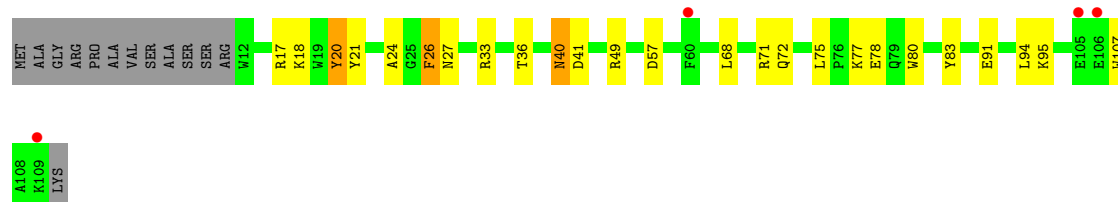


• Molecule 5: CYTOCHROME B-C1 COMPLEX SUBUNIT RIESKE, MITOCHONDRIAL





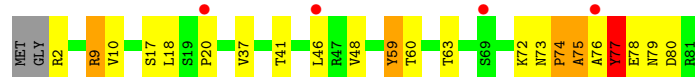
• Molecule 6: CYTOCHROME B-C1 COMPLEX SUBUNIT 7



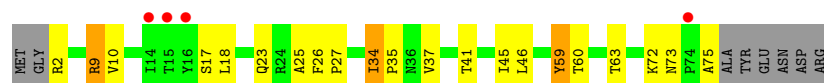
• Molecule 6: CYTOCHROME B-C1 COMPLEX SUBUNIT 7



• Molecule 7: CYTOCHROME B-C1 COMPLEX SUBUNIT 8

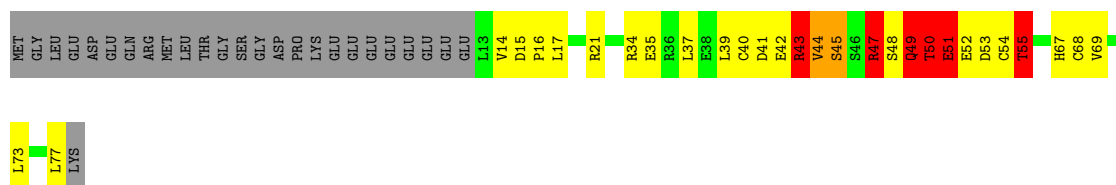


• Molecule 7: CYTOCHROME B-C1 COMPLEX SUBUNIT 8

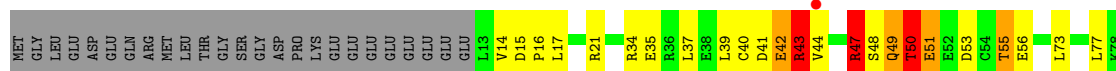


• Molecule 8: CYTOCHROME B-C1 COMPLEX SUBUNIT 6, MITOCHONDRIAL

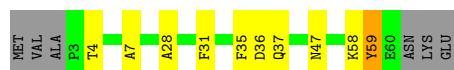




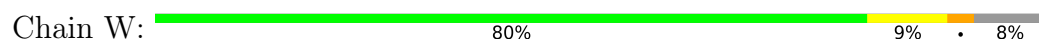
- Molecule 8: CYTOCHROME B-C1 COMPLEX SUBUNIT 6, MITOCHONDRIAL



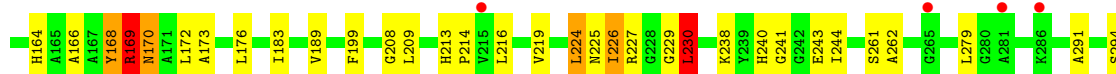
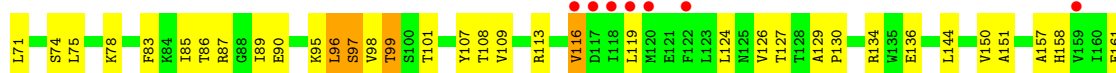
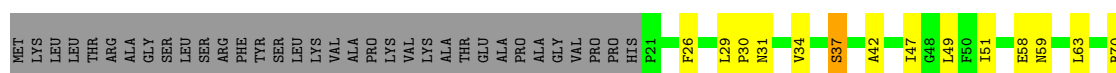
- Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT 9



- Molecule 9: CYTOCHROME B-C1 COMPLEX SUBUNIT 9



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



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



[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	129.90Å 129.90Å 722.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.57 50.00 – 3.57	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-3.57) 99.9 (50.00-3.57)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.206 , 0.252 0.207 , 0.251	Depositor DCC
R_{free} test set	3954 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	122.6	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 67.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.064 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	31051	wwPDB-VP
Average B, all atoms (Å ²)	135.0	wwPDB-VP

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

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, PEE, GOL, CDL, HEC, 4X9, PO4, FES

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	0.60	1/3511 (0.0%)	0.93	8/4766 (0.2%)
1	N	0.58	0/3503	0.94	9/4755 (0.2%)
2	B	0.80	3/3224 (0.1%)	1.20	15/4375 (0.3%)
3	C	0.68	0/3065	0.97	3/4196 (0.1%)
3	P	0.65	0/3031	0.99	4/4150 (0.1%)
4	D	0.58	0/1971	0.90	2/2676 (0.1%)
4	Q	0.60	0/1977	0.88	2/2684 (0.1%)
5	E	0.57	0/557	0.94	0/752
5	I	0.84	0/156	1.58	2/209 (1.0%)
5	R	0.64	0/1552	1.15	9/2100 (0.4%)
6	F	0.59	0/879	0.87	0/1180
6	S	0.59	0/888	0.86	0/1191
7	G	0.64	1/699 (0.1%)	1.77	13/946 (1.4%)
7	T	0.66	0/645	1.03	4/873 (0.5%)
8	H	2.23	6/534 (1.1%)	1.82	14/718 (1.9%)
8	U	1.56	5/543 (0.9%)	1.77	9/729 (1.2%)
9	J	0.60	0/495	0.85	0/667
9	W	0.61	0/500	0.86	0/675
10	O	0.67	2/3197 (0.1%)	1.30	16/4336 (0.4%)
11	V	0.85	0/129	1.24	0/177
All	All	0.73	18/31056 (0.1%)	1.09	110/42155 (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
1	N	0	1
2	B	0	2

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

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	169	ARG	CZ-NH2	28.09	1.70	1.33
8	H	43	ARG	NE-CZ	28.05	1.64	1.33
8	H	47	ARG	CZ-NH2	25.48	1.66	1.33
8	U	47	ARG	CZ-NH2	25.40	1.66	1.33
8	H	43	ARG	CZ-NH1	25.16	1.68	1.32
10	O	169	ARG	NE-CZ	18.42	1.53	1.33
1	A	408	ARG	CZ-NH2	13.66	1.51	1.33
8	H	47	ARG	CD-NE	11.60	1.62	1.46
8	U	43	ARG	CZ-NH2	-10.93	1.19	1.33
2	B	169	ARG	CZ-NH1	-10.62	1.17	1.32
8	U	43	ARG	NE-CZ	10.16	1.44	1.33
8	U	43	ARG	CZ-NH1	9.44	1.46	1.32
2	B	169	ARG	NE-CZ	7.67	1.41	1.33
10	O	169	ARG	CZ-NH1	7.44	1.43	1.32
8	H	43	ARG	N-CA	-5.55	1.39	1.46
8	U	50	THR	CB-CG2	5.44	1.70	1.52
8	H	47	ARG	CZ-NH1	-5.30	1.25	1.32
7	G	74	PRO	N-CD	5.08	1.54	1.47

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	390	GLY	N-CA-C	31.63	151.42	112.83
10	O	390	GLY	N-CA-C	31.48	151.24	112.83
10	O	301	LYS	N-CA-C	25.58	144.84	113.38
2	B	301	LYS	N-CA-C	24.90	143.79	113.41
10	O	169	ARG	N-CA-C	24.53	138.26	111.03
7	G	77	TYR	CA-C-N	20.31	148.06	120.44
7	G	77	TYR	C-N-CA	20.31	148.06	120.44
8	H	47	ARG	NE-CZ-NH2	19.76	136.99	119.20
8	U	47	ARG	NE-CZ-NH2	-19.50	101.65	119.20
5	R	72	SER	N-CA-C	19.27	132.29	111.28
7	G	74	PRO	N-CA-C	18.33	150.22	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	O	301	LYS	CB-CA-C	-16.14	81.56	109.65
8	U	43	ARG	NH1-CZ-NH2	-15.85	98.69	119.30
7	G	75	ALA	N-CA-CB	-15.52	83.10	110.42
10	O	169	ARG	NH1-CZ-NH2	-15.08	99.70	119.30
10	O	168	TYR	CB-CA-C	-14.99	85.27	110.16
7	G	74	PRO	CB-CA-C	-14.87	87.02	111.56
8	H	50	THR	CB-CA-C	-14.11	85.15	109.83
5	R	142	LEU	N-CA-C	-13.88	86.83	108.76
10	O	169	ARG	N-CA-CB	-13.86	89.89	109.98
5	I	53	GLU	N-CA-C	13.34	133.00	113.40
8	U	43	ARG	CB-CG-CD	-13.16	81.03	111.30
5	R	73	LYS	N-CA-C	-13.01	97.32	113.97
8	H	47	ARG	NH1-CZ-NH2	-12.60	102.92	119.30
7	G	77	TYR	N-CA-C	12.54	130.54	114.75
2	B	301	LYS	CA-C-N	12.49	135.75	120.14
2	B	301	LYS	C-N-CA	12.49	135.75	120.14
2	B	301	LYS	CB-CA-C	-12.01	88.22	109.24
8	U	43	ARG	CD-NE-CZ	-11.74	107.97	124.40
8	U	47	ARG	NH1-CZ-NH2	11.47	134.21	119.30
10	O	169	ARG	NE-CZ-NH2	10.81	128.93	119.20
2	B	391	SER	N-CA-CB	10.76	128.03	111.46
8	U	50	THR	CB-CA-C	-10.33	89.01	110.40
1	A	349	ALA	N-CA-C	-10.28	91.20	108.26
10	O	391	SER	N-CA-CB	10.19	127.16	111.46
5	R	141	HIS	N-CA-C	9.86	123.26	111.82
1	N	349	ALA	N-CA-C	-9.62	92.29	108.26
8	H	49	GLN	OE1-CD-NE2	9.35	131.94	122.60
1	A	348	SER	N-CA-C	-9.32	93.04	108.32
8	H	43	ARG	CB-CG-CD	-8.84	90.97	111.30
5	R	141	HIS	CB-CA-C	-8.71	93.95	110.67
8	H	43	ARG	N-CA-CB	-8.61	97.14	110.06
1	A	348	SER	CB-CA-C	8.60	124.42	109.89
7	G	75	ALA	N-CA-C	8.57	123.39	113.19
5	R	142	LEU	N-CA-CB	8.35	126.00	111.39
7	G	77	TYR	CB-CA-C	7.98	119.45	109.16
8	H	43	ARG	NE-CZ-NH2	-7.84	112.15	119.20
1	A	349	ALA	N-CA-CB	7.68	123.29	110.77
5	R	73	LYS	N-CA-CB	7.58	121.20	110.67
2	B	169	ARG	N-CA-CB	-7.57	95.94	111.00
8	U	43	ARG	NE-CZ-NH1	7.50	129.00	121.50
4	D	97	ASN	N-CA-C	7.40	114.79	108.13
5	R	77	LYS	N-CA-C	7.39	118.95	108.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	318	ARG	CA-C-N	7.30	126.56	118.97
3	P	318	ARG	C-N-CA	7.30	126.56	118.97
2	B	169	ARG	N-CA-C	7.25	122.04	111.02
2	B	230	LEU	CB-CA-C	7.22	118.68	109.80
5	R	72	SER	CB-CA-C	-7.14	98.94	110.79
1	N	348	SER	N-CA-C	-7.10	95.68	110.80
10	O	230	LEU	CB-CA-C	7.02	119.47	109.71
8	H	50	THR	CA-C-N	6.85	132.98	122.23
8	H	50	THR	C-N-CA	6.85	132.98	122.23
4	Q	97	ASN	N-CA-C	6.83	114.27	108.13
1	N	220	SER	N-CA-C	-6.82	100.46	110.42
8	H	43	ARG	NE-CZ-NH1	6.72	128.22	121.50
7	G	76	ALA	N-CA-C	6.70	122.88	113.56
8	H	47	ARG	CD-NE-CZ	6.67	133.74	124.40
10	O	230	LEU	N-CA-C	-6.63	100.75	110.42
2	B	389	ALA	N-CA-C	-6.60	100.13	108.45
10	O	169	ARG	NE-CZ-NH1	6.60	128.10	121.50
10	O	389	ALA	N-CA-C	-6.58	99.67	108.74
1	N	349	ALA	N-CA-CB	6.57	121.48	110.77
4	D	198	HIS	N-CA-C	6.38	124.38	110.80
10	O	169	ARG	CD-NE-CZ	-6.38	115.47	124.40
10	O	168	TYR	N-CA-C	6.26	118.62	108.41
2	B	230	LEU	N-CA-C	-6.25	101.39	110.64
1	N	408	ARG	CB-CG-CD	-6.16	97.13	111.30
1	A	326	CYS	N-CA-C	6.15	116.68	108.38
3	P	16	ASN	N-CA-C	-6.14	105.82	113.38
3	C	16	ASN	N-CA-C	-6.04	105.55	113.17
3	P	12	LYS	N-CA-C	-5.85	104.98	111.71
8	U	42	GLU	CA-CB-CG	-5.81	102.48	114.10
5	I	72	VAL	N-CA-CB	-5.78	107.84	111.83
3	C	12	LYS	N-CA-C	-5.67	105.18	111.71
4	Q	198	HIS	N-CA-C	5.64	122.82	110.80
7	T	34	ILE	CB-CA-C	-5.56	108.42	113.70
8	H	67	HIS	N-CA-C	-5.56	104.24	111.02
7	G	48	VAL	N-CA-C	5.53	115.77	110.74
7	T	23	GLN	N-CA-C	5.50	117.76	109.41
7	T	37	VAL	CB-CA-C	-5.47	104.97	111.97
2	B	168	TYR	CB-CA-C	-5.38	100.02	109.71
10	O	37	SER	N-CA-C	5.37	116.33	107.20
2	B	302	GLY	N-CA-C	5.32	120.21	113.24
1	A	408	ARG	CB-CG-CD	-5.29	99.14	111.30
7	T	45	ILE	N-CA-C	5.27	115.99	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	298	ILE	CB-CA-C	-5.26	105.59	111.80
7	G	37	VAL	CB-CA-C	-5.23	105.28	111.97
1	N	326	CYS	N-CA-C	5.22	116.07	108.14
7	G	73	ASN	CA-C-N	-5.19	113.35	119.84
7	G	73	ASN	C-N-CA	-5.19	113.35	119.84
8	H	51	GLU	N-CA-CB	-5.17	103.75	110.88
1	A	408	ARG	CG-CD-NE	5.17	123.37	112.00
2	B	104	ASN	N-CA-C	5.11	117.72	109.40
1	N	220	SER	CB-CA-C	5.09	116.79	109.71
1	N	408	ARG	CD-NE-CZ	-5.09	117.28	124.40
8	H	55	THR	CB-CA-C	-5.06	102.71	110.81
1	A	324	PHE	N-CA-C	5.05	117.06	109.23
1	N	348	SER	CB-CA-C	5.04	120.45	110.42
2	B	303	VAL	N-CA-C	5.02	115.07	107.80
8	U	43	ARG	N-CA-CB	-5.01	102.51	110.28

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	444	LEU	Peptide
2	B	169	ARG	Sidechain
2	B	301	LYS	Peptide
7	G	77	TYR	Peptide
8	H	50	THR	Peptide
1	N	444	LEU	Peptide
10	O	169	ARG	Sidechain
10	O	301	LYS	Peptide
8	U	43	ARG	Sidechain
8	U	47	ARG	Sidechain
8	U	50	THR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3439	0	3337	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	3432	0	3330	48	0
2	B	3164	0	3144	81	0
3	C	2968	0	3028	88	0
3	P	2936	0	2996	79	0
4	D	1912	0	1861	47	0
4	Q	1918	0	1870	41	0
5	E	549	0	547	9	0
5	I	157	0	171	28	0
5	R	1518	0	1504	27	0
6	F	860	0	849	24	1
6	S	869	0	862	28	0
7	G	677	0	673	9	0
7	T	624	0	630	9	0
8	H	529	0	512	48	0
8	U	538	0	522	27	1
9	J	482	0	483	10	0
9	W	487	0	487	9	0
10	O	3140	0	3121	107	0
11	V	127	0	135	40	0
12	C	86	0	60	10	0
12	P	86	0	60	10	0
13	C	28	0	14	5	0
13	P	28	0	14	4	0
14	C	5	0	0	0	0
14	D	15	0	0	0	0
14	E	5	0	0	0	0
14	F	5	0	0	0	0
14	N	10	0	0	0	0
14	Q	10	0	0	0	0
14	S	5	0	0	0	0
15	C	49	0	72	1	0
15	D	26	0	26	1	0
15	P	49	0	72	1	0
15	Q	51	0	82	3	0
16	D	43	0	32	10	0
16	Q	43	0	32	6	0
17	D	39	0	39	0	0
17	G	44	0	32	0	0
17	Q	39	0	39	1	0
17	T	49	0	42	1	0
18	R	4	0	0	3	0
19	R	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	31051	0	30686	688	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (688) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:376:LEU:CD1	6:F:20:TYR:HD2	1.90	0.84
8:H:47:ARG:HH12	8:H:50:THR:C	1.85	0.84
2:B:99:THR:HG22	5:I:67:SER:OG	1.77	0.84
4:Q:37:CYS:SG	16:Q:501:HEC:CBB	2.66	0.83
3:P:276:PHE:HD1	3:P:277:ALA:N	1.74	0.83
4:D:37:CYS:SG	16:D:501:HEC:CAB	2.66	0.83
8:U:48:SER:C	8:U:49:GLN:HG2	2.04	0.83
8:H:44:VAL:HG23	8:H:47:ARG:HH21	1.44	0.83
10:O:90:GLU:CG	11:V:71:ASN:OD1	2.26	0.83
3:C:376:LEU:HD12	6:F:20:TYR:CD2	2.14	0.82
3:C:276:PHE:HD1	3:C:277:ALA:N	1.78	0.82
2:B:168:TYR:CD2	2:B:172:LEU:HB2	2.14	0.81
10:O:169:ARG:HH21	10:O:238:LYS:HG2	1.45	0.81
8:H:50:THR:OG1	8:H:51:GLU:N	2.10	0.80
10:O:168:TYR:CD2	10:O:172:LEU:HB2	2.17	0.80
8:U:50:THR:OG1	8:U:51:GLU:N	2.05	0.80
10:O:169:ARG:NH2	10:O:238:LYS:HG2	1.97	0.79
4:D:40:CYS:SG	16:D:501:HEC:CBC	2.69	0.79
3:C:145:VAL:HG21	3:C:268:ILE:HD12	1.64	0.79
8:H:47:ARG:NH1	8:H:50:THR:O	2.15	0.78
3:P:145:VAL:HG21	3:P:268:ILE:HD12	1.65	0.78
4:D:37:CYS:SG	16:D:501:HEC:CBB	2.72	0.78
4:D:40:CYS:SG	16:D:501:HEC:CAC	2.71	0.78
12:C:502:HEM:HBC2	12:C:502:HEM:HMC2	1.64	0.77
3:C:78:ILE:HD11	4:D:204:MET:HE1	1.67	0.77
8:H:48:SER:C	8:H:49:GLN:HG2	2.09	0.77
4:D:140:GLY:HA3	8:H:53:ASP:HB3	1.64	0.76
4:D:37:CYS:SG	16:D:501:HEC:HBB3	2.25	0.76
10:O:89:ILE:HB	11:V:70:LEU:CD2	2.16	0.75
8:U:44:VAL:HG23	8:U:47:ARG:NH2	2.02	0.74
2:B:99:THR:HG23	5:I:67:SER:OG	1.87	0.74
2:B:169:ARG:NH2	2:B:238:LYS:HG2	2.03	0.74
3:P:78:ILE:HD11	4:Q:204:MET:HE1	1.69	0.74
4:D:120:ARG:NE	16:D:501:HEC:O1A	2.21	0.74
12:C:501:HEM:HMC1	12:C:501:HEM:HBC2	1.70	0.73
5:I:53:GLU:O	5:I:53:GLU:HG3	1.88	0.73
3:C:120:LEU:HG	3:C:124:MET:HE3	1.71	0.72
13:P:503:4X9:C6	13:P:503:4X9:H16	2.18	0.72
7:G:77:TYR:O	7:G:80:ASP:O	2.07	0.72
10:O:89:ILE:CD1	11:V:70:LEU:HD22	2.16	0.72
3:P:120:LEU:HG	3:P:124:MET:HE3	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:276:PHE:HD1	3:P:276:PHE:C	1.97	0.72
6:F:20:TYR:HD1	6:F:20:TYR:O	1.73	0.72
2:B:78:LYS:HB2	2:B:129:ALA:HB1	1.72	0.71
3:C:106:SER:HB3	12:C:502:HEM:HBD2	1.71	0.71
8:H:43:ARG:O	8:H:47:ARG:HG2	1.90	0.71
2:B:438:GLU:OE2	10:O:169:ARG:NH1	2.23	0.71
12:P:501:HEM:HMC1	12:P:501:HEM:HBC2	1.71	0.71
2:B:227:ARG:HE	2:B:227:ARG:HA	1.55	0.70
2:B:168:TYR:O	2:B:173:ALA:HB2	1.92	0.70
1:N:253:VAL:HB	1:N:324:PHE:CE1	2.26	0.70
12:P:501:HEM:HMB1	12:P:501:HEM:HBB2	1.74	0.70
5:R:98:VAL:HG23	5:R:98:VAL:O	1.92	0.70
6:F:20:TYR:HD1	6:F:20:TYR:C	1.99	0.70
2:B:169:ARG:NH1	10:O:438:GLU:OE2	2.24	0.70
8:H:40:CYS:HA	8:H:43:ARG:HG2	1.74	0.70
4:Q:40:CYS:SG	16:Q:501:HEC:HBC3	2.31	0.69
8:H:47:ARG:NH2	8:H:50:THR:OG1	2.23	0.69
10:O:168:TYR:O	10:O:173:ALA:CB	2.30	0.69
1:A:21:ASN:O	1:A:221:GLY:O	2.10	0.69
10:O:78:LYS:HB2	10:O:129:ALA:HB1	1.75	0.69
3:P:276:PHE:CD1	3:P:277:ALA:N	2.60	0.69
3:P:276:PHE:C	3:P:276:PHE:CD1	2.71	0.69
10:O:227:ARG:HE	10:O:227:ARG:HA	1.57	0.68
8:H:44:VAL:HA	8:H:47:ARG:HE	1.58	0.68
10:O:304:HIS:O	10:O:305:GLU:HG3	1.93	0.68
6:F:20:TYR:C	6:F:20:TYR:CD1	2.71	0.68
4:Q:37:CYS:SG	16:Q:501:HEC:HBB3	2.33	0.68
6:S:40:ASN:OD1	6:S:40:ASN:C	2.35	0.68
2:B:29:LEU:HD23	2:B:30:PRO:HD2	1.75	0.67
11:V:72:VAL:HG13	11:V:73:PRO:HD2	1.77	0.67
3:C:187:PHE:CZ	3:P:184:ILE:CD1	2.78	0.66
3:C:276:PHE:CD1	3:C:277:ALA:N	2.61	0.66
3:C:276:PHE:HD1	3:C:276:PHE:C	2.03	0.66
2:B:170:ASN:ND2	2:B:170:ASN:H	1.93	0.65
11:V:72:VAL:HG12	11:V:73:PRO:O	1.95	0.65
3:P:78:ILE:HD11	4:Q:204:MET:CE	2.27	0.65
3:C:220:PHE:HD1	3:C:220:PHE:O	1.80	0.65
5:R:163:SER:HA	5:R:174:GLY:HA3	1.79	0.65
8:H:43:ARG:O	8:H:47:ARG:CG	2.45	0.65
8:H:44:VAL:HA	8:H:47:ARG:NE	2.12	0.65
11:V:70:LEU:O	11:V:70:LEU:HG	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:29:LEU:HD23	10:O:30:PRO:HD2	1.78	0.64
9:W:58:LYS:C	9:W:59:TYR:HD1	2.05	0.64
1:A:253:VAL:HB	1:A:324:PHE:CE1	2.33	0.64
1:N:21:ASN:O	1:N:221:GLY:O	2.16	0.64
1:N:324:PHE:CE2	1:N:334:MET:HB3	2.33	0.64
1:A:117:VAL:HG11	1:A:195:MET:HE1	1.80	0.64
5:I:70:LEU:HG	5:I:70:LEU:O	1.96	0.64
3:C:78:ILE:HD11	4:D:204:MET:CE	2.28	0.63
5:R:175:PRO:HG2	18:R:501:FES:S1	2.38	0.63
6:F:20:TYR:HE1	6:F:24:ALA:HB2	1.64	0.63
3:C:379:TRP:CE2	6:F:33:ARG:HD3	2.34	0.63
5:I:72:VAL:HG12	5:I:73:PRO:O	1.99	0.62
7:G:59:TYR:CD1	7:G:59:TYR:C	2.75	0.62
3:P:220:PHE:CD1	3:P:224:TYR:HB2	2.34	0.62
4:D:178:THR:HG21	8:H:16:PRO:CD	2.29	0.62
1:N:117:VAL:HG11	1:N:195:MET:HE1	1.82	0.62
11:V:62:ARG:O	11:V:78:TYR:HB3	2.00	0.62
3:C:168:PHE:HE2	5:R:72:SER:HB2	1.65	0.62
3:C:276:PHE:CD1	3:C:276:PHE:C	2.77	0.62
10:O:98:VAL:O	11:V:67:SER:HA	2.00	0.62
3:P:103:TYR:HB2	3:P:325:PHE:HE2	1.65	0.61
3:C:220:PHE:CD1	3:C:220:PHE:C	2.78	0.61
4:Q:204:MET:HE3	15:Q:506:PEE:O4	1.99	0.61
1:A:293:PRO:O	1:A:297:ILE:HG12	2.01	0.61
1:N:284:TYR:CE1	11:V:73:PRO:CB	2.71	0.61
10:O:170:ASN:H	10:O:170:ASN:ND2	1.96	0.61
2:B:169:ARG:CD	10:O:435:PHE:CZ	2.83	0.61
2:B:261:SER:OG	2:B:262:ALA:N	2.32	0.61
10:O:169:ARG:HH21	10:O:238:LYS:CG	2.12	0.61
1:N:253:VAL:HB	1:N:324:PHE:HE1	1.64	0.61
2:B:435:PHE:CZ	10:O:169:ARG:CD	2.84	0.61
3:P:376:LEU:HB2	6:S:20:TYR:HD2	1.64	0.61
12:C:501:HEM:HBB2	12:C:501:HEM:HHC	1.83	0.60
11:V:76:VAL:HG12	11:V:76:VAL:O	2.01	0.60
3:C:277:ALA:HB1	3:C:294:LEU:CD1	2.31	0.60
5:I:72:VAL:HG13	5:I:73:PRO:HD2	1.83	0.60
8:H:48:SER:C	8:H:49:GLN:CG	2.75	0.60
2:B:134:ARG:NH2	6:S:49:ARG:O	2.34	0.60
2:B:169:ARG:HD3	10:O:435:PHE:CE2	2.36	0.60
7:G:59:TYR:C	7:G:59:TYR:HD1	2.08	0.60
3:P:277:ALA:HB1	3:P:294:LEU:CD1	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:35:GLU:C	8:H:39:LEU:HD12	2.27	0.60
3:P:376:LEU:CB	6:S:20:TYR:HD2	2.15	0.60
1:A:324:PHE:CE2	1:A:334:MET:HB3	2.37	0.59
4:D:178:THR:CG2	8:H:15:ASP:HA	2.32	0.59
1:A:443:TRP:CD1	1:A:444:LEU:HD23	2.37	0.59
3:C:220:PHE:O	3:C:220:PHE:CD1	2.55	0.59
10:O:89:ILE:HB	11:V:70:LEU:HD23	1.83	0.59
3:C:220:PHE:HD1	3:C:220:PHE:C	2.11	0.59
6:F:40:ASN:C	6:F:40:ASN:OD1	2.44	0.59
5:R:161:HIS:HB2	18:R:501:FES:S1	2.43	0.59
4:D:33:TYR:HA	4:D:37:CYS:SG	2.43	0.58
2:B:279:LEU:HA	2:B:294:SER:HB3	1.85	0.58
4:Q:181:GLN:HB2	8:U:77:LEU:HD22	1.85	0.58
8:U:40:CYS:HA	8:U:43:ARG:HG2	1.84	0.58
8:U:48:SER:C	8:U:49:GLN:CG	2.77	0.58
3:C:78:ILE:CD1	4:D:204:MET:HE1	2.34	0.58
3:C:375:LYS:O	6:F:17:ARG:NH1	2.36	0.58
5:I:64:LEU:HD21	5:I:76:VAL:HG13	1.84	0.58
3:C:106:SER:HB3	12:C:502:HEM:CBD	2.33	0.57
2:B:98:VAL:O	5:I:68:VAL:O	2.22	0.57
3:C:361:LEU:O	3:C:366:MET:HG3	2.04	0.57
3:C:220:PHE:CZ	13:C:503:4X9:H15	2.39	0.57
1:N:3:THR:HG23	1:N:6:GLN:H	1.69	0.57
7:T:59:TYR:CD1	7:T:59:TYR:C	2.82	0.57
8:U:47:ARG:HB2	8:U:50:THR:HG22	1.85	0.57
3:C:103:TYR:HB2	3:C:325:PHE:HE2	1.68	0.57
10:O:261:SER:OG	10:O:262:ALA:N	2.38	0.57
13:P:503:4X9:H16	13:P:503:4X9:H6	1.87	0.57
3:P:78:ILE:CD1	4:Q:204:MET:HE1	2.33	0.56
3:P:349:THR:HA	3:P:352:GLN:HG2	1.86	0.56
1:A:223:TYR:HB2	1:A:228:VAL:HG21	1.87	0.56
3:P:376:LEU:HB2	6:S:20:TYR:CD2	2.40	0.56
3:C:11:MET:SD	3:C:11:MET:C	2.88	0.56
6:F:40:ASN:OD1	6:F:41:ASP:N	2.38	0.56
4:Q:40:CYS:SG	16:Q:501:HEC:CAC	2.93	0.56
2:B:71:LEU:HD23	5:I:68:VAL:HG11	1.88	0.56
6:F:49:ARG:O	10:O:134:ARG:NH2	2.39	0.56
3:P:18:PHE:O	3:P:220:PHE:HD2	1.88	0.56
4:Q:33:TYR:HA	4:Q:37:CYS:SG	2.45	0.56
1:A:253:VAL:HB	1:A:324:PHE:HE1	1.70	0.56
4:D:178:THR:HG21	8:H:15:ASP:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:97:SER:HA	11:V:69:SER:OG	2.06	0.56
2:B:169:ARG:NH2	2:B:238:LYS:CG	2.69	0.56
9:J:58:LYS:C	9:J:59:TYR:HD1	2.13	0.56
5:E:58:PHE:O	5:E:61:SER:HB3	2.06	0.56
5:I:52:ARG:HD2	5:I:53:GLU:H	1.71	0.56
3:P:145:VAL:HG21	3:P:268:ILE:CD1	2.36	0.56
6:S:40:ASN:OD1	6:S:41:ASP:N	2.38	0.56
10:O:86:THR:HA	11:V:70:LEU:HD11	1.87	0.56
10:O:71:LEU:HD23	11:V:68:VAL:HG21	1.87	0.55
3:P:103:TYR:HD1	3:P:325:PHE:HD2	1.53	0.55
3:P:70:CYS:SG	3:P:80:ARG:HD3	2.46	0.55
8:H:40:CYS:CA	8:H:43:ARG:HG2	2.36	0.55
2:B:176:LEU:HD13	5:I:66:ALA:HB2	1.88	0.55
3:C:21:LEU:HD23	3:C:220:PHE:HD2	1.72	0.55
1:A:27:SER:HA	1:A:199:ALA:O	2.06	0.55
4:Q:1:SER:CA	4:Q:155:GLY:HA2	2.32	0.55
10:O:31:ASN:ND2	10:O:225:ASN:OD1	2.39	0.55
8:H:35:GLU:O	8:H:39:LEU:HD12	2.07	0.55
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.89	0.55
16:D:501:HEC:HBD2	16:D:501:HEC:HHA	1.88	0.55
3:P:325:PHE:C	3:P:325:PHE:CD1	2.85	0.55
3:C:10:LEU:HD12	3:C:10:LEU:C	2.32	0.55
3:C:105:GLY:HA2	3:C:107:TYR:CE2	2.42	0.55
4:Q:204:MET:HG2	15:Q:506:PEE:H2	1.88	0.55
1:A:3:THR:HG23	1:A:6:GLN:H	1.71	0.54
10:O:90:GLU:HA	11:V:71:ASN:HD21	1.71	0.54
16:D:501:HEC:HHA	16:D:501:HEC:CBD	2.37	0.54
5:I:53:GLU:O	5:I:53:GLU:CG	2.56	0.54
10:O:176:LEU:HD12	11:V:64:VAL:HG23	1.90	0.54
1:N:284:TYR:CD1	11:V:73:PRO:HB3	2.38	0.54
3:P:138:MET:HA	3:P:138:MET:HE2	1.90	0.54
10:O:226:ILE:HD12	10:O:227:ARG:N	2.23	0.54
3:C:8:HIS:N	3:C:9:PRO:HD3	2.23	0.54
1:A:233:PRO:O	5:E:22:THR:HA	2.07	0.54
1:N:288:ALA:HB2	1:N:300:THR:HG22	1.90	0.54
2:B:169:ARG:HD3	10:O:435:PHE:CZ	2.43	0.53
3:C:75:TYR:CE2	5:E:57:GLN:HG2	2.42	0.53
2:B:99:THR:CG2	5:I:67:SER:HG	2.22	0.53
2:B:101:THR:HG1	2:B:103:GLU:H	1.55	0.53
3:C:184:ILE:CD1	3:P:187:PHE:CZ	2.91	0.53
1:N:294:LEU:HD11	1:N:334:MET:HE1	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:299:VAL:HG11	2:B:336:VAL:HG13	1.90	0.53
3:C:104:TYR:CD1	3:C:208:PRO:HA	2.43	0.53
3:C:205:SER:OG	13:C:503:4X9:H26B	2.09	0.53
3:P:221:HIS:ND1	3:P:222:PRO:HA	2.24	0.53
4:D:211:MET:HG2	9:J:35:PHE:CE2	2.43	0.53
8:U:35:GLU:C	8:U:39:LEU:HD12	2.34	0.53
10:O:229:GLY:O	10:O:230:LEU:C	2.51	0.53
3:P:376:LEU:HD12	6:S:20:TYR:CD2	2.44	0.53
1:N:219:LEU:HG	1:N:220:SER:O	2.08	0.53
13:P:503:4X9:C6	13:P:503:4X9:C16	2.84	0.53
1:A:162:PRO:HD2	1:A:234:CYS:SG	2.48	0.52
8:H:44:VAL:HG23	8:H:47:ARG:NH2	2.14	0.52
2:B:229:GLY:O	2:B:230:LEU:C	2.53	0.52
3:C:325:PHE:CD1	3:C:325:PHE:C	2.87	0.52
2:B:157:ALA:O	2:B:161:GLU:HG2	2.09	0.52
2:B:168:TYR:CE2	2:B:172:LEU:HD12	2.44	0.52
1:N:106:LEU:HB3	1:N:107:PRO:HD3	1.91	0.52
10:O:299:VAL:HG11	10:O:336:VAL:HG13	1.91	0.52
3:P:375:LYS:O	6:S:17:ARG:NH1	2.37	0.52
4:Q:178:THR:HG21	8:U:16:PRO:HD2	1.90	0.52
6:S:20:TYR:CD1	6:S:20:TYR:C	2.85	0.52
1:N:283:THR:HB	11:V:74:ALA:HB3	1.91	0.52
3:C:138:MET:HE2	3:C:138:MET:HA	1.91	0.52
6:F:107:TRP:HE1	10:O:87:ARG:HB3	1.75	0.52
3:C:11:MET:SD	3:C:11:MET:O	2.67	0.52
4:D:204:MET:HE3	15:D:506:PEE:H7	1.91	0.52
6:F:20:TYR:CE1	6:F:24:ALA:HB2	2.43	0.52
12:P:502:HEM:HMB1	12:P:502:HEM:HBB2	1.92	0.52
9:W:59:TYR:N	9:W:59:TYR:CD1	2.75	0.52
2:B:169:ARG:NH2	2:B:169:ARG:NH1	2.41	0.52
10:O:42:ALA:O	10:O:113:ARG:NH1	2.41	0.52
3:P:103:TYR:HD1	3:P:325:PHE:CD2	2.28	0.52
4:Q:139:THR:HG1	8:U:41:ASP:CG	2.17	0.52
3:C:246:ALA:HB1	3:C:249:LEU:HB2	1.92	0.51
5:I:64:LEU:HD23	5:I:65:VAL:N	2.24	0.51
10:O:96:LEU:O	11:V:69:SER:HA	2.10	0.51
10:O:279:LEU:HA	10:O:294:SER:HB3	1.91	0.51
3:P:226:ILE:HA	3:P:229:ILE:HD12	1.92	0.51
3:P:361:LEU:O	3:P:366:MET:HG3	2.10	0.51
3:C:277:ALA:HB1	3:C:294:LEU:HD12	1.92	0.51
4:D:141:VAL:HG23	8:H:53:ASP:OD2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:10:LEU:HD12	3:P:10:LEU:C	2.35	0.51
2:B:435:PHE:CE2	10:O:169:ARG:HD3	2.45	0.51
10:O:49:LEU:HD23	10:O:127:THR:HG21	1.91	0.51
3:P:103:TYR:HB2	3:P:325:PHE:CE2	2.44	0.51
7:T:59:TYR:C	7:T:59:TYR:HD1	2.17	0.51
10:O:168:TYR:CE2	10:O:172:LEU:HD12	2.45	0.51
3:C:145:VAL:HG21	3:C:268:ILE:CD1	2.36	0.51
3:P:211:ILE:HD11	6:S:36:THR:HG22	1.93	0.51
7:T:73:ASN:HB3	7:T:75:ALA:H	1.76	0.51
2:B:226:ILE:HD12	2:B:227:ARG:N	2.25	0.51
5:I:65:VAL:HG23	5:I:77:ARG:HB2	1.91	0.51
10:O:85:ILE:HG22	11:V:70:LEU:HD11	1.90	0.51
2:B:435:PHE:CZ	10:O:169:ARG:HD2	2.46	0.51
1:N:27:SER:HA	1:N:199:ALA:O	2.11	0.51
3:C:181:PHE:HA	3:C:184:ILE:HG22	1.92	0.51
5:I:76:VAL:HG12	5:I:76:VAL:O	2.10	0.51
3:C:349:THR:HA	3:C:352:GLN:HG2	1.93	0.51
12:C:502:HEM:HBC2	12:C:502:HEM:CMC	2.38	0.51
3:P:246:ALA:HB1	3:P:249:LEU:HB2	1.92	0.51
3:P:277:ALA:HB1	3:P:294:LEU:HD12	1.93	0.51
10:O:75:LEU:HD22	10:O:136:GLU:HB3	1.93	0.51
1:A:244:ARG:CZ	7:G:10:VAL:HB	2.41	0.50
3:C:19:ILE:HG22	3:C:20:ASP:OD1	2.11	0.50
3:C:138:MET:HE1	3:C:268:ILE:HA	1.93	0.50
1:N:219:LEU:O	1:N:220:SER:C	2.54	0.50
10:O:90:GLU:HG3	11:V:71:ASN:OD1	2.09	0.50
1:N:442:PHE:CD1	1:N:442:PHE:C	2.89	0.50
6:S:71:ARG:O	6:S:72:GLN:HB2	2.12	0.50
4:D:137:PRO:HA	4:D:149:PHE:CD2	2.46	0.50
10:O:98:VAL:HG22	10:O:107:TYR:CD1	2.46	0.50
17:Q:505:CDL:C42	17:T:501:CDL:C78	2.90	0.50
3:C:75:TYR:CD2	5:E:57:GLN:HG2	2.47	0.50
1:N:442:PHE:C	1:N:442:PHE:HD1	2.20	0.50
12:P:502:HEM:HBB2	12:P:502:HEM:CMB	2.42	0.50
4:Q:40:CYS:SG	16:Q:501:HEC:CBC	2.98	0.50
5:R:134:ILE:HD11	5:R:185:TYR:CG	2.47	0.50
2:B:177:TYR:OH	5:I:76:VAL:CG2	2.60	0.50
1:N:223:TYR:CB	1:N:228:VAL:HG21	2.41	0.49
1:N:293:PRO:O	1:N:297:ILE:HG12	2.12	0.49
10:O:157:ALA:O	10:O:161:GLU:HG2	2.12	0.49
6:S:12:TRP:CD1	6:S:13:LEU:HD23	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:124:MET:HE1	3:C:298:ILE:HD12	1.95	0.49
3:C:226:ILE:HA	3:C:229:ILE:HD12	1.94	0.49
3:P:51:LEU:HD13	12:P:501:HEM:HBD1	1.94	0.49
5:R:150:ALA:O	5:R:157:TYR:HB2	2.12	0.49
10:O:385:GLN:O	10:O:389:ALA:O	2.29	0.49
3:P:14:VAL:HG12	3:P:14:VAL:O	2.11	0.49
3:P:137:GLN:OE1	3:P:260:ASN:N	2.45	0.49
1:A:288:ALA:HB2	1:A:300:THR:HG22	1.93	0.49
1:A:294:LEU:HD11	1:A:334:MET:HE1	1.94	0.49
3:C:70:CYS:SG	3:C:80:ARG:HD3	2.52	0.49
1:N:3:THR:OG1	1:N:4:TYR:N	2.46	0.49
6:S:35:ASP:OD1	6:S:89:TYR:OH	2.27	0.49
2:B:83:PHE:CZ	6:S:107:TRP:HD1	2.31	0.49
2:B:308:ASP:HB2	5:I:55:LEU:CB	2.42	0.49
2:B:435:PHE:CZ	10:O:169:ARG:HD3	2.47	0.49
5:R:171:ILE:HD11	5:R:176:ALA:HB3	1.95	0.49
1:A:106:LEU:HB3	1:A:107:PRO:HD3	1.95	0.49
1:A:223:TYR:CB	1:A:228:VAL:HG21	2.42	0.49
2:B:100:SER:O	5:I:66:ALA:O	2.30	0.49
4:D:231:LYS:O	6:F:71:ARG:HD3	2.13	0.49
4:Q:211:MET:HG2	9:W:35:PHE:CE2	2.48	0.49
5:R:140:THR:HB	5:R:177:PRO:HD2	1.95	0.49
1:A:223:TYR:HB2	1:A:228:VAL:CG2	2.42	0.49
2:B:316:TYR:CD1	2:B:316:TYR:N	2.80	0.49
2:B:380:ASP:O	2:B:384:SER:HB2	2.13	0.49
10:O:169:ARG:HH21	10:O:238:LYS:HB3	1.77	0.49
3:P:105:GLY:HA2	3:P:107:TYR:CE2	2.48	0.49
1:N:443:TRP:CD1	1:N:444:LEU:HD23	2.48	0.49
3:C:120:LEU:HG	3:C:124:MET:CE	2.40	0.48
1:A:294:LEU:HD13	1:A:337:VAL:HG12	1.95	0.48
2:B:169:ARG:HD2	10:O:435:PHE:CZ	2.48	0.48
1:N:386:TYR:CD2	1:N:390:ILE:HD12	2.47	0.48
2:B:129:ALA:N	2:B:130:PRO:CD	2.77	0.48
9:J:59:TYR:CD1	9:J:59:TYR:N	2.82	0.48
10:O:95:LYS:HG3	11:V:72:VAL:CG2	2.44	0.48
10:O:164:HIS:NE2	10:O:316:TYR:OH	2.40	0.48
3:P:13:ILE:O	3:P:16:ASN:ND2	2.46	0.48
12:P:502:HEM:HBC2	12:P:502:HEM:HHD	1.95	0.48
4:Q:149:PHE:CE1	4:Q:156:GLN:HB3	2.48	0.48
7:T:25:ALA:O	7:T:27:PRO:HD3	2.14	0.48
1:A:53:ASN:HD21	1:A:165:GLN:HB3	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:99:GLY:O	3:C:100:ARG:C	2.57	0.48
3:C:137:GLN:OE1	3:C:260:ASN:N	2.46	0.48
3:C:312:GLN:HG3	3:C:379:TRP:CZ3	2.47	0.48
2:B:49:LEU:HD23	2:B:127:THR:HG21	1.94	0.48
2:B:97:SER:HA	5:I:69:SER:HB3	1.96	0.48
3:C:103:TYR:HB2	3:C:325:PHE:CE2	2.48	0.48
10:O:95:LYS:HG3	11:V:72:VAL:HG23	1.95	0.48
10:O:96:LEU:O	10:O:96:LEU:HG	2.13	0.48
6:S:20:TYR:CD1	6:S:20:TYR:O	2.66	0.48
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.49	0.48
1:A:442:PHE:CD1	1:A:442:PHE:C	2.91	0.48
3:C:15:ASN:N	3:C:15:ASN:OD1	2.46	0.48
4:D:140:GLY:CA	8:H:53:ASP:HB3	2.39	0.48
3:P:131:TYR:HA	12:P:501:HEM:HAA1	1.94	0.48
3:C:103:TYR:HD1	3:C:325:PHE:HD2	1.61	0.48
1:N:245:GLU:HG3	1:N:248:LEU:HG	1.96	0.48
2:B:209:LEU:CD2	2:B:375:SER:HB2	2.43	0.48
3:C:14:VAL:HG12	3:C:14:VAL:O	2.14	0.48
3:C:29:SER:O	3:C:32:ASN:HB2	2.13	0.48
8:H:41:ASP:O	8:H:45:SER:OG	2.19	0.48
5:I:52:ARG:HD2	5:I:53:GLU:N	2.28	0.48
3:P:104:TYR:CD1	3:P:208:PRO:HA	2.48	0.48
1:A:386:TYR:CD2	1:A:390:ILE:HD12	2.49	0.48
4:D:33:TYR:HA	4:D:37:CYS:HG	1.79	0.48
10:O:243:GLU:HA	10:O:424:MET:O	2.13	0.48
10:O:312:PHE:HD1	10:O:313:ASN:N	2.11	0.48
4:D:225:HIS:CE1	7:G:20:PRO:HB2	2.49	0.47
1:N:85:HIS:HB2	1:N:100:LYS:HB2	1.96	0.47
10:O:85:ILE:CG2	11:V:70:LEU:HD13	2.29	0.47
3:P:75:TYR:CE2	5:R:57:GLN:HG2	2.49	0.47
1:A:3:THR:OG1	1:A:4:TYR:N	2.47	0.47
1:A:430:GLN:O	1:A:431:LEU:C	2.56	0.47
2:B:29:LEU:CD2	2:B:30:PRO:HD2	2.43	0.47
2:B:385:GLN:O	2:B:389:ALA:O	2.32	0.47
6:F:20:TYR:O	6:F:21:TYR:C	2.57	0.47
1:A:267:ASN:O	1:A:271:GLN:HG2	2.15	0.47
3:C:211:ILE:HD11	6:F:36:THR:HG22	1.95	0.47
4:D:211:MET:HG2	9:J:35:PHE:HE2	1.79	0.47
10:O:301:LYS:HG3	10:O:301:LYS:O	2.13	0.47
10:O:316:TYR:CD1	10:O:316:TYR:N	2.80	0.47
3:P:11:MET:SD	3:P:11:MET:C	2.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:3:LEU:HD21	8:U:56:GLU:HG3	1.96	0.47
2:B:227:ARG:HA	2:B:227:ARG:NE	2.26	0.47
4:D:218:LEU:O	4:D:221:ALA:HB3	2.13	0.47
2:B:354:ASN:N	2:B:355:PRO:HD2	2.30	0.47
10:O:86:THR:HA	11:V:70:LEU:HD21	1.97	0.47
3:P:14:VAL:O	3:P:14:VAL:CG1	2.63	0.47
3:P:77:TRP:CZ3	3:P:78:ILE:HG13	2.50	0.47
5:R:98:VAL:O	5:R:98:VAL:CG2	2.62	0.47
8:U:35:GLU:O	8:U:39:LEU:HD12	2.15	0.47
2:B:435:PHE:N	2:B:435:PHE:CD1	2.82	0.47
5:R:45:VAL:HG13	9:W:28:ALA:HA	1.96	0.47
11:V:62:ARG:HB3	11:V:63:PRO:HD2	1.97	0.47
1:N:204:GLU:O	1:N:205:HIS:C	2.57	0.47
15:Q:506:PEE:H11	5:R:53:ASN:OD1	2.15	0.47
10:O:209:LEU:CD2	10:O:375:SER:HB2	2.45	0.46
12:P:501:HEM:HHA	12:P:501:HEM:CBA	2.45	0.46
4:Q:126:TYR:CD1	4:Q:126:TYR:C	2.93	0.46
5:R:171:ILE:CD1	5:R:176:ALA:HB3	2.45	0.46
13:C:503:4X9:C6	13:C:503:4X9:C12	2.89	0.46
3:P:120:LEU:HG	3:P:124:MET:CE	2.43	0.46
5:E:31:ALA:HB2	9:J:7:ALA:HB2	1.96	0.46
3:P:379:TRP:CE3	6:S:33:ARG:HD3	2.51	0.46
4:D:138:PRO:HG3	8:H:55:THR:HA	1.98	0.46
10:O:96:LEU:C	11:V:69:SER:HB3	2.41	0.46
3:P:124:MET:HE1	3:P:298:ILE:HD12	1.97	0.46
3:P:358:TYR:HE1	3:P:362:ILE:HD11	1.80	0.46
8:H:40:CYS:O	8:H:43:ARG:CG	2.64	0.46
1:N:294:LEU:HD13	1:N:337:VAL:HG12	1.97	0.46
10:O:34:VAL:HG11	10:O:386:ALA:HB1	1.98	0.46
12:P:501:HEM:HBB2	12:P:501:HEM:CMB	2.42	0.46
3:C:373:GLU:HA	6:F:20:TYR:HE2	1.80	0.46
8:U:17:LEU:HD11	8:U:21:ARG:NE	2.30	0.46
4:D:198:HIS:ND1	4:D:198:HIS:C	2.73	0.46
5:R:91:TRP:HZ3	5:R:136:ILE:HD11	1.81	0.46
1:A:245:GLU:HG3	1:A:248:LEU:HG	1.97	0.46
2:B:308:ASP:HB2	5:I:55:LEU:HB2	1.97	0.46
4:D:138:PRO:HD3	4:D:149:PHE:CE2	2.50	0.46
4:D:181:GLN:OE1	8:H:77:LEU:HB3	2.16	0.46
3:P:103:TYR:CD1	3:P:325:PHE:CD2	3.04	0.46
2:B:87:ARG:HB3	6:S:107:TRP:NE1	2.30	0.46
3:C:186:PRO:HG2	12:C:501:HEM:HMC3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:417:PHE:CD1	10:O:417:PHE:C	2.94	0.46
1:A:77:LYS:HE3	2:B:291:ALA:HB1	1.97	0.46
1:A:442:PHE:C	1:A:442:PHE:HD1	2.23	0.46
2:B:70:ARG:HG2	5:I:68:VAL:HB	1.98	0.46
2:B:109:VAL:HB	2:B:119:LEU:HD12	1.98	0.46
10:O:169:ARG:HH21	10:O:238:LYS:CB	2.29	0.46
10:O:354:ASN:N	10:O:355:PRO:HD2	2.31	0.45
3:P:319:PRO:HD2	6:S:20:TYR:CE1	2.51	0.45
3:C:14:VAL:O	3:C:14:VAL:CG1	2.64	0.45
12:C:502:HEM:HBB2	12:C:502:HEM:CMB	2.47	0.45
4:D:40:CYS:SG	16:D:501:HEC:C3C	3.04	0.45
8:H:53:ASP:CG	8:H:55:THR:HG1	2.24	0.45
10:O:26:PHE:CE2	10:O:391:SER:HA	2.52	0.45
10:O:99:THR:HG23	11:V:67:SER:OG	2.15	0.45
4:Q:149:PHE:CD1	4:Q:156:GLN:HB3	2.50	0.45
3:C:10:LEU:HD21	3:P:202:GLU:HG3	1.99	0.45
3:C:233:LEU:HD22	4:D:216:LEU:HG	1.98	0.45
8:H:17:LEU:HD11	8:H:21:ARG:NE	2.31	0.45
10:O:213:HIS:N	10:O:214:PRO:CD	2.79	0.45
4:Q:137:PRO:HA	4:Q:149:PHE:CD2	2.52	0.45
10:O:129:ALA:N	10:O:130:PRO:CD	2.80	0.45
3:P:103:TYR:CD1	3:P:325:PHE:HD2	2.34	0.45
4:Q:3:LEU:CD2	8:U:56:GLU:HG3	2.47	0.45
3:C:140:PHE:CD1	3:C:140:PHE:C	2.93	0.45
4:D:216:LEU:N	4:D:217:PRO:HD2	2.31	0.45
1:N:77:LYS:HE3	10:O:291:ALA:HB1	1.98	0.45
1:A:111:GLU:HG3	1:A:215:HIS:CE1	2.52	0.45
7:G:75:ALA:O	7:G:77:TYR:CD2	2.69	0.45
1:N:233:PRO:O	5:R:22:THR:HA	2.17	0.45
10:O:291:ALA:HA	10:O:297:GLN:NE2	2.31	0.45
6:S:68:LEU:HD11	6:S:75:LEU:HG	1.99	0.45
3:C:221:HIS:ND1	3:C:222:PRO:HA	2.32	0.45
8:H:73:LEU:O	8:H:73:LEU:HD23	2.17	0.45
5:I:70:LEU:O	5:I:70:LEU:CG	2.64	0.45
3:P:103:TYR:CE2	15:P:505:PEE:H2	2.51	0.45
8:U:53:ASP:CG	8:U:55:THR:HG1	2.24	0.45
9:W:58:LYS:C	9:W:59:TYR:CD1	2.90	0.45
1:A:140:GLU:OE2	5:I:52:ARG:O	2.35	0.45
2:B:87:ARG:HB3	6:S:107:TRP:HE1	1.82	0.45
1:N:184:GLU:O	1:N:185:TYR:C	2.59	0.45
3:P:15:ASN:OD1	3:P:15:ASN:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:26:PHE:HD1	6:F:27:ASN:N	2.15	0.44
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.52	0.44
13:P:503:4X9:H6	13:P:503:4X9:C16	2.47	0.44
5:R:175:PRO:CG	18:R:501:FES:S1	3.04	0.44
7:T:25:ALA:C	7:T:27:PRO:HD3	2.42	0.44
3:C:144:THR:O	3:C:148:ASN:HB2	2.17	0.44
5:E:45:VAL:HG13	9:J:28:ALA:HA	1.99	0.44
8:H:40:CYS:CB	8:H:54:CYS:SG	3.05	0.44
10:O:227:ARG:HA	10:O:227:ARG:NE	2.28	0.44
10:O:325:TYR:HD1	10:O:326:THR:N	2.14	0.44
8:U:73:LEU:HD23	8:U:73:LEU:O	2.17	0.44
1:A:84:ALA:HB1	1:A:100:LYS:O	2.18	0.44
1:A:149:VAL:HG23	1:A:425:PHE:CB	2.47	0.44
4:Q:31:GLN:O	4:Q:35:GLN:HG2	2.17	0.44
1:A:120:CYS:SG	1:A:122:LEU:HG	2.57	0.44
5:E:72:SER:HB2	3:P:168:PHE:HE2	1.81	0.44
8:U:40:CYS:O	8:U:43:ARG:HG3	2.18	0.44
2:B:164:HIS:NE2	2:B:316:TYR:OH	2.43	0.44
13:C:503:4X9:C6	13:C:503:4X9:H12	2.47	0.44
10:O:58:GLU:OE1	10:O:63:LEU:HA	2.16	0.44
10:O:85:ILE:O	11:V:70:LEU:HD21	2.17	0.44
10:O:151:ALA:HB2	11:V:76:VAL:HG21	1.98	0.44
6:S:20:TYR:O	6:S:21:TYR:C	2.58	0.44
2:B:31:ASN:ND2	2:B:225:ASN:OD1	2.51	0.44
2:B:34:VAL:HG11	2:B:386:ALA:HB1	1.99	0.44
2:B:213:HIS:N	2:B:214:PRO:CD	2.81	0.44
3:C:312:GLN:HG3	3:C:379:TRP:HZ3	1.82	0.44
10:O:70:ARG:NE	11:V:66:ALA:HB3	2.33	0.44
10:O:124:LEU:HD22	10:O:224:LEU:HD12	2.00	0.44
10:O:312:PHE:CD1	10:O:312:PHE:C	2.95	0.44
3:P:29:SER:O	3:P:32:ASN:HB2	2.18	0.44
3:P:99:GLY:O	3:P:100:ARG:C	2.60	0.44
3:P:140:PHE:CD1	3:P:140:PHE:C	2.96	0.44
3:P:181:PHE:HA	3:P:184:ILE:HG22	2.00	0.44
4:Q:138:PRO:HD3	4:Q:149:PHE:CE2	2.53	0.44
2:B:83:PHE:CZ	6:S:107:TRP:CD1	3.06	0.44
3:C:103:TYR:HD1	3:C:325:PHE:CD2	2.35	0.44
3:C:220:PHE:CE2	13:C:503:4X9:H15	2.52	0.44
1:N:41:ILE:HG12	1:N:195:MET:HG2	1.99	0.44
3:P:219:PRO:HB2	3:P:221:HIS:O	2.17	0.44
2:B:303:VAL:HG23	2:B:303:VAL:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:162:PRO:HD2	1:N:234:CYS:SG	2.58	0.44
10:O:168:TYR:N	10:O:168:TYR:CD1	2.86	0.44
10:O:208:GLY:HA3	10:O:216:LEU:HD11	2.00	0.44
2:B:98:VAL:HG22	2:B:107:TYR:CD1	2.53	0.43
3:C:50:PHE:HE2	5:E:58:PHE:HB3	1.82	0.43
3:C:377:LEU:C	3:C:378:LYS:HG3	2.42	0.43
1:N:84:ALA:HB1	1:N:100:LYS:O	2.18	0.43
5:R:72:SER:O	5:R:92:ARG:NE	2.50	0.43
2:B:47:ILE:HD11	2:B:116:VAL:HG12	1.99	0.43
12:C:501:HEM:HBC2	12:C:501:HEM:CMC	2.43	0.43
9:J:35:PHE:O	9:J:36:ASP:C	2.62	0.43
3:P:26:ASN:ND2	3:P:208:PRO:HD2	2.33	0.43
4:Q:178:THR:HG21	8:U:15:ASP:HA	2.00	0.43
2:B:291:ALA:HA	2:B:297:GLN:NE2	2.33	0.43
3:C:358:TYR:HE1	3:C:362:ILE:HD11	1.83	0.43
4:Q:48:TYR:CE2	4:Q:65:ALA:HA	2.54	0.43
1:A:369:LEU:HD12	1:A:392:LEU:HD21	2.00	0.43
2:B:299:VAL:O	2:B:299:VAL:HG12	2.18	0.43
2:B:417:PHE:CD1	2:B:417:PHE:C	2.96	0.43
4:D:137:PRO:HA	4:D:149:PHE:HD2	1.83	0.43
1:N:252:HIS:CE1	1:N:325:VAL:HG22	2.54	0.43
5:R:75:GLU:OE1	5:R:75:GLU:HA	2.19	0.43
4:D:39:SER:C	4:D:40:CYS:SG	3.02	0.43
10:O:47:ILE:HD11	10:O:116:VAL:HG12	1.99	0.43
2:B:243:GLU:HA	2:B:424:MET:O	2.18	0.43
1:N:267:ASN:O	1:N:271:GLN:HG2	2.18	0.43
1:A:41:ILE:HD13	1:A:190:TYR:CE1	2.54	0.43
4:D:240:PRO:O	4:D:241:LYS:HG3	2.19	0.43
5:I:68:VAL:HG12	5:I:69:SER:N	2.34	0.43
1:N:185:TYR:C	1:N:185:TYR:CD1	2.97	0.43
6:S:76:PRO:O	6:S:77:LYS:C	2.62	0.43
1:A:192:ALA:N	1:A:193:PRO:HD2	2.34	0.43
2:B:26:PHE:CE1	2:B:391:SER:HA	2.54	0.43
3:C:77:TRP:CZ3	3:C:78:ILE:HG13	2.54	0.43
10:O:37:SER:HA	10:O:208:GLY:O	2.19	0.43
3:P:94:LEU:O	3:P:98:VAL:HG23	2.19	0.43
4:Q:139:THR:OG1	8:U:41:ASP:CG	2.52	0.43
1:A:246:ASP:OD2	7:G:9:ARG:HA	2.18	0.43
3:C:187:PHE:HZ	3:P:184:ILE:CD1	2.31	0.42
1:N:192:ALA:N	1:N:193:PRO:HD2	2.33	0.42
4:Q:227:TRP:O	4:Q:228:SER:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:18:LYS:HA	6:S:83:TYR:CD2	2.54	0.42
1:A:185:TYR:CD1	1:A:189:HIS:CD2	3.07	0.42
3:C:211:ILE:O	3:C:212:SER:C	2.62	0.42
1:N:123:GLU:HB2	1:N:126:GLN:HB2	2.00	0.42
1:N:379:ILE:HG12	1:N:389:ARG:CD	2.49	0.42
3:P:75:TYR:CD2	5:R:57:GLN:HG2	2.55	0.42
5:R:141:HIS:O	5:R:141:HIS:CG	2.72	0.42
1:A:21:ASN:HB2	1:A:221:GLY:CA	2.49	0.42
2:B:42:ALA:O	2:B:113:ARG:NH1	2.49	0.42
4:Q:216:LEU:N	4:Q:217:PRO:HD2	2.35	0.42
2:B:169:ARG:HH22	2:B:238:LYS:HG2	1.78	0.42
2:B:312:PHE:HD1	2:B:313:ASN:N	2.17	0.42
5:I:55:LEU:O	5:I:56:ARG:C	2.62	0.42
10:O:312:PHE:HD1	10:O:312:PHE:C	2.28	0.42
3:C:21:LEU:HD23	3:C:220:PHE:CD2	2.53	0.42
10:O:299:VAL:HG21	10:O:340:ALA:HB2	2.01	0.42
3:P:174:THR:O	3:P:177:ARG:HG2	2.20	0.42
8:U:44:VAL:HA	8:U:47:ARG:CZ	2.49	0.42
3:C:26:ASN:ND2	3:C:208:PRO:HD2	2.35	0.42
3:C:310:SER:HA	3:C:374:ASN:HD21	1.85	0.42
10:O:26:PHE:HZ	10:O:390:GLY:O	2.01	0.42
10:O:83:PHE:CE1	10:O:87:ARG:HG3	2.55	0.42
3:P:17:ALA:O	3:P:18:PHE:CD1	2.72	0.42
3:P:19:ILE:HG22	3:P:20:ASP:OD1	2.19	0.42
1:A:270:LEU:HD21	1:A:414:TYR:HD2	1.85	0.42
2:B:208:GLY:HA3	2:B:216:LEU:HD11	2.01	0.42
3:C:118:ILE:O	3:C:119:LEU:C	2.62	0.42
4:D:149:PHE:CD1	4:D:156:GLN:HB3	2.55	0.42
3:P:16:ASN:N	3:P:16:ASN:HD22	2.17	0.42
3:P:325:PHE:C	3:P:325:PHE:HD1	2.27	0.42
4:D:143:LEU:HD11	4:D:149:PHE:HB2	2.02	0.42
10:O:59:ASN:OD1	10:O:59:ASN:C	2.62	0.42
4:Q:182:VAL:HG12	4:Q:183:ALA:N	2.35	0.42
8:U:53:ASP:OD1	8:U:55:THR:OG1	2.36	0.42
1:N:40:TRP:C	1:N:41:ILE:HG13	2.45	0.42
10:O:240:HIS:ND1	10:O:241:GLY:O	2.52	0.42
5:R:44:THR:HG21	9:W:24:ILE:HD13	2.02	0.42
1:A:46:ARG:NH1	1:A:93:GLU:OE2	2.49	0.41
2:B:51:ILE:HG12	2:B:204:MET:HG2	2.02	0.41
4:Q:90:TYR:O	4:Q:91:PHE:C	2.63	0.41
4:Q:118:ARG:HD2	4:Q:194:ALA:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:224:ARG:HG3	7:T:26:PHE:CE1	2.55	0.41
3:C:284:ILE:HD12	3:C:293:ALA:HB2	2.01	0.41
4:D:48:TYR:CE2	4:D:65:ALA:HA	2.55	0.41
1:N:280:TYR:HB3	1:N:307:PHE:CE2	2.55	0.41
3:P:310:SER:HA	3:P:374:ASN:HD21	1.85	0.41
2:B:299:VAL:HG21	2:B:340:ALA:HB2	2.02	0.41
3:C:13:ILE:O	3:C:16:ASN:ND2	2.52	0.41
8:H:47:ARG:NH1	8:H:50:THR:C	2.38	0.41
1:N:40:TRP:CZ2	1:N:377:GLU:HA	2.56	0.41
1:N:327:ASP:OD1	1:N:328:HIS:N	2.53	0.41
10:O:435:PHE:CD1	10:O:435:PHE:N	2.88	0.41
3:P:118:ILE:O	3:P:119:LEU:C	2.63	0.41
4:Q:237:TYR:HB2	6:S:60:PHE:CD1	2.54	0.41
5:R:113:GLU:OE1	5:R:115:SER:N	2.52	0.41
1:A:184:GLU:O	1:A:185:TYR:C	2.62	0.41
3:C:17:ALA:O	3:C:18:PHE:CD1	2.74	0.41
3:C:193:ALA:O	3:C:196:HIS:HB3	2.21	0.41
1:N:149:VAL:HG23	1:N:425:PHE:CB	2.50	0.41
4:D:28:ARG:HA	4:D:31:GLN:HE21	1.85	0.41
1:N:158:PHE:O	1:N:159:GLN:C	2.64	0.41
6:S:83:TYR:C	6:S:83:TYR:CD1	2.99	0.41
11:V:70:LEU:O	11:V:70:LEU:CG	2.66	0.41
3:C:187:PHE:CZ	3:P:184:ILE:HD11	2.56	0.41
4:D:126:TYR:CD1	4:D:126:TYR:C	2.98	0.41
10:O:303:VAL:HG23	10:O:303:VAL:O	2.20	0.41
4:Q:110:PRO:HA	4:Q:111:PRO:HD2	1.97	0.41
7:T:34:ILE:N	7:T:35:PRO:HD2	2.35	0.41
1:A:37:VAL:HG23	1:A:199:ALA:HB2	2.03	0.41
1:A:41:ILE:HG12	1:A:195:MET:HG2	2.03	0.41
4:D:140:GLY:HA3	8:H:53:ASP:CB	2.42	0.41
7:G:79:ASN:ND2	8:H:52:GLU:OE2	2.53	0.41
10:O:172:LEU:HD13	10:O:316:TYR:CD2	2.56	0.41
3:P:186:PRO:HG2	12:P:501:HEM:HMC3	2.03	0.41
1:A:294:LEU:HG	1:A:307:PHE:CZ	2.56	0.41
3:C:30:TRP:NE1	15:C:505:PEE:O4	2.53	0.41
3:C:311:LYS:HE2	3:C:379:TRP:CD1	2.56	0.41
12:C:502:HEM:HBB2	12:C:502:HEM:HMB1	2.02	0.41
6:F:71:ARG:O	6:F:72:GLN:HB2	2.20	0.41
8:H:68:CYS:O	8:H:69:VAL:C	2.64	0.41
1:N:246:ASP:OD2	7:T:9:ARG:HA	2.20	0.41
10:O:86:THR:N	11:V:70:LEU:HD11	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:O:144:LEU:HB2	10:O:183:ILE:HG23	2.02	0.41
10:O:166:ALA:HB2	10:O:244:ILE:HG13	2.03	0.41
5:R:14:ARG:NH1	5:R:18:VAL:O	2.52	0.41
5:R:137:GLY:O	5:R:146:PRO:HD2	2.21	0.41
5:R:188:THR:HG23	5:R:192:MET:HB2	2.02	0.41
4:D:7:PRO:HA	4:D:8:PRO:HD3	1.92	0.41
4:Q:198:HIS:ND1	4:Q:198:HIS:C	2.78	0.41
5:R:82:PRO:HD2	5:R:85:LYS:HD3	2.03	0.41
8:U:47:ARG:CD	8:U:50:THR:CG2	2.99	0.41
2:B:209:LEU:HD23	2:B:375:SER:HB2	2.02	0.40
4:D:27:ARG:NH1	9:J:59:TYR:CE2	2.90	0.40
6:F:18:LYS:HG3	6:F:83:TYR:HD2	1.86	0.40
10:O:74:SER:CB	11:V:70:LEU:HD12	2.51	0.40
3:P:376:LEU:CD1	6:S:20:TYR:CD2	3.03	0.40
4:Q:60:GLU:OE2	9:W:59:TYR:HB3	2.20	0.40
2:B:365:LYS:HG2	2:B:399:LEU:HD23	2.03	0.40
4:D:179:MET:HB3	8:H:15:ASP:OD2	2.21	0.40
5:E:16:PRO:HA	5:E:19:LEU:HD12	2.03	0.40
6:F:18:LYS:HA	6:F:83:TYR:CD2	2.57	0.40
4:Q:211:MET:HG2	9:W:35:PHE:HE2	1.84	0.40
4:D:19:SER:HA	9:J:47:ASN:OD1	2.21	0.40
1:N:244:ARG:CZ	7:T:10:VAL:HB	2.51	0.40
10:O:109:VAL:HB	10:O:119:LEU:HD12	2.02	0.40
10:O:309:VAL:HA	10:O:325:TYR:O	2.20	0.40
3:P:17:ALA:O	3:P:18:PHE:HD1	2.04	0.40
3:P:276:PHE:CE1	3:P:277:ALA:HB2	2.57	0.40
8:U:40:CYS:O	8:U:43:ARG:CG	2.69	0.40
9:W:4:THR:HG22	9:W:5:LEU:H	1.86	0.40
1:A:26:ALA:O	1:A:198:ALA:HA	2.21	0.40
1:A:261:GLY:O	1:A:262:TRP:C	2.64	0.40
2:B:240:HIS:ND1	2:B:241:GLY:O	2.54	0.40
3:C:186:PRO:O	3:C:189:ILE:HB	2.21	0.40
6:F:68:LEU:HD11	6:F:75:LEU:HG	2.04	0.40
10:O:29:LEU:CD2	10:O:30:PRO:HD2	2.47	0.40
10:O:89:ILE:CG1	11:V:70:LEU:HD22	2.52	0.40
3:P:211:ILE:O	3:P:212:SER:C	2.64	0.40
6:S:77:LYS:HA	6:S:80:TRP:CE2	2.56	0.40
7:G:79:ASN:ND2	7:G:79:ASN:H	2.19	0.40
9:J:31:PHE:CD1	9:J:31:PHE:C	2.99	0.40
10:O:51:ILE:HD13	10:O:199:PHE:CE2	2.55	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	442/480 (92%)	405 (92%)	35 (8%)	2 (0%)	24	57
1	N	442/480 (92%)	407 (92%)	33 (8%)	2 (0%)	24	57
2	B	420/453 (93%)	375 (89%)	44 (10%)	1 (0%)	43	72
3	C	372/379 (98%)	347 (93%)	23 (6%)	2 (0%)	24	57
3	P	368/379 (97%)	337 (92%)	30 (8%)	1 (0%)	36	65
4	D	238/265 (90%)	216 (91%)	21 (9%)	1 (0%)	30	60
4	Q	239/265 (90%)	218 (91%)	20 (8%)	1 (0%)	30	60
5	E	71/274 (26%)	64 (90%)	7 (10%)	0	100	100
5	I	17/274 (6%)	12 (71%)	5 (29%)	0	100	100
5	R	194/274 (71%)	174 (90%)	19 (10%)	1 (0%)	24	57
6	F	96/111 (86%)	87 (91%)	9 (9%)	0	100	100
6	S	97/111 (87%)	89 (92%)	8 (8%)	0	100	100
7	G	78/82 (95%)	67 (86%)	10 (13%)	1 (1%)	9	39
7	T	72/82 (88%)	62 (86%)	10 (14%)	0	100	100
8	H	63/91 (69%)	59 (94%)	4 (6%)	0	100	100
8	U	64/91 (70%)	61 (95%)	3 (5%)	0	100	100
9	J	56/64 (88%)	51 (91%)	5 (9%)	0	100	100
9	W	57/64 (89%)	51 (90%)	6 (10%)	0	100	100
10	O	417/453 (92%)	376 (90%)	41 (10%)	0	100	100
11	V	15/274 (6%)	12 (80%)	3 (20%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3818/4946 (77%)	3470 (91%)	336 (9%)	12 (0%)	36	65

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	267	ASN
1	N	267	ASN
3	P	107	TYR
5	R	177	PRO
3	C	107	TYR
2	B	394	PRO
7	G	74	PRO
1	N	260	PRO
4	D	240	PRO
1	A	260	PRO
3	C	266	PRO
4	Q	240	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	368/394 (93%)	350 (95%)	18 (5%)	22	49
1	N	367/394 (93%)	349 (95%)	18 (5%)	22	49
2	B	331/355 (93%)	310 (94%)	21 (6%)	16	43
3	C	322/327 (98%)	301 (94%)	21 (6%)	15	42
3	P	318/327 (97%)	300 (94%)	18 (6%)	18	46
4	D	205/218 (94%)	195 (95%)	10 (5%)	22	49
4	Q	206/218 (94%)	196 (95%)	10 (5%)	22	49
5	E	63/228 (28%)	54 (86%)	9 (14%)	3	18
5	I	19/228 (8%)	13 (68%)	6 (32%)	0	2
5	R	168/228 (74%)	154 (92%)	14 (8%)	10	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	90/99 (91%)	83 (92%)	7 (8%)	11	37
6	S	91/99 (92%)	84 (92%)	7 (8%)	12	37
7	G	71/72 (99%)	60 (84%)	11 (16%)	2	16
7	T	66/72 (92%)	56 (85%)	10 (15%)	3	16
8	H	62/85 (73%)	51 (82%)	11 (18%)	2	11
8	U	63/85 (74%)	55 (87%)	8 (13%)	4	22
9	J	49/54 (91%)	46 (94%)	3 (6%)	17	44
9	W	49/54 (91%)	46 (94%)	3 (6%)	17	44
10	O	328/355 (92%)	306 (93%)	22 (7%)	15	42
11	V	15/228 (7%)	10 (67%)	5 (33%)	0	2
All	All	3251/4120 (79%)	3019 (93%)	232 (7%)	13	40

All (232) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LYS
1	A	58	PHE
1	A	149	VAL
1	A	150	PHE
1	A	156	THR
1	A	185	TYR
1	A	186	LEU
1	A	206	ARG
1	A	230	THR
1	A	302	LYS
1	A	305	GLN
1	A	324	PHE
1	A	348	SER
1	A	388	ARG
1	A	397	SER
1	A	442	PHE
1	A	444	LEU
1	A	445	ARG
2	B	96	LEU
2	B	97	SER
2	B	99	THR
2	B	101	THR
2	B	108	THR

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Mol	Chain	Res	Type
2	B	116	VAL
2	B	126	VAL
2	B	150	VAL
2	B	158	HIS
2	B	170	ASN
2	B	189	VAL
2	B	219	VAL
2	B	224	LEU
2	B	226	ILE
2	B	230	LEU
2	B	301	LYS
2	B	310	SER
2	B	316	TYR
2	B	324	PHE
2	B	379	LEU
2	B	436	ILE
3	C	10	LEU
3	C	11	MET
3	C	15	ASN
3	C	21	LEU
3	C	32	ASN
3	C	35	SER
3	C	39	ILE
3	C	64	SER
3	C	78	ILE
3	C	138	MET
3	C	156	ILE
3	C	161	VAL
3	C	171	ASP
3	C	257	THR
3	C	268	ILE
3	C	276	PHE
3	C	282	ARG
3	C	287	LYS
3	C	310	SER
3	C	311	LYS
3	C	349	THR
4	D	3	LEU
4	D	17	LEU
4	D	19	SER
4	D	37	CYS
4	D	40	CYS

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Mol	Chain	Res	Type
4	D	68	VAL
4	D	178	THR
4	D	182	VAL
4	D	216	LEU
4	D	232	SER
5	E	7	VAL
5	E	11	SER
5	E	27	GLU
5	E	36	SER
5	E	40	THR
5	E	42	THR
5	E	47	VAL
5	E	54	VAL
5	E	72	SER
6	F	20	TYR
6	F	26	PHE
6	F	40	ASN
6	F	78	GLU
6	F	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	60	THR
7	G	63	THR
7	G	72	LYS
7	G	78	GLU
8	H	14	VAL
8	H	34	ARG
8	H	42	GLU
8	H	43	ARG
8	H	44	VAL
8	H	45	SER
8	H	47	ARG
8	H	49	GLN
8	H	50	THR
8	H	51	GLU

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Mol	Chain	Res	Type
8	H	55	THR
5	I	50	LEU
5	I	54	SER
5	I	65	VAL
5	I	67	SER
5	I	70	LEU
5	I	72	VAL
9	J	4	THR
9	J	37	GLN
9	J	59	TYR
1	N	27	SER
1	N	51	LYS
1	N	58	PHE
1	N	149	VAL
1	N	156	THR
1	N	168	GLU
1	N	185	TYR
1	N	186	LEU
1	N	206	ARG
1	N	230	THR
1	N	305	GLN
1	N	324	PHE
1	N	348	SER
1	N	388	ARG
1	N	397	SER
1	N	442	PHE
1	N	444	LEU
1	N	445	ARG
10	O	96	LEU
10	O	97	SER
10	O	99	THR
10	O	101	THR
10	O	108	THR
10	O	116	VAL
10	O	126	VAL
10	O	150	VAL
10	O	158	HIS
10	O	170	ASN
10	O	189	VAL
10	O	219	VAL
10	O	224	LEU
10	O	226	ILE

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Mol	Chain	Res	Type
10	O	230	LEU
10	O	301	LYS
10	O	310	SER
10	O	316	TYR
10	O	324	PHE
10	O	328	SER
10	O	379	LEU
10	O	436	ILE
3	P	10	LEU
3	P	11	MET
3	P	15	ASN
3	P	21	LEU
3	P	32	ASN
3	P	35	SER
3	P	39	ILE
3	P	64	SER
3	P	78	ILE
3	P	138	MET
3	P	156	ILE
3	P	257	THR
3	P	268	ILE
3	P	276	PHE
3	P	287	LYS
3	P	310	SER
3	P	311	LYS
3	P	349	THR
4	Q	3	LEU
4	Q	17	LEU
4	Q	19	SER
4	Q	37	CYS
4	Q	40	CYS
4	Q	68	VAL
4	Q	178	THR
4	Q	182	VAL
4	Q	216	LEU
4	Q	232	SER
5	R	7	VAL
5	R	27	GLU
5	R	36	SER
5	R	40	THR
5	R	42	THR
5	R	47	VAL

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Mol	Chain	Res	Type
5	R	54	VAL
5	R	72	SER
5	R	78	LEU
5	R	102	THR
5	R	113	GLU
5	R	136	ILE
5	R	140	THR
5	R	194	ILE
6	S	26	PHE
6	S	40	ASN
6	S	78	GLU
6	S	91	GLU
6	S	94	LEU
6	S	95	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
7	T	60	THR
7	T	63	THR
7	T	72	LYS
8	U	14	VAL
8	U	34	ARG
8	U	43	ARG
8	U	47	ARG
8	U	49	GLN
8	U	50	THR
8	U	51	GLU
8	U	55	THR
11	V	65	VAL
11	V	67	SER
11	V	70	LEU
11	V	72	VAL
11	V	76	VAL
9	W	4	THR
9	W	37	GLN
9	W	59	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	32	GLN
1	A	118	GLN
1	A	165	GLN
1	A	189	HIS
1	A	240	GLN
1	A	271	GLN
2	B	31	ASN
2	B	104	ASN
2	B	290	ASN
2	B	297	GLN
2	B	305	GLN
2	B	343	GLN
2	B	412	ASN
3	C	8	HIS
3	C	16	ASN
3	C	148	ASN
3	C	260	ASN
3	C	267	HIS
3	C	341	GLN
3	C	345	HIS
4	D	31	GLN
4	D	97	ASN
4	D	225	HIS
6	F	72	GLN
7	G	6	HIS
7	G	73	ASN
7	G	79	ASN
9	J	57	HIS
1	N	32	GLN
1	N	118	GLN
1	N	165	GLN
1	N	189	HIS
1	N	240	GLN
1	N	271	GLN
10	O	31	ASN
10	O	104	ASN
10	O	277	HIS
10	O	343	GLN
10	O	412	ASN
3	P	16	ASN
3	P	148	ASN

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Mol	Chain	Res	Type
3	P	341	GLN
3	P	345	HIS
3	P	374	ASN
4	Q	31	GLN
4	Q	97	ASN
4	Q	166	ASN
6	S	22	ASN
9	W	57	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](#)

29 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
14	PO4	D	504	-	4,4,4	0.90	0	6,6,6	0.61	0
14	PO4	D	503	-	4,4,4	0.93	0	6,6,6	0.70	0
14	PO4	Q	1002	-	4,4,4	0.94	0	6,6,6	0.51	0
17	CDL	D	505	-	38,38,99	1.28	3 (7%)	42,47,111	1.17	4 (9%)
14	PO4	N	1001	-	4,4,4	0.85	0	6,6,6	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	CDL	G	501	-	43,43,99	1.56	4 (9%)	49,55,111	1.55	8 (16%)
14	PO4	C	504	-	4,4,4	1.00	0	6,6,6	0.44	0
15	PEE	Q	506	-	50,50,50	1.32	4 (8%)	53,55,55	1.32	7 (13%)
16	HEC	Q	501	4	46,50,50	2.62	24 (52%)	58,82,82	2.10	22 (37%)
15	PEE	C	505	-	48,48,50	1.28	4 (8%)	51,53,55	1.05	4 (7%)
19	GOL	R	502	-	5,5,5	0.34	0	5,5,5	0.48	0
16	HEC	D	501	4	46,50,50	2.67	25 (54%)	58,82,82	2.28	24 (41%)
17	CDL	Q	505	-	38,38,99	1.28	3 (7%)	42,47,111	1.17	4 (9%)
15	PEE	P	505	-	48,48,50	1.35	4 (8%)	51,53,55	0.95	1 (1%)
12	HEM	C	501	3	50,50,50	1.66	8 (16%)	67,82,82	1.64	14 (20%)
12	HEM	C	502	3	50,50,50	1.71	11 (22%)	67,82,82	1.47	10 (14%)
12	HEM	P	502	3	50,50,50	1.69	10 (20%)	67,82,82	1.76	16 (23%)
14	PO4	E	501	-	4,4,4	0.73	0	6,6,6	0.85	0
12	HEM	P	501	3	50,50,50	1.59	11 (22%)	67,82,82	1.62	15 (22%)
14	PO4	F	501	-	4,4,4	0.92	0	6,6,6	0.66	0
14	PO4	D	502	-	4,4,4	0.80	0	6,6,6	0.66	0
18	FES	R	501	5	0,4,4	-	-	-	-	-
13	4X9	C	503	-	30,30,30	2.99	7 (23%)	41,44,44	1.22	2 (4%)
14	PO4	S	501	-	4,4,4	0.90	0	6,6,6	0.51	0
15	PEE	D	506	-	25,25,50	1.50	2 (8%)	28,30,55	1.48	4 (14%)
17	CDL	T	501	-	48,48,99	1.41	4 (8%)	54,60,111	1.21	5 (9%)
13	4X9	P	503	-	30,30,30	2.80	6 (20%)	41,44,44	1.69	7 (17%)
14	PO4	N	501	-	4,4,4	0.77	0	6,6,6	1.02	1 (16%)
14	PO4	Q	1001	-	4,4,4	0.91	0	6,6,6	0.50	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	HEC	Q	501	4	-	5/14/54/54	-
15	PEE	P	505	-	1/1/4/8	22/52/52/54	-
15	PEE	C	505	-	1/1/4/8	23/52/52/54	-
12	HEM	C	501	3	-	5/14/54/54	-
15	PEE	D	506	-	1/1/4/8	13/29/29/54	-
12	HEM	C	502	3	-	5/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	HEM	P	502	3	-	8/14/54/54	-
13	4X9	P	503	-	-	3/13/13/13	0/3/3/3
16	HEC	D	501	4	-	9/14/54/54	-
17	CDL	D	505	-	-	20/43/43/110	-
12	HEM	P	501	3	-	8/14/54/54	-
17	CDL	Q	505	-	-	12/43/43/110	-
17	CDL	T	501	-	-	28/57/57/110	-
19	GOL	R	502	-	-	2/4/4/4	-
18	FES	R	501	5	-	-	0/1/1/1
17	CDL	G	501	-	-	24/52/52/110	-
15	PEE	Q	506	-	1/1/4/8	24/54/54/54	-
13	4X9	C	503	-	-	5/13/13/13	0/3/3/3

All (130) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	P	503	4X9	C19-C20	8.48	1.50	1.38
13	C	503	4X9	C17-C18	8.41	1.50	1.40
13	C	503	4X9	C19-C20	7.66	1.49	1.38
13	C	503	4X9	C17-C22	7.38	1.49	1.40
13	P	503	4X9	C17-C18	7.02	1.48	1.40
13	P	503	4X9	C17-C22	6.49	1.48	1.40
13	C	503	4X9	C18-C19	6.03	1.49	1.39
17	G	501	CDL	OA6-CA5	5.37	1.47	1.35
16	D	501	HEC	CHC-C4B	5.36	1.48	1.38
12	P	502	HEM	FE-NB	5.34	2.11	1.94
15	D	506	PEE	O3-C30	5.02	1.48	1.33
16	Q	501	HEC	CHA-C1A	4.99	1.48	1.38
17	T	501	CDL	OB6-CB5	4.95	1.48	1.34
16	Q	501	HEC	C2A-C3A	4.95	1.47	1.36
16	D	501	HEC	C2A-C3A	4.91	1.47	1.36
12	P	501	HEM	FE-NB	4.89	2.10	1.94
17	G	501	CDL	OB6-CB5	4.89	1.48	1.34
17	Q	505	CDL	OA6-CA5	4.87	1.48	1.34
17	G	501	CDL	OB8-CB7	4.87	1.47	1.33
15	P	505	PEE	O2-C10	4.84	1.48	1.34
13	P	503	4X9	O28-C18	-4.82	1.25	1.36
16	Q	501	HEC	CHC-C4B	4.80	1.47	1.38
16	D	501	HEC	CHD-C4C	4.80	1.47	1.38
12	C	501	HEM	FE-NB	4.79	2.09	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	T	501	CDL	OA6-CA5	4.79	1.45	1.35
15	Q	506	PEE	O2-C10	4.78	1.47	1.34
16	Q	501	HEC	CHB-C4A	4.77	1.47	1.38
17	D	505	CDL	OA6-CA5	4.76	1.47	1.34
17	T	501	CDL	OB8-CB7	4.74	1.47	1.33
16	D	501	HEC	CAC-C3C	4.72	1.50	1.35
15	P	505	PEE	O3-C30	4.71	1.47	1.33
15	C	505	PEE	O2-C10	4.66	1.47	1.34
13	C	503	4X9	O28-C18	-4.59	1.26	1.36
16	Q	501	HEC	CHD-C4C	4.56	1.47	1.38
13	P	503	4X9	C18-C19	4.56	1.46	1.39
17	Q	505	CDL	OA8-CA7	4.55	1.46	1.33
15	D	506	PEE	O2-C10	4.53	1.47	1.34
17	D	505	CDL	OA8-CA7	4.50	1.46	1.33
12	C	502	HEM	FE-NB	4.43	2.08	1.94
16	D	501	HEC	CHA-C1A	4.32	1.46	1.38
16	Q	501	HEC	CAC-C3C	4.31	1.49	1.35
15	Q	506	PEE	O3-C30	4.29	1.45	1.33
16	Q	501	HEC	CAB-C3B	4.25	1.48	1.35
16	D	501	HEC	CAB-C3B	4.25	1.48	1.35
12	P	502	HEM	FE-NC	4.20	2.09	1.95
12	C	501	HEM	C1B-NB	-4.17	1.33	1.40
15	C	505	PEE	O3-C30	4.13	1.45	1.33
16	D	501	HEC	CHC-C1C	4.09	1.48	1.39
12	C	501	HEM	FE-NC	4.09	2.08	1.95
12	C	502	HEM	C1B-NB	-4.05	1.33	1.40
16	D	501	HEC	CHB-C4A	3.98	1.46	1.38
15	Q	506	PEE	C18-C19	3.96	1.54	1.31
16	Q	501	HEC	CHB-C1B	3.95	1.48	1.39
12	P	501	HEM	FE-NC	3.91	2.08	1.95
15	C	505	PEE	C18-C19	3.90	1.53	1.31
15	P	505	PEE	C39-C38	3.89	1.53	1.31
15	P	505	PEE	C18-C19	3.89	1.53	1.31
15	C	505	PEE	C39-C38	3.86	1.53	1.31
12	C	502	HEM	FE-NC	3.83	2.07	1.95
15	Q	506	PEE	C39-C38	3.82	1.53	1.31
16	Q	501	HEC	CHC-C1C	3.77	1.47	1.39
12	P	502	HEM	C1B-NB	-3.62	1.34	1.40
16	Q	501	HEC	CHD-C1D	3.61	1.47	1.39
12	P	501	HEM	C1B-NB	-3.58	1.34	1.40
16	D	501	HEC	CHB-C1B	3.55	1.47	1.39
16	D	501	HEC	CHD-C1D	3.54	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	D	501	HEC	C4A-NA	-3.50	1.33	1.39
16	D	501	HEC	C1A-NA	-3.36	1.33	1.39
12	C	502	HEM	C4D-ND	-3.33	1.34	1.40
13	P	503	4X9	C19-CL	3.30	1.79	1.72
16	D	501	HEC	CHA-C4D	3.26	1.46	1.39
12	C	501	HEM	C4D-ND	-3.23	1.34	1.40
16	Q	501	HEC	C3D-C2D	3.15	1.47	1.38
16	Q	501	HEC	C4D-ND	-3.11	1.33	1.39
16	D	501	HEC	C1B-NB	-3.10	1.33	1.39
17	G	501	CDL	OA8-CA7	3.09	1.48	1.33
16	Q	501	HEC	CHA-C4D	3.03	1.46	1.39
12	C	502	HEM	C4B-NB	-2.98	1.33	1.38
16	Q	501	HEC	C1C-C2C	2.96	1.50	1.43
13	C	503	4X9	C19-CL	2.94	1.79	1.72
12	P	501	HEM	C4D-ND	-2.92	1.35	1.40
16	D	501	HEC	C3D-C2D	2.89	1.46	1.38
12	C	502	HEM	C1D-ND	-2.89	1.33	1.38
12	C	502	HEM	C1C-C2C	-2.82	1.39	1.45
16	D	501	HEC	C1D-ND	-2.82	1.34	1.39
16	D	501	HEC	C1B-C2B	2.81	1.49	1.43
16	Q	501	HEC	C4B-NB	-2.80	1.34	1.39
12	C	501	HEM	C4B-NB	-2.73	1.33	1.38
16	D	501	HEC	C4C-NC	-2.73	1.34	1.39
12	P	501	HEM	C4B-NB	-2.71	1.33	1.38
17	Q	505	CDL	PB2-OB5	2.69	1.64	1.54
12	P	502	HEM	C4D-ND	-2.68	1.35	1.40
16	D	501	HEC	C4B-NB	-2.67	1.34	1.39
12	P	502	HEM	C4B-NB	-2.63	1.33	1.38
12	C	502	HEM	C3B-C4B	2.60	1.50	1.44
16	Q	501	HEC	C4A-NA	-2.60	1.34	1.39
16	D	501	HEC	C1C-NC	-2.59	1.34	1.39
17	D	505	CDL	PB2-OB5	2.55	1.64	1.54
12	P	502	HEM	C1C-C2C	-2.55	1.40	1.45
17	T	501	CDL	OA8-CA7	2.54	1.45	1.33
16	D	501	HEC	C1D-C2D	2.52	1.49	1.43
16	D	501	HEC	C4D-ND	-2.49	1.34	1.39
13	C	503	4X9	O3-C1	2.49	1.44	1.31
16	Q	501	HEC	C1B-NB	-2.49	1.34	1.39
16	Q	501	HEC	C1C-NC	-2.41	1.35	1.39
12	P	502	HEM	C1D-ND	-2.41	1.34	1.38
16	Q	501	HEC	C1A-NA	-2.40	1.35	1.39
12	C	502	HEM	C1C-NC	-2.40	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	501	HEC	C1B-C2B	2.39	1.48	1.43
16	D	501	HEC	C1C-C2C	2.37	1.48	1.43
16	Q	501	HEC	C1A-C2A	2.37	1.49	1.45
12	P	501	HEM	C1C-NC	-2.36	1.35	1.39
12	C	501	HEM	C1C-NC	-2.36	1.35	1.39
16	D	501	HEC	C4D-C3D	2.36	1.49	1.44
12	C	502	HEM	C4C-NC	-2.35	1.35	1.39
12	C	502	HEM	C3C-C4C	-2.34	1.41	1.46
12	C	501	HEM	C4A-NA	-2.31	1.35	1.39
12	P	501	HEM	C3C-C4C	-2.28	1.42	1.46
12	P	501	HEM	C1D-C2D	2.23	1.49	1.44
16	Q	501	HEC	C1D-ND	-2.23	1.35	1.39
12	P	502	HEM	C4D-C3D	2.22	1.48	1.45
12	P	501	HEM	C1C-C2C	-2.21	1.41	1.45
12	C	501	HEM	C1D-ND	-2.20	1.34	1.38
16	Q	501	HEC	C1D-C2D	2.18	1.48	1.43
12	P	501	HEM	FE-NA	2.17	2.02	1.95
16	Q	501	HEC	C4A-C3A	2.16	1.49	1.45
12	P	502	HEM	FE-ND	-2.14	1.88	1.94
12	P	502	HEM	C1A-C2A	-2.07	1.40	1.44
12	P	501	HEM	C1D-ND	-2.03	1.34	1.38
16	D	501	HEC	C3C-C2C	2.01	1.47	1.41

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	501	HEC	C2A-C1A-NA	5.28	115.42	110.32
16	D	501	HEC	C2A-C1A-NA	5.24	115.38	110.32
15	D	506	PEE	O2-C10-C11	5.06	122.42	111.48
13	P	503	4X9	C20-C19-CL	4.97	128.27	121.05
17	G	501	CDL	OA6-CA5-C11	4.97	119.95	111.09
12	P	501	HEM	CHC-C4B-NB	4.89	129.69	124.42
12	P	502	HEM	CAD-C3D-C4D	4.86	133.17	124.70
15	Q	506	PEE	C2-O2-C10	4.76	129.18	117.80
16	D	501	HEC	CAD-C3D-C4D	4.68	134.07	124.94
12	P	502	HEM	CHD-C1D-ND	4.56	129.33	124.42
16	D	501	HEC	C3D-C4D-ND	4.50	115.15	110.15
16	Q	501	HEC	C3D-C4D-ND	4.36	114.99	110.15
17	T	501	CDL	OA6-CA5-C11	4.35	118.85	111.09
12	C	501	HEM	C1B-NB-C4B	4.27	110.26	105.21
17	G	501	CDL	OB8-CB7-C71	4.09	124.29	111.83
13	P	503	4X9	C20-C19-C18	-4.05	118.33	122.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	501	HEC	C1D-C2D-C3D	-4.01	102.23	106.82
12	P	501	HEM	C1B-NB-C4B	3.98	109.92	105.21
17	D	505	CDL	OA6-CA5-C11	3.98	120.08	111.48
12	C	501	HEM	C3B-C4B-NB	-3.96	106.63	109.47
16	D	501	HEC	CBA-CAA-C2A	3.94	123.43	112.53
12	P	502	HEM	CHC-C4B-NB	3.91	128.63	124.42
12	P	502	HEM	CAC-C3C-C4C	3.88	134.08	124.82
13	P	503	4X9	C18-C19-CL	-3.87	113.39	118.09
15	Q	506	PEE	O2-C10-C11	3.79	119.68	111.48
17	Q	505	CDL	OA6-CA5-C11	3.76	119.61	111.48
12	C	501	HEM	CHC-C4B-NB	3.76	128.47	124.42
17	T	501	CDL	OB6-CB5-C51	3.73	119.55	111.48
12	P	501	HEM	CMD-C2D-C1D	3.72	130.85	125.03
12	C	502	HEM	C1B-NB-C4B	3.69	109.57	105.21
12	C	501	HEM	CHB-C1B-NB	3.68	128.92	124.37
16	D	501	HEC	C2B-C1B-NB	3.67	116.03	110.14
16	D	501	HEC	C1D-C2D-C3D	-3.55	102.75	106.82
17	D	505	CDL	OA8-CA7-C31	3.54	122.63	111.83
16	Q	501	HEC	C1A-C2A-C3A	-3.53	102.46	107.11
16	D	501	HEC	C4A-C3A-C2A	-3.53	101.74	106.97
12	C	502	HEM	CHC-C4B-NB	3.48	128.17	124.42
12	C	502	HEM	CHA-C4D-ND	3.46	128.65	124.37
12	C	502	HEM	CHD-C1D-ND	3.45	128.13	124.42
16	D	501	HEC	CAA-CBA-CGA	-3.44	104.54	113.67
16	Q	501	HEC	C2B-C1B-NB	3.44	115.65	110.14
17	G	501	CDL	OB6-CB5-C51	3.39	123.37	110.93
13	C	503	4X9	C22-N30-C20	3.37	124.37	119.58
16	D	501	HEC	CMD-C2D-C1D	3.35	130.52	125.42
15	P	505	PEE	O2-C10-C11	3.35	118.73	111.48
16	D	501	HEC	C2D-C1D-ND	3.30	115.43	110.14
16	Q	501	HEC	C2C-C1C-NC	3.27	115.39	110.14
15	D	506	PEE	O3-C30-C31	3.25	121.75	111.83
12	P	501	HEM	CHA-C4D-ND	3.25	128.39	124.37
12	C	501	HEM	CHD-C1D-ND	3.23	127.90	124.42
16	D	501	HEC	C1A-C2A-C3A	-3.22	102.87	107.11
16	D	501	HEC	CHA-C1A-C2A	-3.18	119.85	124.86
16	Q	501	HEC	C2D-C1D-ND	3.17	115.22	110.14
16	D	501	HEC	C3A-C4A-NA	3.15	115.46	109.64
16	D	501	HEC	C2C-C1C-NC	3.14	115.18	110.14
13	P	503	4X9	C29-C22-C17	-3.10	117.85	122.31
12	C	502	HEM	CHA-C4D-C3D	-3.09	119.52	125.23
15	C	505	PEE	O3-C30-C31	3.05	121.15	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	P	502	HEM	CHB-C1B-NB	3.04	128.12	124.37
17	G	501	CDL	CA6-OA8-CA7	3.03	124.55	117.08
16	Q	501	HEC	C3A-C4A-NA	3.01	115.20	109.64
13	P	503	4X9	C29-C22-N30	2.99	121.18	116.53
17	T	501	CDL	OB8-CB7-C71	2.98	120.92	111.83
15	Q	506	PEE	O3-C3-C2	2.97	116.95	108.40
15	C	505	PEE	O2-C10-C11	2.96	117.88	111.48
12	C	501	HEM	CHD-C1D-C2D	-2.91	120.43	125.03
17	Q	505	CDL	OA8-CA7-C31	2.91	120.70	111.83
16	Q	501	HEC	CMD-C2D-C1D	2.88	129.81	125.42
12	P	502	HEM	CAC-C3C-C2C	-2.87	119.10	128.43
16	Q	501	HEC	C4A-C3A-C2A	-2.84	102.76	106.97
16	Q	501	HEC	CAD-C3D-C4D	2.83	130.47	124.94
12	P	502	HEM	C1B-NB-C4B	2.83	108.56	105.21
17	G	501	CDL	OB8-CB6-CB4	2.83	116.56	108.40
12	C	501	HEM	CBA-CAA-C2A	-2.83	104.71	112.53
16	Q	501	HEC	CHA-C1A-C2A	-2.82	120.41	124.86
12	P	501	HEM	CHB-C1B-NB	2.81	127.84	124.37
13	P	503	4X9	C22-N30-C20	2.81	123.56	119.58
15	Q	506	PEE	O3-C30-C31	2.79	120.34	111.83
12	P	502	HEM	CAD-C3D-C2D	-2.79	122.65	127.87
17	D	505	CDL	OA8-CA7-OA9	-2.77	116.71	123.63
15	D	506	PEE	O2-C10-O4	-2.76	117.25	123.70
13	C	503	4X9	C20-C19-C18	-2.74	119.73	122.65
16	D	501	HEC	C4D-C3D-C2D	-2.72	102.66	106.87
12	C	502	HEM	CHD-C1D-C2D	-2.71	120.74	125.03
17	T	501	CDL	OA6-CA5-OA7	-2.71	117.76	122.99
12	P	501	HEM	CHD-C1D-C2D	-2.71	120.76	125.03
17	G	501	CDL	OB6-CB5-OB7	-2.68	117.44	123.70
16	Q	501	HEC	CMA-C3A-C4A	2.68	129.44	124.73
16	D	501	HEC	CMA-C3A-C4A	2.67	129.42	124.73
16	D	501	HEC	CAA-C2A-C3A	2.65	132.84	127.87
16	Q	501	HEC	CHD-C1D-C2D	-2.65	119.74	127.43
12	P	501	HEM	CHD-C1D-ND	2.61	127.24	124.42
12	P	501	HEM	CHD-C4C-NC	2.61	127.29	124.45
15	C	505	PEE	O3-C30-O5	-2.60	117.12	123.63
12	P	501	HEM	CHA-C4D-C3D	-2.60	120.43	125.23
12	C	502	HEM	CHB-C1B-NB	2.59	127.58	124.37
17	Q	505	CDL	OA8-CA7-OA9	-2.59	117.16	123.63
16	D	501	HEC	CAD-CBD-CGD	-2.55	106.91	113.67
12	P	501	HEM	O2D-CGD-CBD	2.55	122.04	114.00
16	Q	501	HEC	CBB-CAB-C3B	-2.54	122.37	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	501	HEC	CBC-CAC-C3C	-2.54	122.37	127.43
17	Q	505	CDL	OB4-PB2-OB3	2.53	120.68	110.83
16	Q	501	HEC	CAD-CBD-CGD	-2.52	106.97	113.67
17	G	501	CDL	OB8-CB7-OB9	-2.49	117.40	123.63
12	C	501	HEM	CAB-C3B-C2B	-2.48	120.36	128.43
16	Q	501	HEC	CHB-C1B-C2B	-2.46	120.28	127.43
12	C	501	HEM	CMB-C2B-C1B	2.44	128.85	125.03
16	Q	501	HEC	CHD-C4C-C3C	-2.43	121.12	125.21
12	P	501	HEM	O2A-CGA-CBA	2.42	121.65	114.00
12	C	501	HEM	CHD-C4C-NC	2.38	127.05	124.45
12	C	502	HEM	C3B-C4B-NB	-2.37	107.77	109.47
16	D	501	HEC	CHB-C1B-C2B	-2.37	120.55	127.43
16	D	501	HEC	CHB-C4A-NA	-2.37	121.88	124.45
12	C	501	HEM	CAD-C3D-C4D	2.36	128.81	124.70
17	G	501	CDL	OA8-CA7-C31	2.36	122.39	112.38
12	P	502	HEM	CHA-C4D-ND	2.36	127.28	124.37
16	Q	501	HEC	C4D-C3D-C2D	-2.36	103.22	106.87
12	P	501	HEM	CAD-C3D-C4D	2.30	128.70	124.70
16	D	501	HEC	CMC-C2C-C3C	2.28	131.91	126.55
16	D	501	HEC	CBB-CAB-C3B	-2.26	122.91	127.43
12	P	502	HEM	CHD-C1D-C2D	-2.24	121.50	125.03
12	P	502	HEM	CMD-C2D-C1D	2.21	128.48	125.03
12	C	502	HEM	O2A-CGA-CBA	2.19	120.91	114.00
12	P	502	HEM	CBA-CAA-C2A	-2.16	106.57	112.53
15	Q	506	PEE	C40-C39-C38	-2.16	108.67	124.83
12	C	501	HEM	CHA-C4D-C3D	-2.15	121.27	125.23
16	Q	501	HEC	CAA-CBA-CGA	-2.15	107.97	113.67
15	Q	506	PEE	O3-C30-O5	-2.13	118.29	123.63
16	D	501	HEC	O2A-CGA-CBA	2.13	120.73	114.00
12	P	502	HEM	CHB-C1B-C2B	-2.12	120.92	126.95
15	D	506	PEE	O3-C30-O5	-2.12	118.33	123.63
17	D	505	CDL	OB4-PB2-OB3	2.10	119.00	110.83
12	C	501	HEM	CMB-C2B-C3B	-2.09	123.37	128.43
12	P	502	HEM	C4C-NC-C1C	2.06	109.18	105.82
12	P	501	HEM	C1D-C2D-C3D	-2.06	104.81	106.98
12	P	502	HEM	CHD-C4C-C3C	2.05	128.67	125.21
12	P	502	HEM	C2A-C1A-NA	-2.05	107.88	110.15
12	C	501	HEM	CAB-C3B-C4B	2.04	133.39	124.39
12	P	501	HEM	CAD-CBD-CGD	-2.04	108.27	113.67
15	Q	506	PEE	O2-C2-C3	2.03	115.64	108.34
15	C	505	PEE	C3-C2-C1	-2.03	107.06	111.78
17	T	501	CDL	OB8-CB7-OB9	-2.02	118.58	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	D	501	HEC	CHD-C1D-C2D	-2.02	121.57	127.43
14	N	501	PO4	O4-P-O2	2.02	114.19	107.91
12	C	502	HEM	CHD-C4C-NC	2.01	126.64	124.45
13	P	503	4X9	O28-C18-C17	2.01	124.34	119.57
12	P	501	HEM	C4B-C3B-C2B	-2.00	105.44	107.28
16	Q	501	HEC	O1D-CGD-CBD	-2.00	116.74	123.09

All (4) chirality outliers are listed below:

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

All (216) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	C	502	HEM	C2D-C3D-CAD-CBD
12	C	502	HEM	C4D-C3D-CAD-CBD
12	P	501	HEM	C1A-C2A-CAA-CBA
15	D	506	PEE	C1-O3P-P-O2P
15	D	506	PEE	C1-O3P-P-O4P
15	D	506	PEE	C4-O4P-P-O3P
15	D	506	PEE	C5-C4-O4P-P
15	D	506	PEE	O4P-C4-C5-N
15	P	505	PEE	C1-O3P-P-O4P
15	P	505	PEE	O4P-C4-C5-N
15	Q	506	PEE	C17-C18-C19-C20
15	Q	506	PEE	C1-O3P-P-O2P
15	Q	506	PEE	C1-O3P-P-O4P
16	Q	501	HEC	C1A-C2A-CAA-CBA
16	Q	501	HEC	C3A-C2A-CAA-CBA
17	D	505	CDL	CB2-OB2-PB2-OB4
17	D	505	CDL	CB2-OB2-PB2-OB5
17	G	501	CDL	O1-C1-CB2-OB2
17	G	501	CDL	CA2-C1-CB2-OB2
17	G	501	CDL	CA3-OA5-PA1-OA2
17	G	501	CDL	CA3-OA5-PA1-OA4
17	G	501	CDL	CB4-CB3-OB5-PB2
17	G	501	CDL	C51-CB5-OB6-CB4
17	Q	505	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
17	Q	505	CDL	CB2-OB2-PB2-OB4
17	Q	505	CDL	CB2-OB2-PB2-OB5
17	T	501	CDL	O1-C1-CB2-OB2
17	T	501	CDL	CA2-OA2-PA1-OA4
17	T	501	CDL	CA2-OA2-PA1-OA5
17	T	501	CDL	CA3-OA5-PA1-OA3
17	T	501	CDL	CB2-OB2-PB2-OB3
17	T	501	CDL	CB3-OB5-PB2-OB2
17	T	501	CDL	CB3-OB5-PB2-OB3
17	T	501	CDL	CB3-OB5-PB2-OB4
17	T	501	CDL	C11-CA5-OA6-CA4
17	Q	505	CDL	OA9-CA7-OA8-CA6
17	T	501	CDL	OA7-CA5-OA6-CA4
17	G	501	CDL	OB7-CB5-OB6-CB4
17	Q	505	CDL	C31-CA7-OA8-CA6
17	G	501	CDL	C11-CA5-OA6-CA4
15	C	505	PEE	C37-C38-C39-C40
12	P	502	HEM	C4D-C3D-CAD-CBD
17	G	501	CDL	O1-C1-CA2-OA2
16	D	501	HEC	C4D-C3D-CAD-CBD
13	C	503	4X9	F23-C1-O3-C4
17	T	501	CDL	OA9-CA7-OA8-CA6
17	T	501	CDL	C31-CA7-OA8-CA6
17	D	505	CDL	CA2-C1-CB2-OB2
17	G	501	CDL	CB2-C1-CA2-OA2
15	D	506	PEE	C31-C30-O3-C3
15	D	506	PEE	O5-C30-O3-C3
12	P	501	HEM	C3A-C2A-CAA-CBA
16	D	501	HEC	C2D-C3D-CAD-CBD
17	G	501	CDL	OA6-CA4-CA6-OA8
17	D	505	CDL	C31-CA7-OA8-CA6
15	P	505	PEE	C10-C11-C12-C13
15	Q	506	PEE	C10-C11-C12-C13
15	P	505	PEE	C11-C10-O2-C2
17	T	501	CDL	CB4-CB3-OB5-PB2
12	C	502	HEM	C3D-CAD-CBD-CGD
15	P	505	PEE	C30-C31-C32-C33
17	Q	505	CDL	CA7-C31-C32-C33
17	D	505	CDL	O1-C1-CB2-OB2
15	P	505	PEE	C37-C38-C39-C40
17	G	501	CDL	OA7-CA5-OA6-CA4
12	P	502	HEM	C2D-C3D-CAD-CBD

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Mol	Chain	Res	Type	Atoms
16	D	501	HEC	C1A-C2A-CAA-CBA
15	P	505	PEE	O4-C10-O2-C2
17	T	501	CDL	CA2-C1-CB2-OB2
17	D	505	CDL	OA9-CA7-OA8-CA6
13	C	503	4X9	F24-C1-O3-C4
19	R	502	GOL	C1-C2-C3-O3
15	C	505	PEE	C21-C22-C23-C24
15	Q	506	PEE	C31-C32-C33-C34
15	C	505	PEE	C30-C31-C32-C33
13	C	503	4X9	F25-C1-O3-C4
15	P	505	PEE	C13-C14-C15-C16
15	Q	506	PEE	C32-C33-C34-C35
15	P	505	PEE	C1-C2-C3-O3
17	T	501	CDL	C52-C53-C54-C55
17	T	501	CDL	C73-C74-C75-C76
15	Q	506	PEE	C21-C22-C23-C24
15	D	506	PEE	C11-C10-O2-C2
17	G	501	CDL	C71-CB7-OB8-CB6
17	D	505	CDL	CA4-CA3-OA5-PA1
17	G	501	CDL	C31-CA7-OA8-CA6
17	D	505	CDL	C38-C39-C40-C41
15	C	505	PEE	C20-C21-C22-C23
15	Q	506	PEE	C11-C12-C13-C14
15	P	505	PEE	C42-C43-C44-C45
15	Q	506	PEE	C22-C23-C24-C25
17	Q	505	CDL	C38-C39-C40-C41
15	P	505	PEE	C34-C35-C36-C37
15	P	505	PEE	C16-C17-C18-C19
15	C	505	PEE	C42-C43-C44-C45
15	C	505	PEE	C11-C10-O2-C2
17	D	505	CDL	C11-CA5-OA6-CA4
15	C	505	PEE	O4-C10-O2-C2
15	C	505	PEE	C15-C16-C17-C18
15	Q	506	PEE	C19-C20-C21-C22
15	Q	506	PEE	C39-C40-C41-C42
15	P	505	PEE	C32-C33-C34-C35
17	D	505	CDL	C37-C38-C39-C40
15	C	505	PEE	C10-C11-C12-C13
15	Q	506	PEE	C34-C35-C36-C37
17	T	501	CDL	CB7-C71-C72-C73
15	P	505	PEE	O2-C2-C3-O3
17	T	501	CDL	C72-C73-C74-C75

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Mol	Chain	Res	Type	Atoms
15	C	505	PEE	C40-C41-C42-C43
12	P	501	HEM	C2A-CAA-CBA-CGA
17	Q	505	CDL	C34-C35-C36-C37
17	Q	505	CDL	C36-C37-C38-C39
17	G	501	CDL	OB5-CB3-CB4-CB6
15	D	506	PEE	O4-C10-O2-C2
17	G	501	CDL	OB9-CB7-OB8-CB6
15	C	505	PEE	C31-C30-O3-C3
15	C	505	PEE	C19-C20-C21-C22
15	P	505	PEE	C12-C13-C14-C15
17	D	505	CDL	CB2-OB2-PB2-OB3
15	P	505	PEE	C1-C2-O2-C10
15	D	506	PEE	O3P-C1-C2-O2
17	D	505	CDL	OA5-CA3-CA4-OA6
15	P	505	PEE	C23-C24-C25-C26
15	Q	506	PEE	C42-C43-C44-C45
17	D	505	CDL	OA7-CA5-OA6-CA4
19	R	502	GOL	O2-C2-C3-O3
12	P	501	HEM	C3D-CAD-CBD-CGD
15	D	506	PEE	O3P-C1-C2-C3
15	Q	506	PEE	O3P-C1-C2-C3
17	D	505	CDL	OA5-CA3-CA4-CA6
15	C	505	PEE	C22-C23-C24-C25
17	D	505	CDL	C36-C37-C38-C39
15	C	505	PEE	O5-C30-O3-C3
15	P	505	PEE	C33-C34-C35-C36
17	G	501	CDL	CA3-CA4-CA6-OA8
17	T	501	CDL	C51-C52-C53-C54
15	P	505	PEE	C21-C22-C23-C24
17	G	501	CDL	OB5-CB3-CB4-OB6
17	G	501	CDL	OA9-CA7-OA8-CA6
12	C	501	HEM	C3D-CAD-CBD-CGD
17	Q	505	CDL	C33-C34-C35-C36
15	C	505	PEE	O3P-C1-C2-C3
17	T	501	CDL	C75-C76-C77-C78
16	Q	501	HEC	C3D-CAD-CBD-CGD
15	Q	506	PEE	C1-C2-O2-C10
15	C	505	PEE	C12-C13-C14-C15
12	C	501	HEM	C4B-C3B-CAB-CBB
12	P	502	HEM	C4C-C3C-CAC-CBC
17	T	501	CDL	C71-CB7-OB8-CB6
15	P	505	PEE	C5-C4-O4P-P

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Mol	Chain	Res	Type	Atoms
17	D	505	CDL	C33-C34-C35-C36
13	P	503	4X9	F24-C1-O3-C4
17	G	501	CDL	C72-C73-C74-C75
15	C	505	PEE	O3P-C1-C2-O2
17	G	501	CDL	OA5-CA3-CA4-OA6
17	T	501	CDL	OB9-CB7-OB8-CB6
15	Q	506	PEE	C40-C41-C42-C43
15	C	505	PEE	C1-O3P-P-O4P
15	C	505	PEE	O4P-C4-C5-N
15	D	506	PEE	C4-O4P-P-O1P
15	P	505	PEE	C1-O3P-P-O1P
15	Q	506	PEE	C1-O3P-P-O1P
15	Q	506	PEE	O4P-C4-C5-N
17	Q	505	CDL	CA3-OA5-PA1-OA3
17	T	501	CDL	CB2-OB2-PB2-OB5
15	C	505	PEE	C1-C2-O2-C10
17	T	501	CDL	OA5-CA3-CA4-CA6
17	T	501	CDL	OA5-CA3-CA4-OA6
15	Q	506	PEE	C1-C2-C3-O3
16	D	501	HEC	C3A-C2A-CAA-CBA
15	Q	506	PEE	C41-C42-C43-C44
17	D	505	CDL	C34-C35-C36-C37
16	D	501	HEC	C2A-CAA-CBA-CGA
17	Q	505	CDL	C37-C38-C39-C40
12	P	502	HEM	C3D-CAD-CBD-CGD
15	C	505	PEE	C36-C37-C38-C39
17	T	501	CDL	C71-C72-C73-C74
12	C	502	HEM	CAA-CBA-CGA-O1A
12	P	502	HEM	CAA-CBA-CGA-O1A
15	P	505	PEE	C19-C20-C21-C22
15	C	505	PEE	C16-C17-C18-C19
12	C	502	HEM	CAA-CBA-CGA-O2A
12	P	501	HEM	CAA-CBA-CGA-O2A
12	P	501	HEM	CAD-CBD-CGD-O2D
12	P	502	HEM	CAA-CBA-CGA-O2A
17	D	505	CDL	CA3-CA4-CA6-OA8
15	Q	506	PEE	C13-C14-C15-C16
17	G	501	CDL	OA5-CA3-CA4-CA6
15	Q	506	PEE	O2-C2-C3-O3
13	P	503	4X9	F25-C1-O3-C4
16	D	501	HEC	CAD-CBD-CGD-O1D
16	D	501	HEC	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
12	C	501	HEM	CAD-CBD-CGD-O2D
12	P	501	HEM	CAA-CBA-CGA-O1A
12	P	501	HEM	CAD-CBD-CGD-O1D
16	Q	501	HEC	CAD-CBD-CGD-O2D
17	T	501	CDL	C53-C54-C55-C56
15	Q	506	PEE	C38-C39-C40-C41
17	G	501	CDL	C1-CA2-OA2-PA1
16	Q	501	HEC	CAD-CBD-CGD-O1D
15	D	506	PEE	C32-C33-C34-C35
12	P	502	HEM	CAD-CBD-CGD-O1D
17	G	501	CDL	C74-C75-C76-C77
12	C	501	HEM	CAD-CBD-CGD-O1D
13	P	503	4X9	F23-C1-O3-C4
17	D	505	CDL	C35-C36-C37-C38
12	P	502	HEM	CAD-CBD-CGD-O2D
13	C	503	4X9	C5-C4-O3-C1
13	C	503	4X9	C9-C4-O3-C1
15	C	505	PEE	C13-C14-C15-C16
17	D	505	CDL	C12-C11-CA5-OA6
17	T	501	CDL	C74-C75-C76-C77
15	Q	506	PEE	C18-C19-C20-C21
12	C	501	HEM	C2C-C3C-CAC-CBC
16	D	501	HEC	CAA-CBA-CGA-O2A
16	D	501	HEC	CAA-CBA-CGA-O1A

There are no ring outliers.

15 monomers are involved in 55 short contacts:

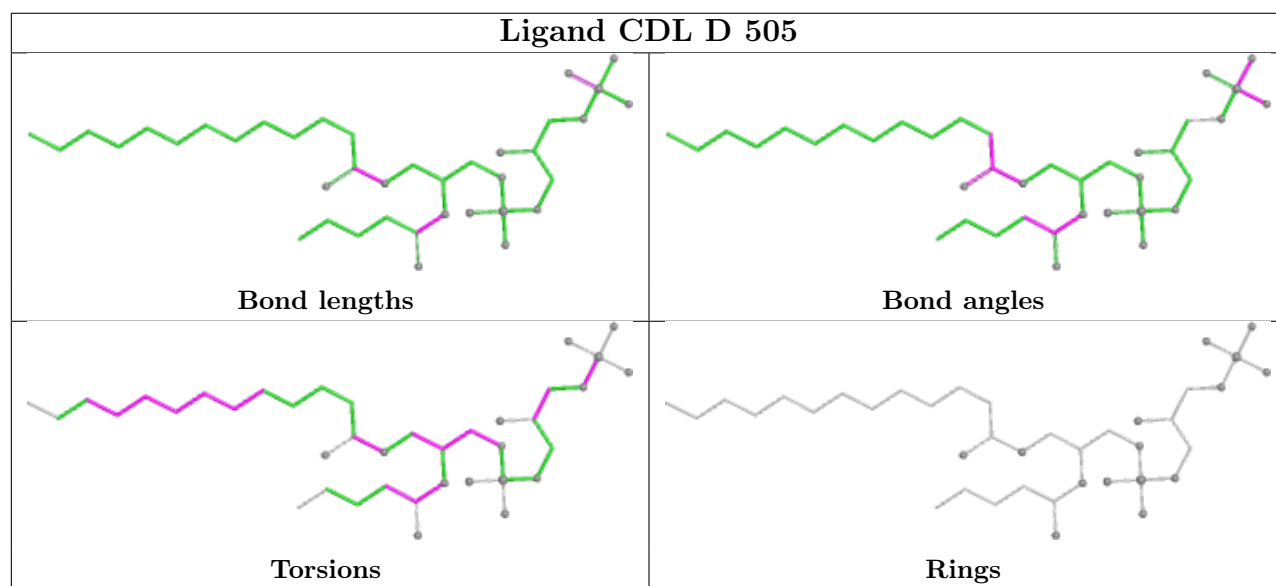
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	Q	506	PEE	3	0
16	Q	501	HEC	6	0
15	C	505	PEE	1	0
16	D	501	HEC	10	0
17	Q	505	CDL	1	0
15	P	505	PEE	1	0
12	C	501	HEM	4	0
12	C	502	HEM	6	0
12	P	502	HEM	3	0
12	P	501	HEM	7	0
18	R	501	FES	3	0
13	C	503	4X9	5	0
15	D	506	PEE	1	0

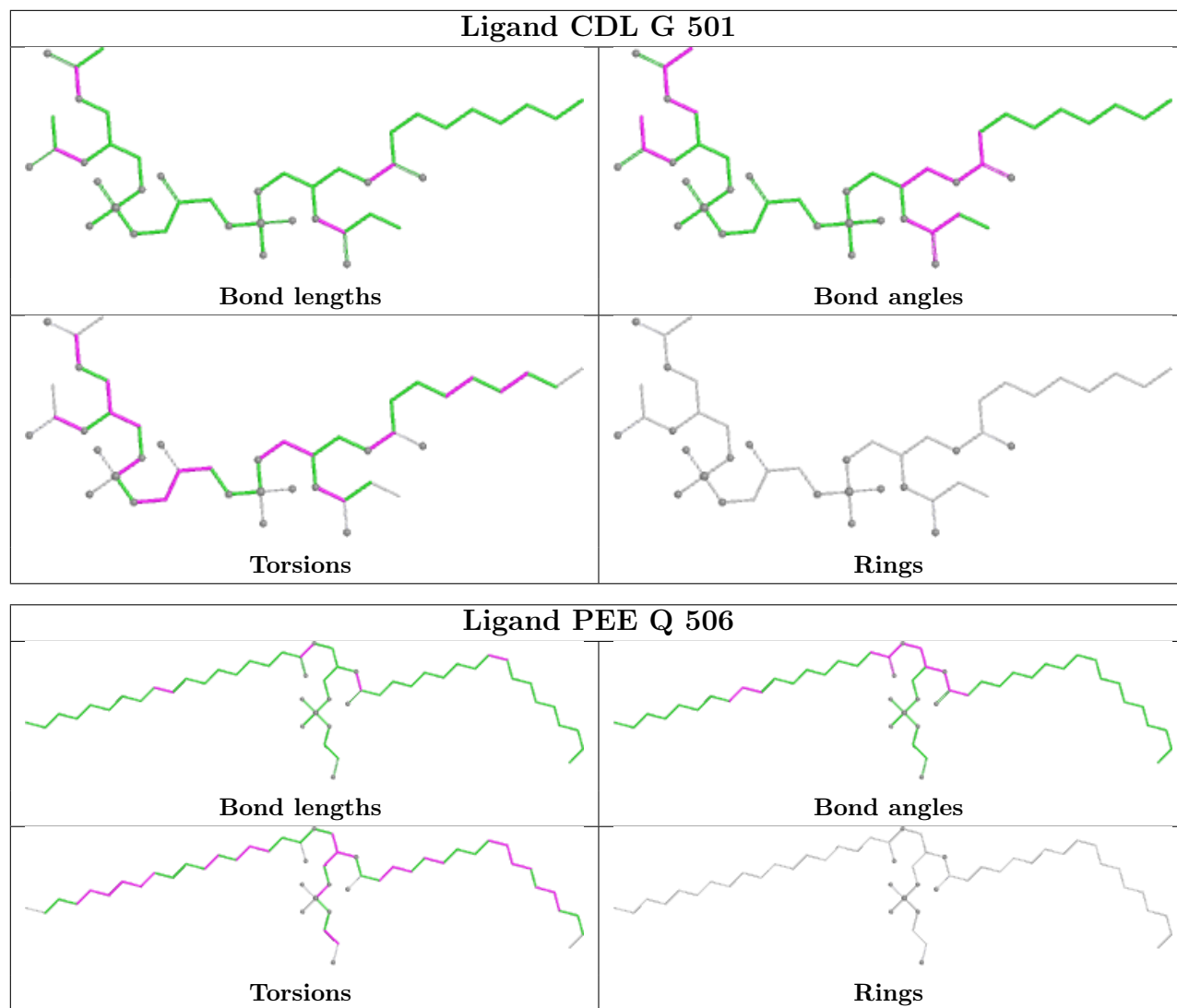
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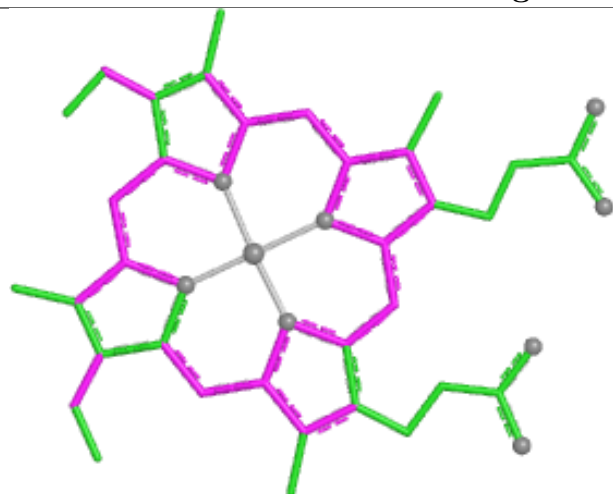
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	T	501	CDL	1	0
13	P	503	4X9	4	0

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

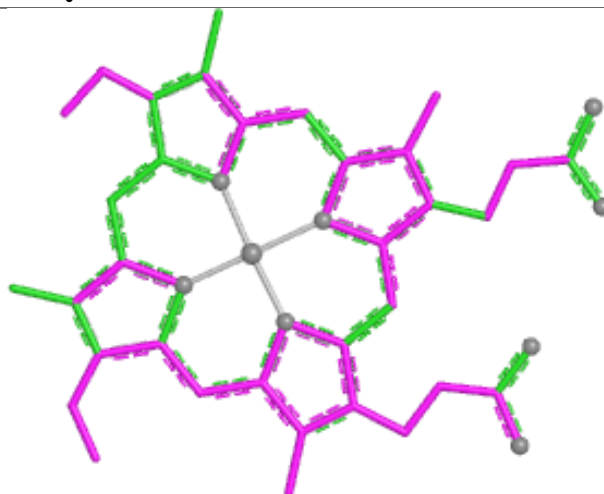




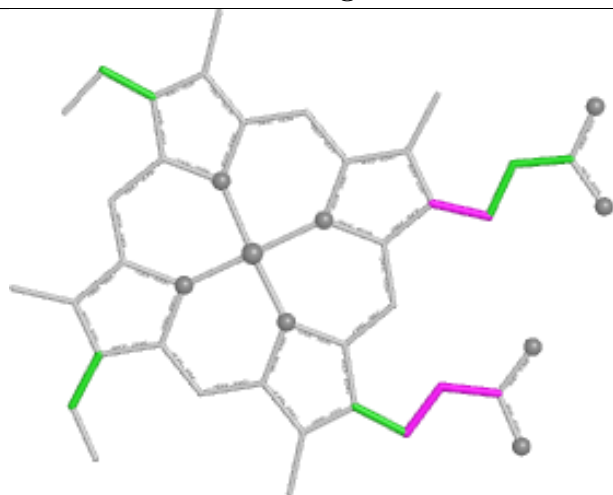
Ligand HEC Q 501



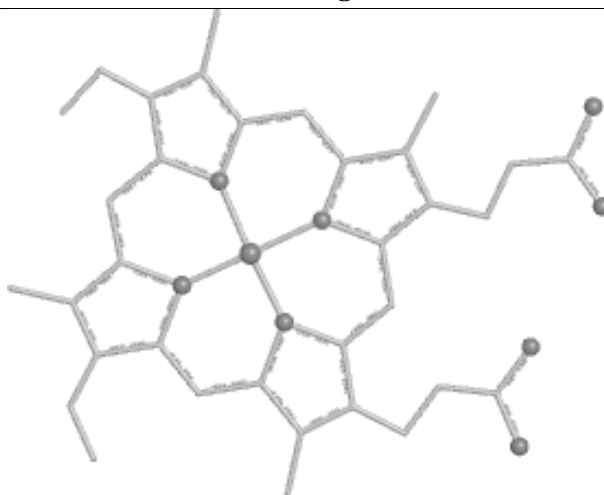
Bond lengths



Bond angles



Torsions



Rings

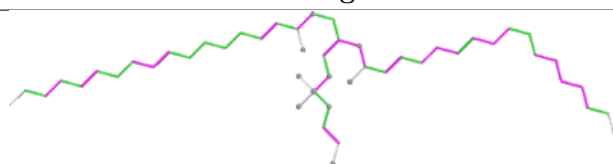
Ligand PEE C 505



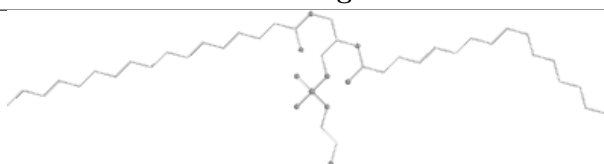
Bond lengths



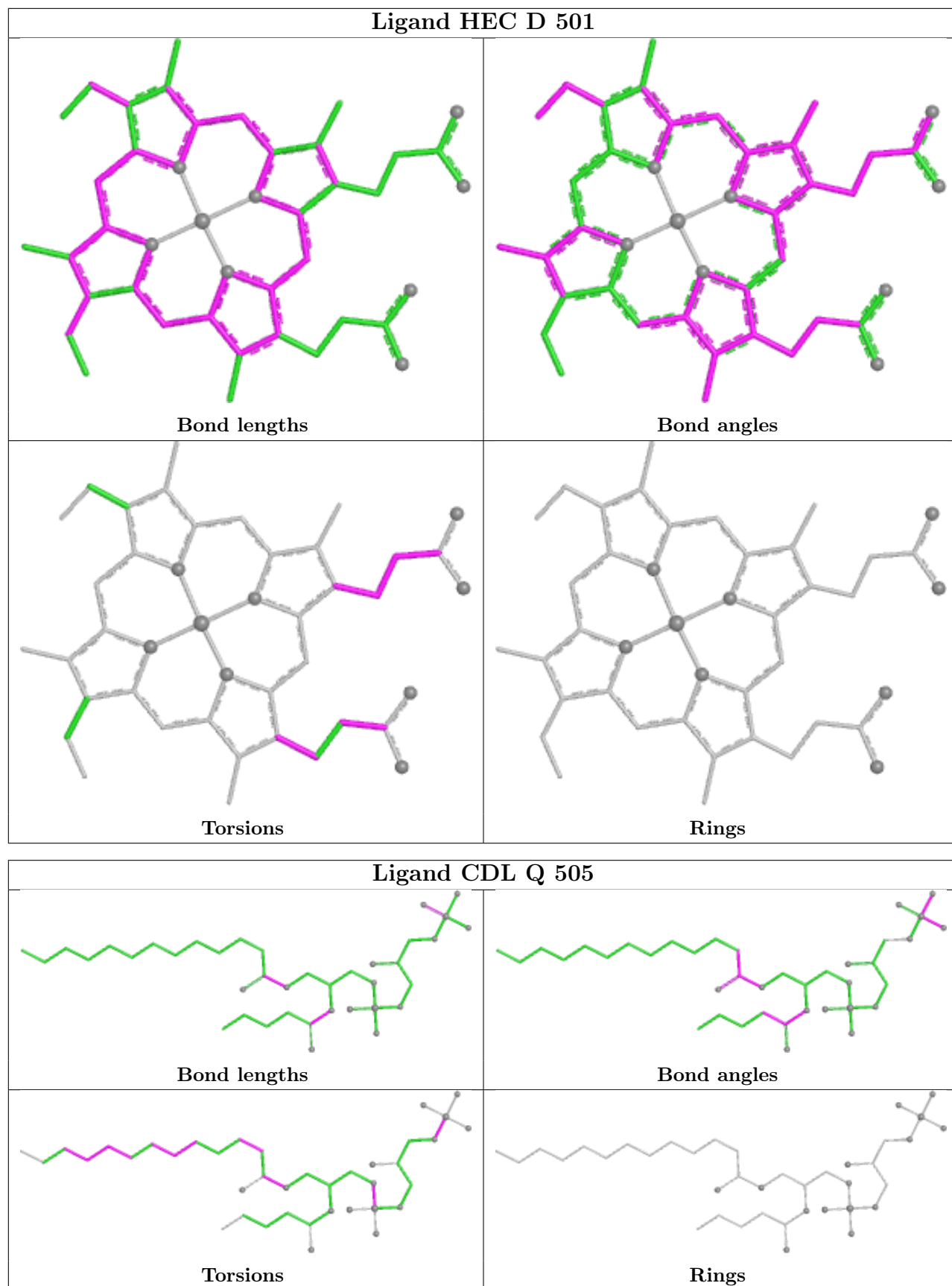
Bond angles



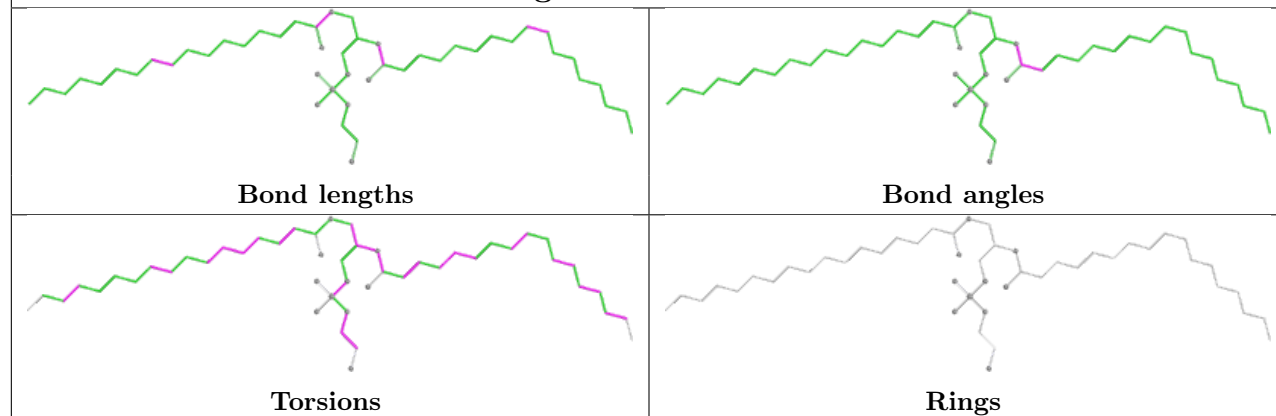
Torsions



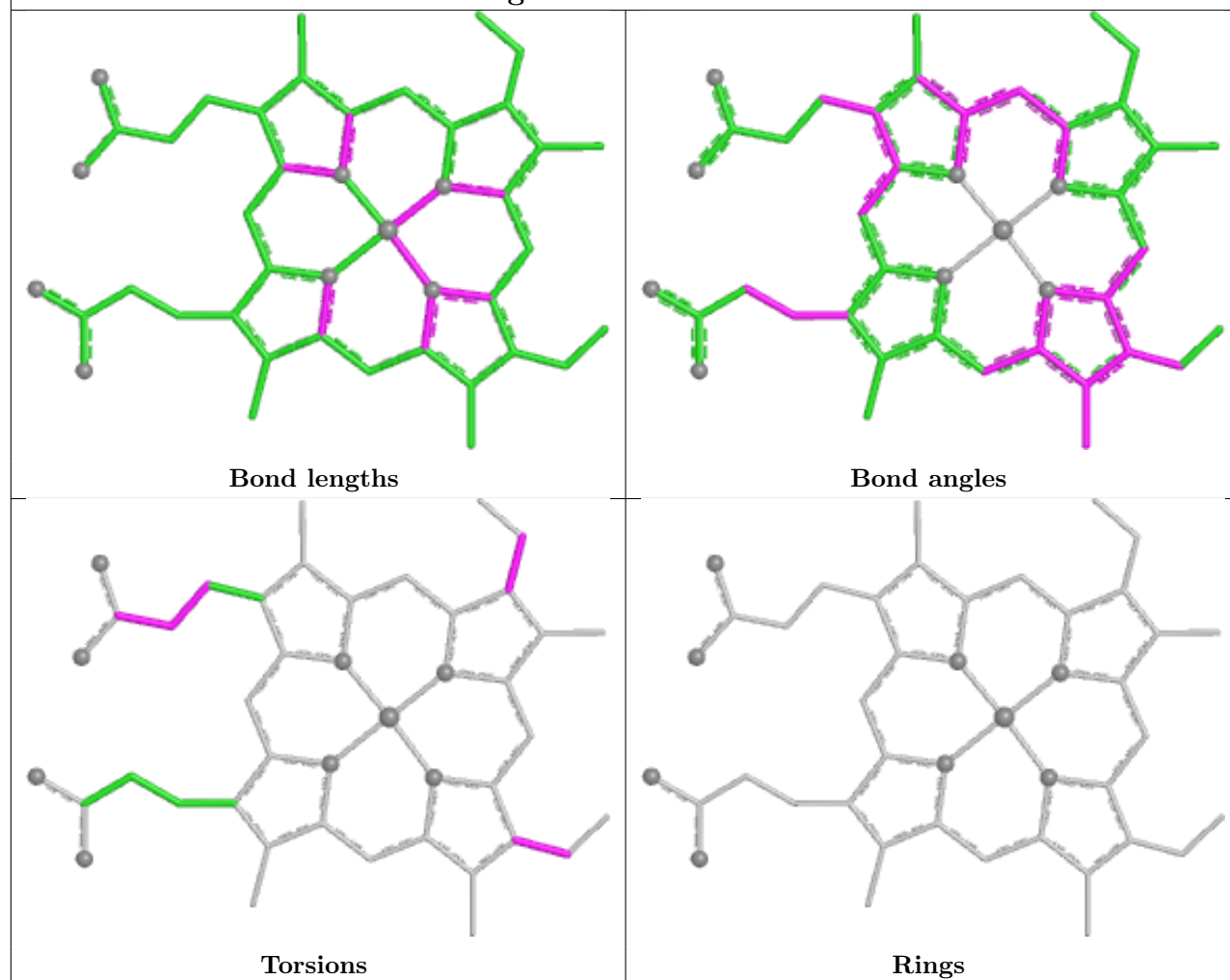
Rings

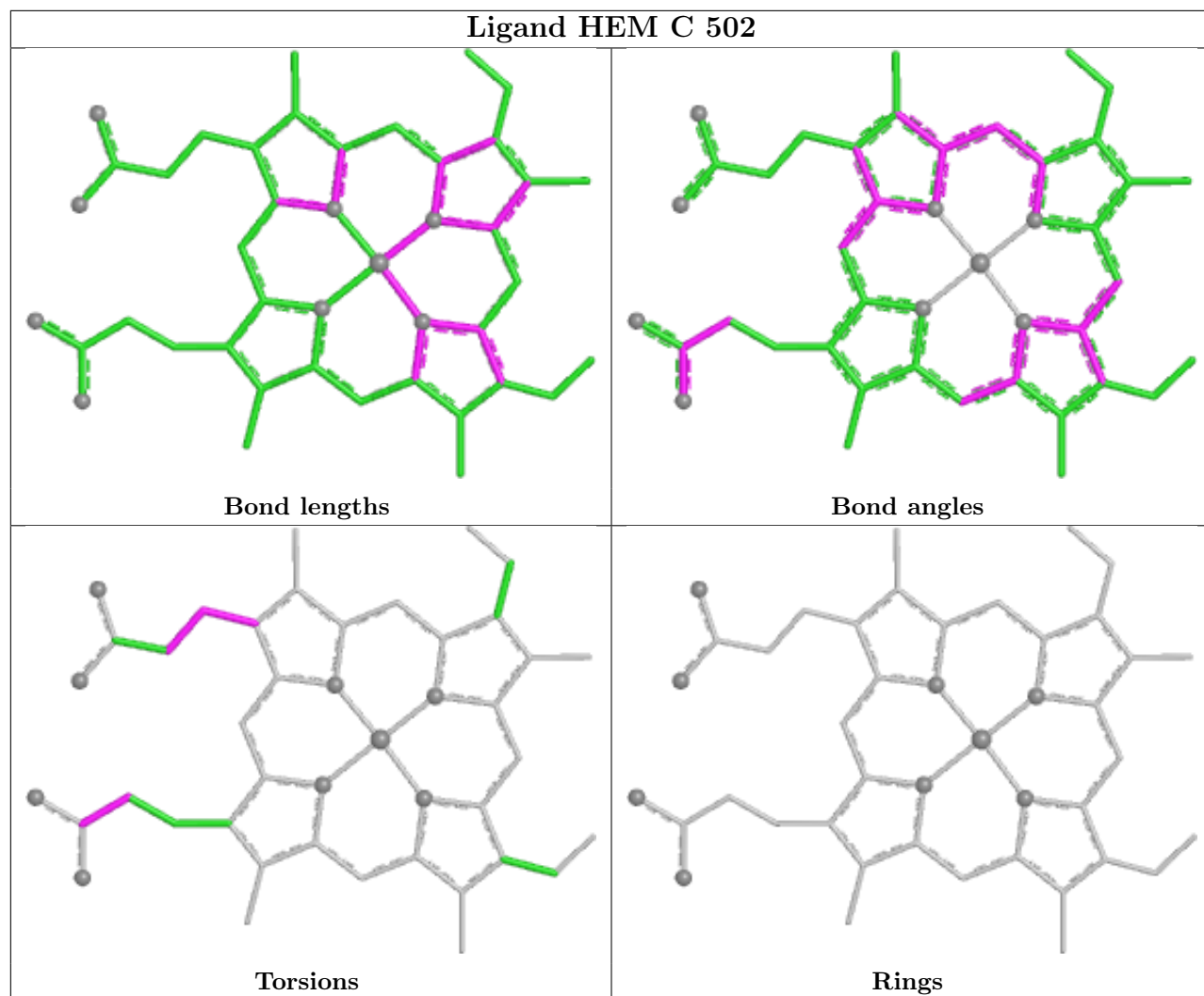


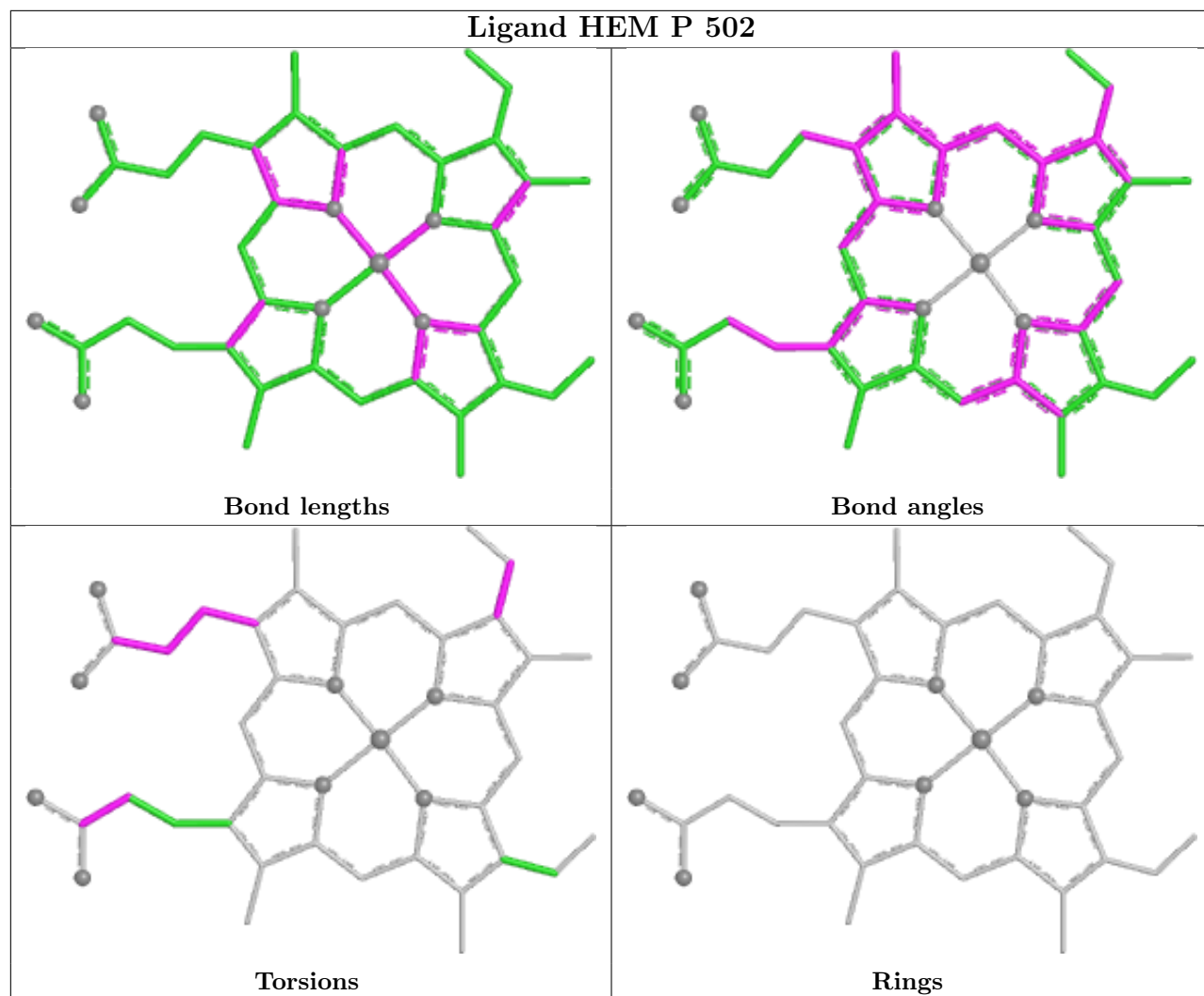
Ligand PEE P 505

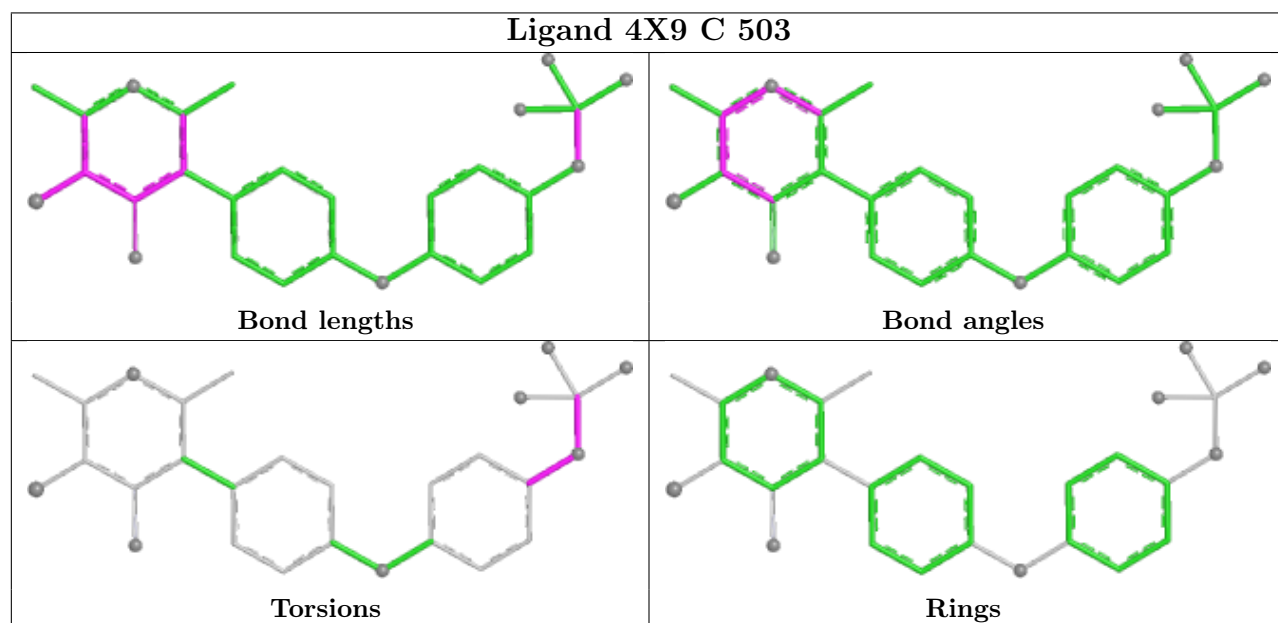
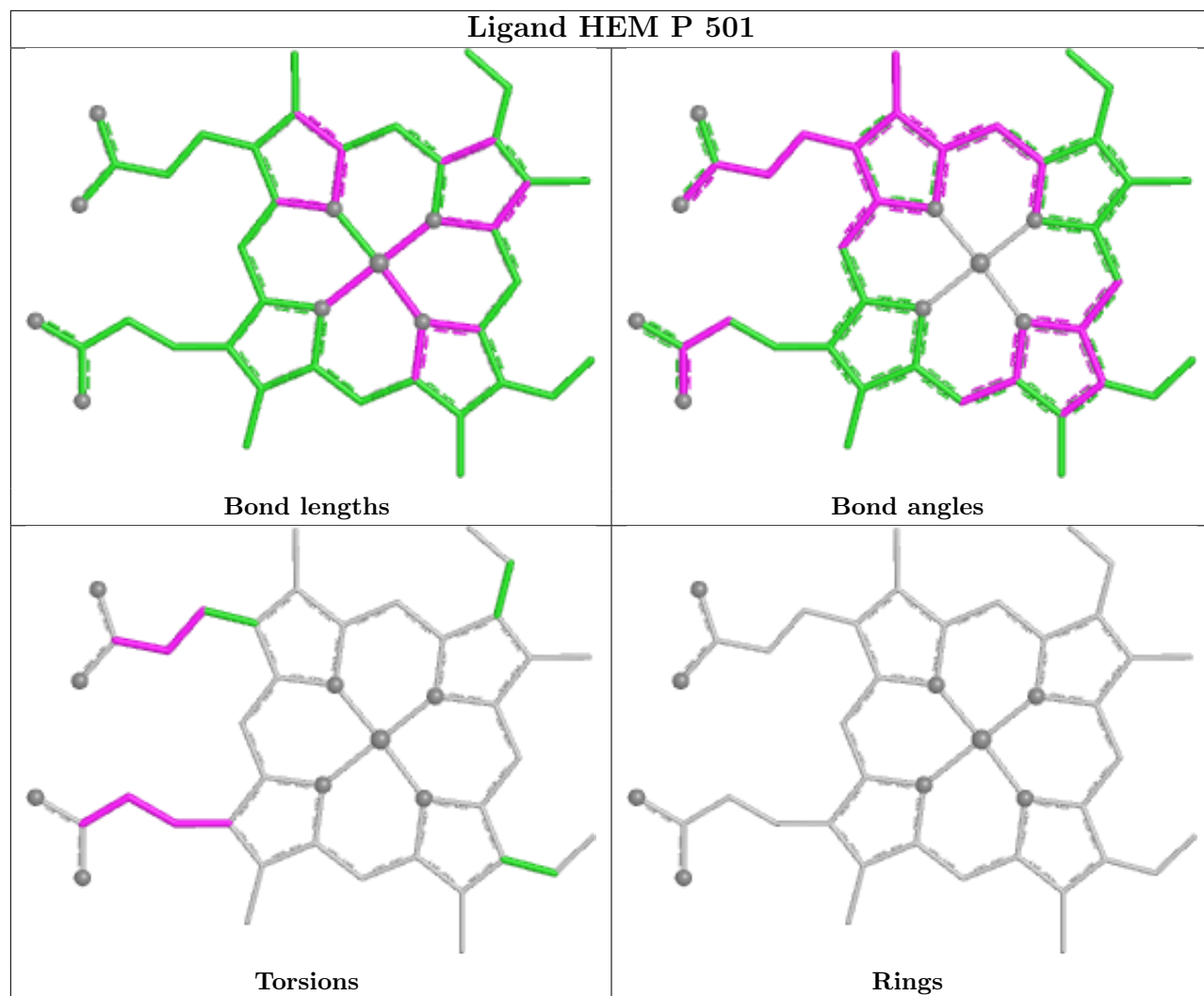


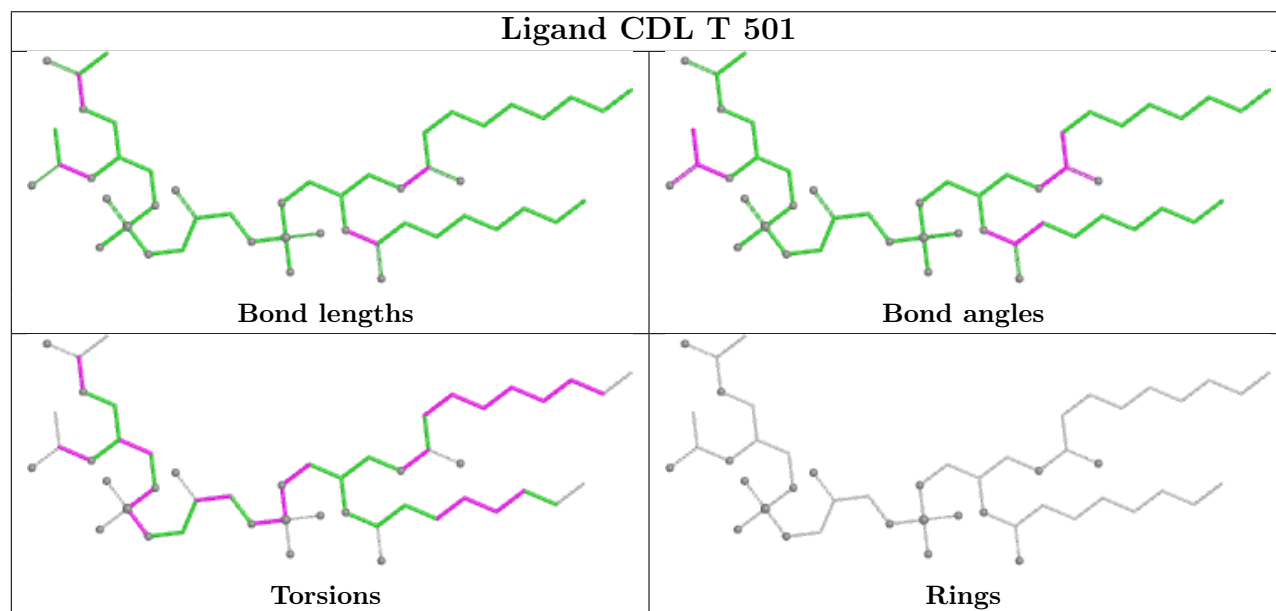
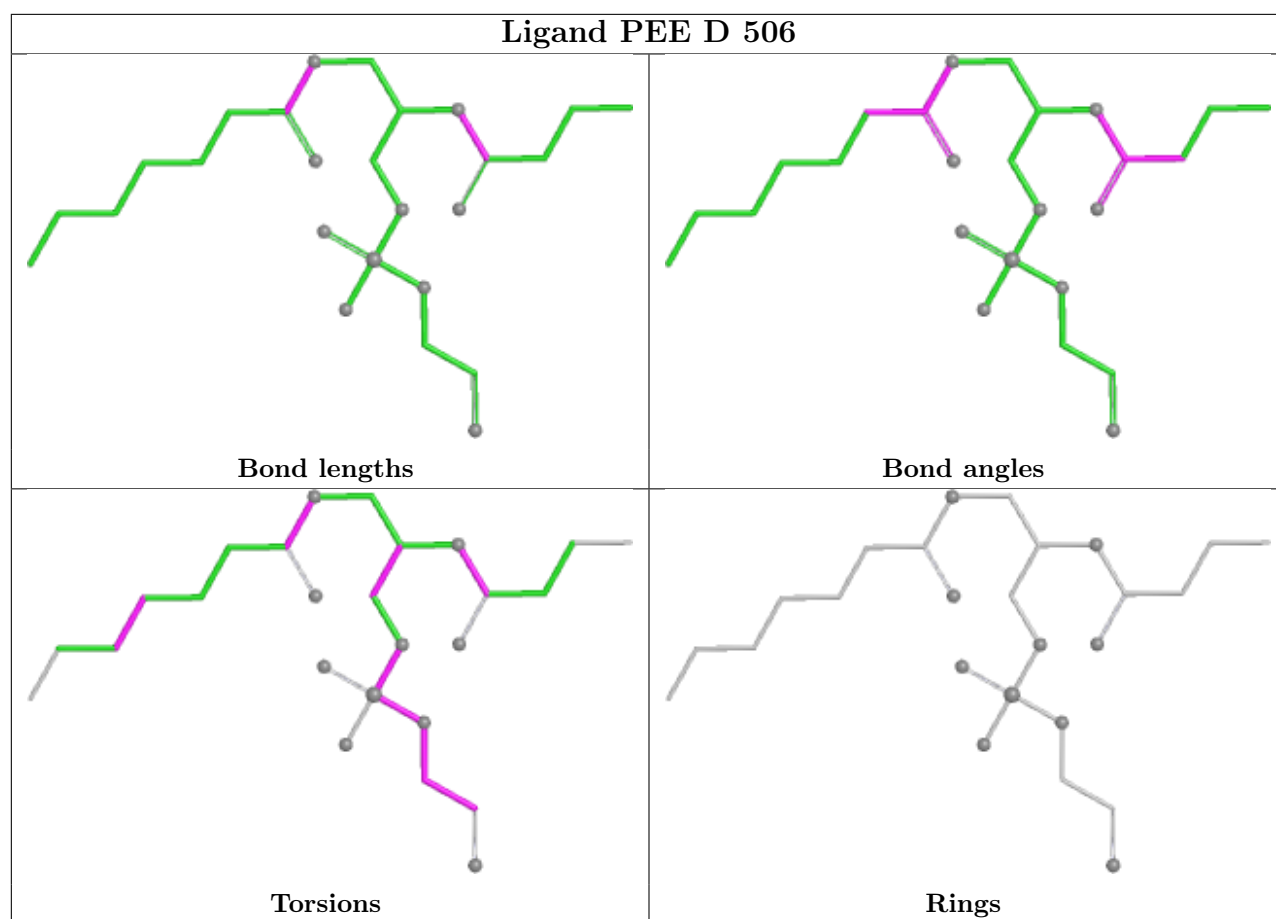
Ligand HEM C 501

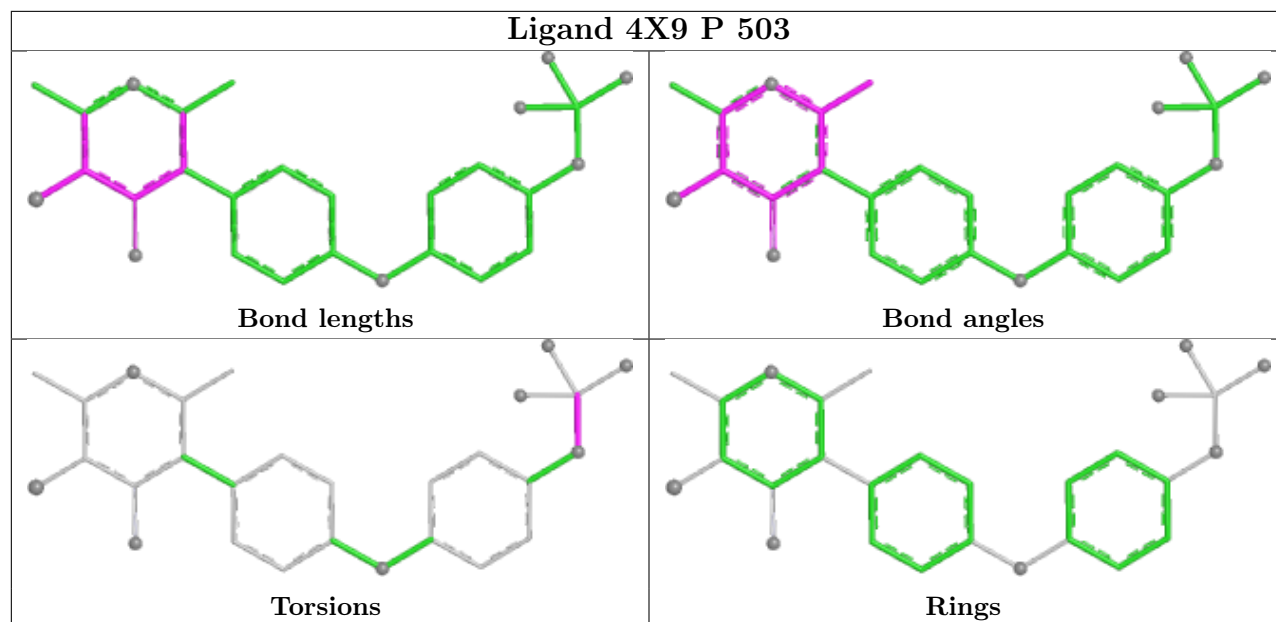












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	444/480 (92%)	0.12	22 (4%) 34 19	92, 150, 191, 255	0
1	N	444/480 (92%)	-0.05	24 (5%) 31 17	87, 132, 176, 243	0
2	B	422/453 (93%)	0.03	15 (3%) 46 25	108, 157, 200, 247	0
3	C	374/379 (98%)	-0.21	7 (1%) 66 38	77, 103, 137, 225	0
3	P	370/379 (97%)	-0.23	5 (1%) 73 45	79, 112, 148, 183	0
4	D	240/265 (90%)	-0.26	4 (1%) 69 40	92, 121, 153, 178	0
4	Q	241/265 (90%)	-0.26	3 (1%) 76 49	86, 131, 168, 211	0
5	E	73/274 (26%)	-0.02	4 (5%) 30 17	93, 130, 158, 170	0
5	I	21/274 (7%)	1.68	10 (47%) 0 1	146, 192, 220, 228	0
5	R	196/274 (71%)	-0.19	6 (3%) 51 28	91, 150, 193, 230	0
6	F	98/111 (88%)	-0.17	4 (4%) 41 22	91, 124, 157, 171	0
6	S	99/111 (89%)	0.06	6 (6%) 27 15	85, 122, 168, 182	0
7	G	80/82 (97%)	-0.04	4 (5%) 34 19	88, 119, 189, 293	0
7	T	74/82 (90%)	-0.24	4 (5%) 31 17	83, 124, 181, 200	0
8	H	65/91 (71%)	0.16	0 100 100	103, 136, 171, 223	0
8	U	66/91 (72%)	-0.16	1 (1%) 72 44	132, 163, 213, 245	0
9	J	58/64 (90%)	-0.58	0 100 100	103, 137, 165, 175	0
9	W	59/64 (92%)	-0.34	0 100 100	102, 121, 153, 162	0
10	O	419/453 (92%)	-0.02	18 (4%) 40 21	97, 146, 193, 250	0
11	V	17/274 (6%)	2.44	10 (58%) 0 0	176, 209, 228, 268	0
All	All	3860/4946 (78%)	-0.08	147 (3%) 44 24	77, 133, 189, 293	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	V	78	TYR	8.5
10	O	117	ASP	7.7
6	F	106	GLU	7.4
10	O	313	ASN	5.9
2	B	313	ASN	5.7
6	F	109	LYS	5.6
2	B	276	GLN	5.6
10	O	312	PHE	5.5
6	S	15	GLY	5.4
1	N	98	TYR	5.1
6	S	16	ILE	5.1
5	I	73	PRO	5.0
7	T	74	PRO	4.9
6	S	19	TRP	4.9
6	S	22	ASN	4.8
1	A	305	GLN	4.7
1	A	175	ARG	4.6
4	D	241	LYS	4.6
11	V	63	PRO	4.5
10	O	371	SER	4.4
5	I	64	LEU	4.4
5	I	65	VAL	4.3
5	I	72	VAL	4.3
1	N	146	ARG	4.3
1	N	394	GLU	4.2
5	E	9	ASP	4.2
1	N	242	CYS	4.2
1	N	243	HIS	4.2
10	O	118	ILE	4.1
1	A	303	LEU	4.0
11	V	76	VAL	4.0
1	A	327	ASP	4.0
1	N	87	ASN	3.9
6	S	21	TYR	3.9
2	B	312	PHE	3.8
6	S	18	LYS	3.8
1	A	249	PRO	3.8
1	A	325	VAL	3.8
1	A	326	CYS	3.8
10	O	368	TYR	3.7
3	P	262	LEU	3.6
1	N	89	TYR	3.5
10	O	314	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	N	232	SER	3.5
1	N	85	HIS	3.5
10	O	215	VAL	3.4
1	A	117	VAL	3.3
10	O	281	ALA	3.3
11	V	64	VAL	3.3
1	A	282	CYS	3.3
1	A	304	CYS	3.3
3	C	328	LEU	3.2
2	B	94	GLY	3.2
11	V	62	ARG	3.2
2	B	311	ALA	3.2
1	A	280	TYR	3.1
1	N	241	ILE	3.0
4	D	167	GLU	3.0
3	C	171	ASP	3.0
1	N	395	TRP	3.0
1	A	306	SER	3.0
7	G	69	SER	3.0
1	N	424	GLY	2.9
4	D	177	ALA	2.9
10	O	327	ILE	2.9
11	V	68	VAL	2.9
7	T	15	THR	2.9
3	P	11	MET	2.8
10	O	120	MET	2.8
4	Q	191	ARG	2.8
1	N	100	LYS	2.8
5	I	74	ALA	2.8
1	N	425	PHE	2.7
10	O	265	GLY	2.7
10	O	119	LEU	2.7
1	A	226	ASP	2.7
2	B	280	GLY	2.7
1	A	250	LEU	2.7
6	F	60	PHE	2.7
3	P	306	LEU	2.7
7	T	14	ILE	2.7
3	C	172	LYS	2.6
1	A	247	GLY	2.6
1	A	168	GLU	2.6
2	B	277	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
5	R	13	TYR	2.6
1	N	230	THR	2.5
10	O	122	PHE	2.5
1	N	398	ARG	2.5
5	R	142	LEU	2.5
1	N	377	GLU	2.5
5	R	12	ASP	2.5
10	O	116	VAL	2.5
11	V	73	PRO	2.5
3	C	331	ASP	2.5
2	B	417	PHE	2.4
5	E	54	VAL	2.4
2	B	347	ILE	2.4
5	I	71	ASN	2.4
1	N	88	ALA	2.4
2	B	314	ALA	2.4
11	V	70	LEU	2.4
3	C	8	HIS	2.4
7	G	76	ALA	2.4
1	A	91	THR	2.4
2	B	344	VAL	2.4
3	P	102	LEU	2.4
5	I	50	LEU	2.4
5	I	70	LEU	2.4
2	B	371	SER	2.3
2	B	23	ASP	2.3
1	N	393	ALA	2.3
6	F	105	GLU	2.3
11	V	72	VAL	2.3
4	D	136	GLU	2.3
1	A	167	VAL	2.3
11	V	65	VAL	2.3
3	C	135	TRP	2.3
1	N	152	TYR	2.3
1	N	264	HIS	2.2
5	I	75	SER	2.2
8	U	44	VAL	2.2
5	E	69	LEU	2.2
5	R	75	GLU	2.2
7	G	46	LEU	2.2
3	P	167	GLY	2.2
5	E	11	SER	2.2

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Mol	Chain	Res	Type	RSRZ
7	T	16	TYR	2.1
3	C	178	PHE	2.1
1	N	373	THR	2.1
7	G	20	PRO	2.1
10	O	159	VAL	2.1
5	I	77	ARG	2.1
1	A	90	SER	2.1
4	Q	183	ALA	2.1
1	A	94	HIS	2.1
1	A	97	TYR	2.1
4	Q	187	CYS	2.1
10	O	286	LYS	2.1
2	B	236	LYS	2.0
1	A	251	ALA	2.0
10	O	401	GLN	2.0
2	B	93	GLY	2.0
1	N	277	ILE	2.0
1	N	225	GLU	2.0
5	R	89	PHE	2.0
5	R	91	TRP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	PO4	Q	1001	5/5	0.41	0.10	194,205,216,232	0
14	PO4	D	502	5/5	0.52	0.08	176,192,199,203	0
14	PO4	F	501	5/5	0.58	0.10	242,243,245,246	0

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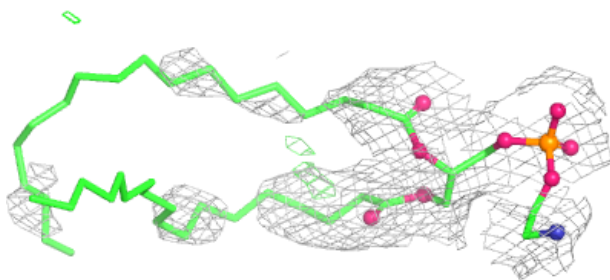
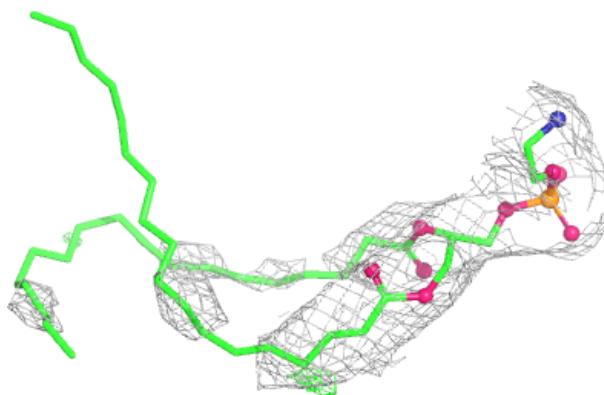
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
14	PO4	D	503	5/5	0.58	0.08	168,169,177,181	0
14	PO4	S	501	5/5	0.64	0.08	225,226,243,252	0
14	PO4	D	504	5/5	0.65	0.08	179,190,194,195	0
14	PO4	N	501	5/5	0.73	0.11	112,126,127,137	0
14	PO4	C	504	5/5	0.78	0.08	121,121,134,149	0
14	PO4	Q	1002	5/5	0.83	0.06	210,211,220,230	0
14	PO4	E	501	5/5	0.88	0.07	124,134,144,145	0
19	GOL	R	502	6/6	0.88	0.11	169,181,193,193	0
14	PO4	N	1001	5/5	0.90	0.06	120,127,135,137	0
15	PEE	Q	506	51/51	0.93	0.21	100,134,171,187	0
13	4X9	P	503	28/28	0.93	0.16	109,147,226,261	0
13	4X9	C	503	28/28	0.94	0.12	116,143,206,215	0
17	CDL	D	505	39/100	0.95	0.11	85,124,146,148	0
15	PEE	D	506	26/51	0.96	0.12	107,127,169,176	0
17	CDL	G	501	44/100	0.96	0.11	95,115,153,168	0
15	PEE	C	505	49/51	0.96	0.15	94,116,135,137	0
17	CDL	T	501	49/100	0.97	0.09	93,129,160,167	0
17	CDL	Q	505	39/100	0.97	0.10	100,126,146,148	0
12	HEM	C	502	43/43	0.98	0.07	71,85,99,106	0
15	PEE	P	505	49/51	0.98	0.12	100,122,154,156	0
12	HEM	P	502	43/43	0.98	0.07	74,89,104,106	0
16	HEC	D	501	43/43	0.98	0.09	80,111,127,138	0
18	FES	R	501	4/4	0.98	0.03	125,158,164,170	0
16	HEC	Q	501	43/43	0.98	0.07	106,117,136,143	0
12	HEM	C	501	43/43	0.99	0.07	89,99,107,115	0
12	HEM	P	501	43/43	0.99	0.07	86,101,116,124	0

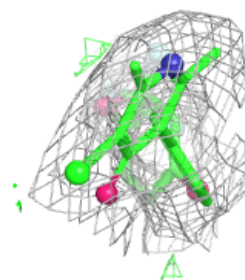
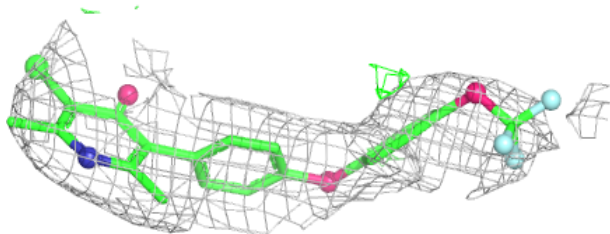
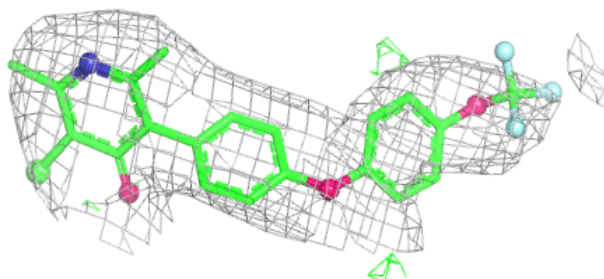
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PEE Q 506:

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

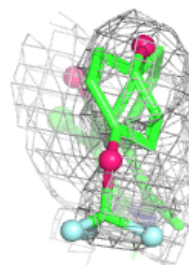
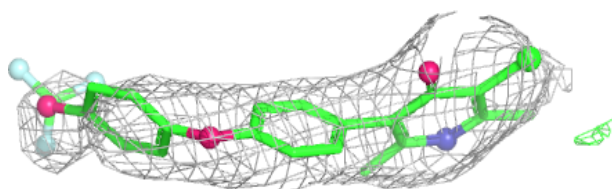
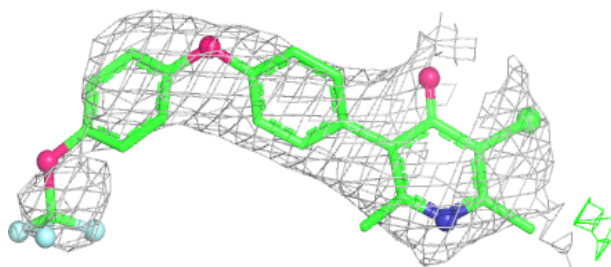
**Electron density around 4X9 P 503:**

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

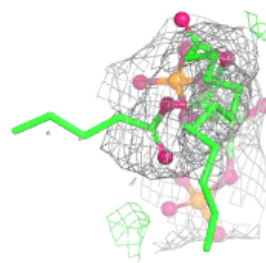
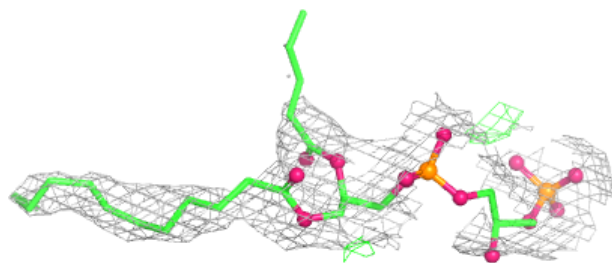
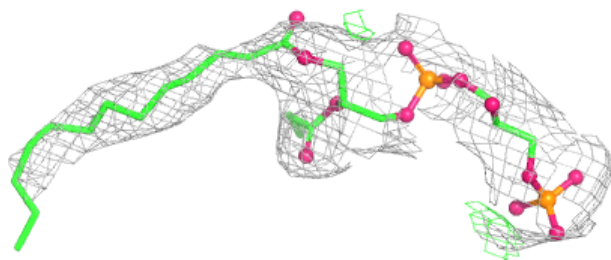


Electron density around 4X9 C 503:

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

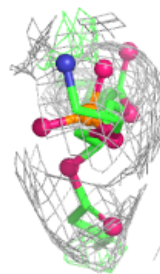
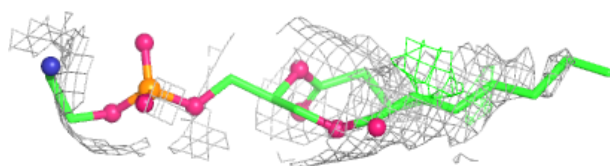
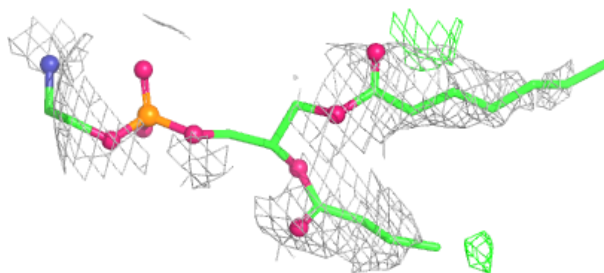
**Electron density around CDL D 505:**

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

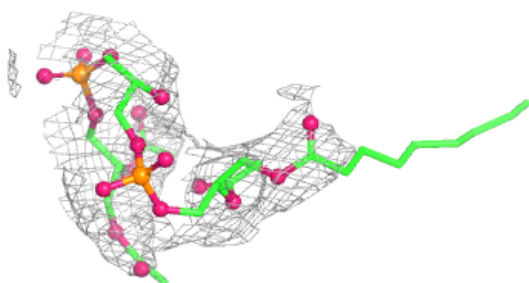
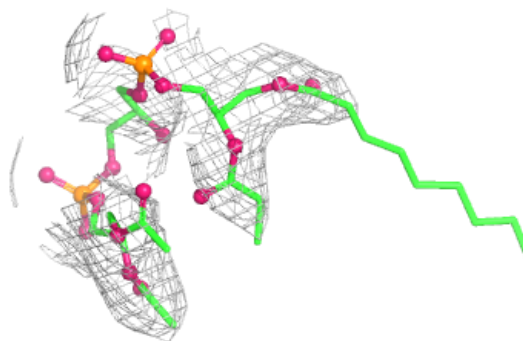


Electron density around PEE D 506:

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

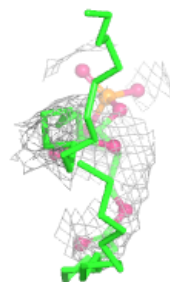
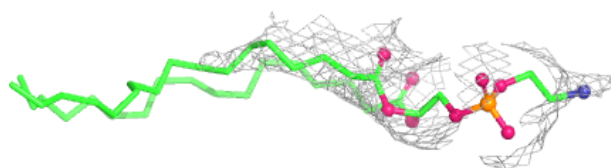
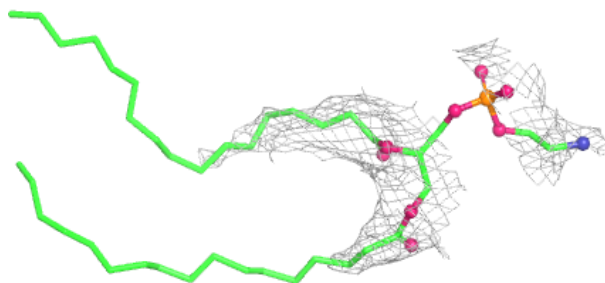
**Electron density around CDL G 501:**

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

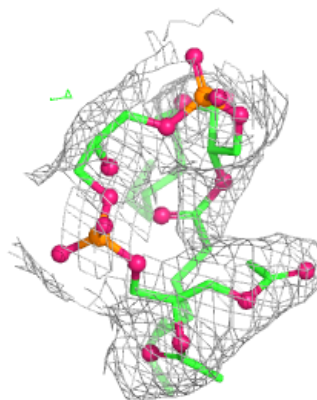
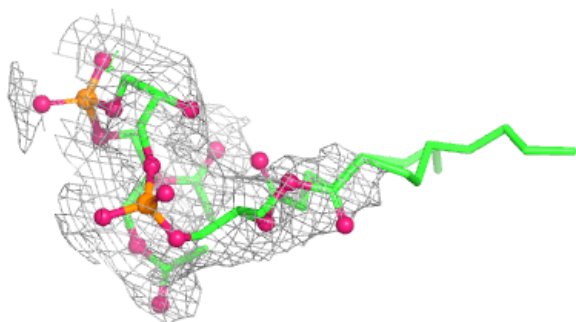
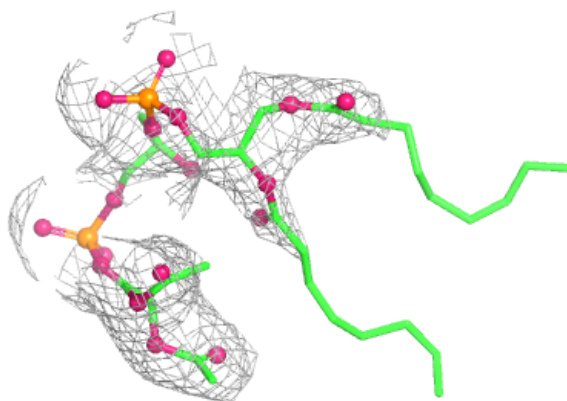


Electron density around PEE C 505:

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

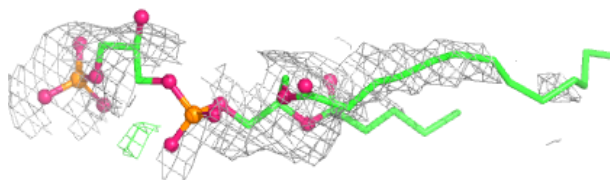
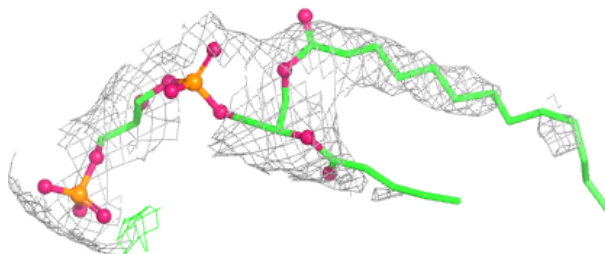
**Electron density around CDL T 501:**

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



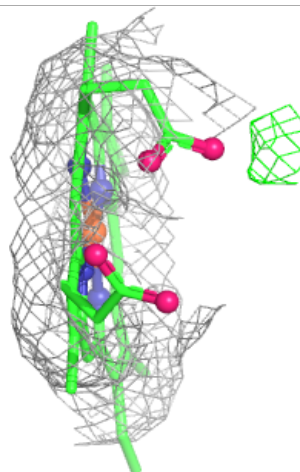
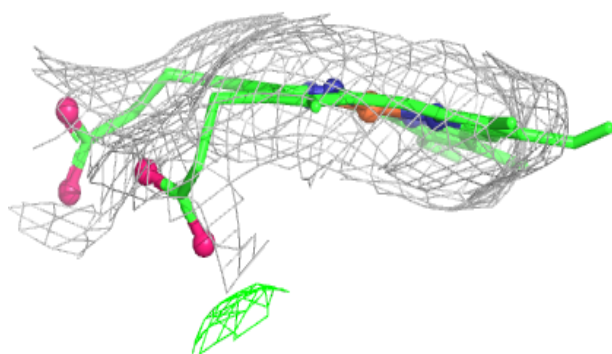
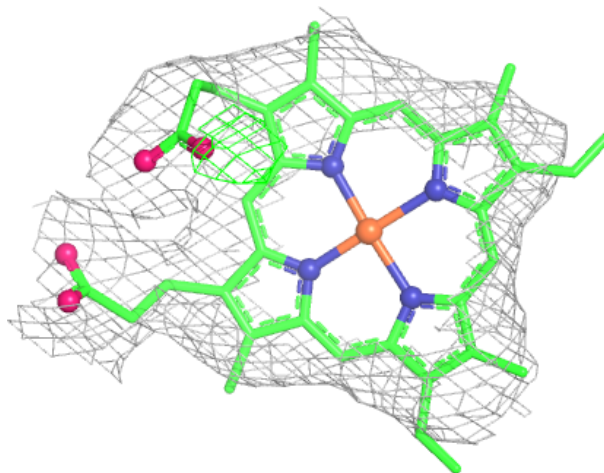
Electron density around CDL Q 505:

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



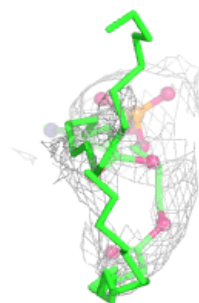
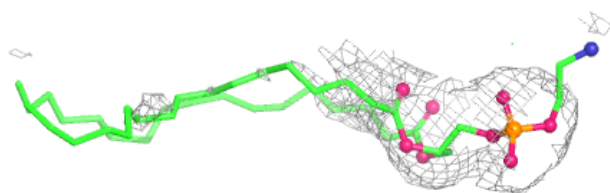
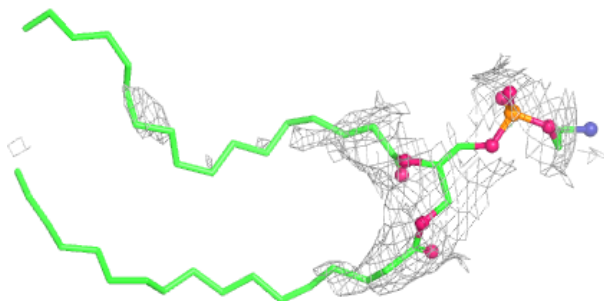
Electron density around HEM C 502:

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



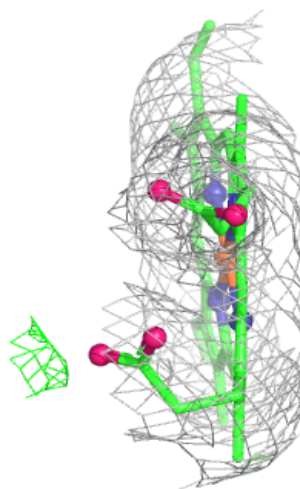
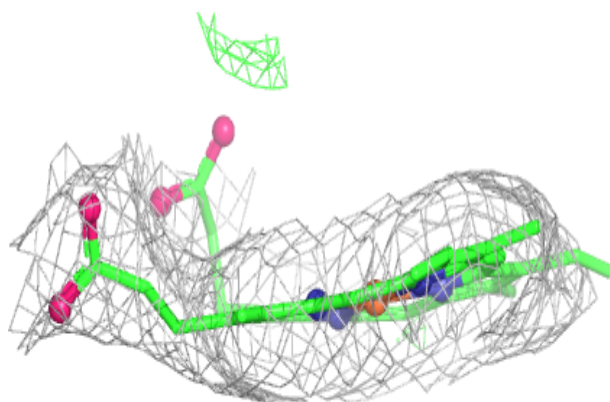
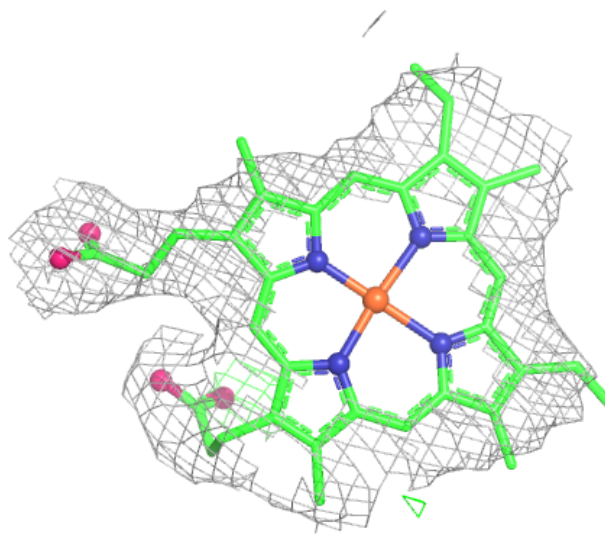
Electron density around PEE P 505:

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



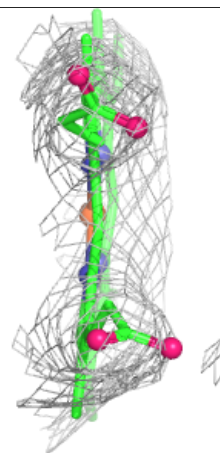
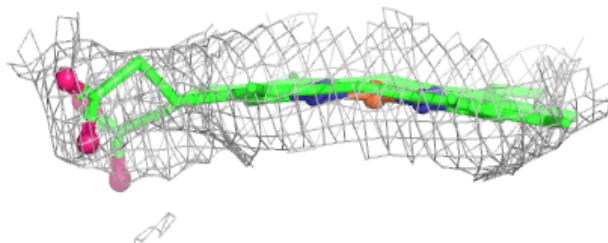
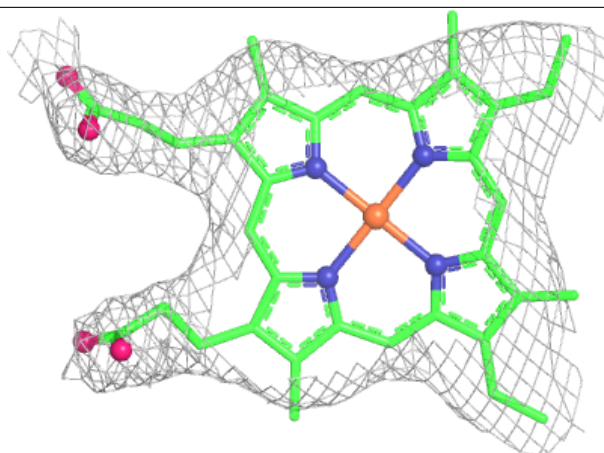
Electron density around HEM P 502:

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



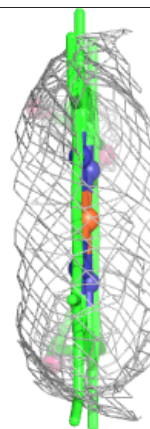
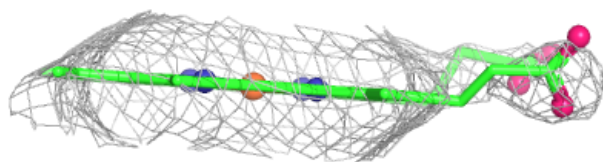
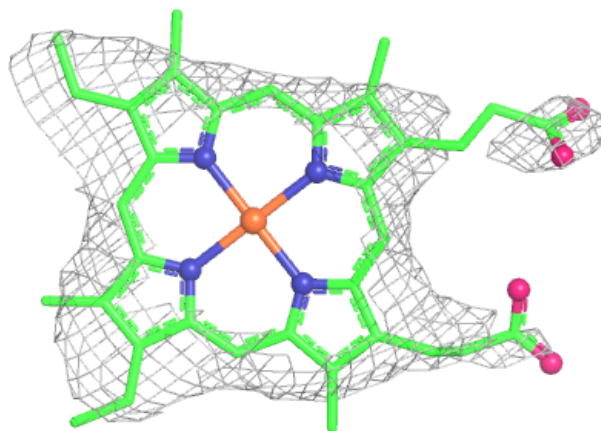
Electron density around HEC D 501:

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



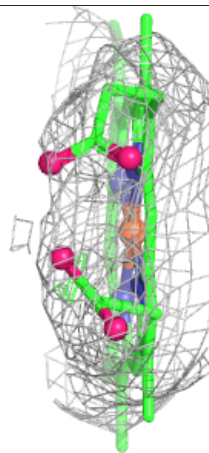
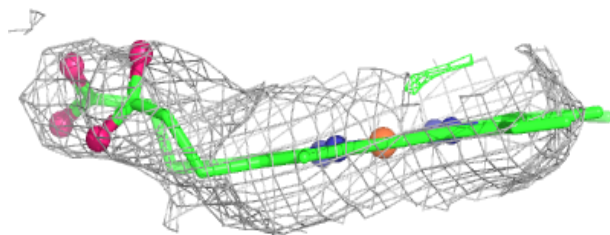
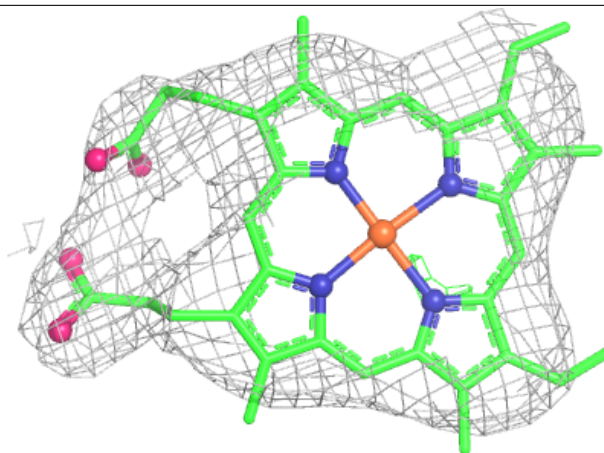
Electron density around HEC Q 501:

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



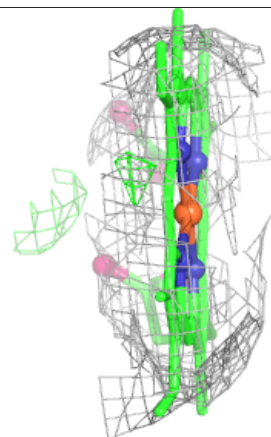
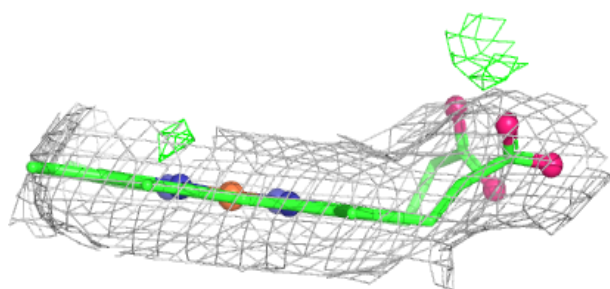
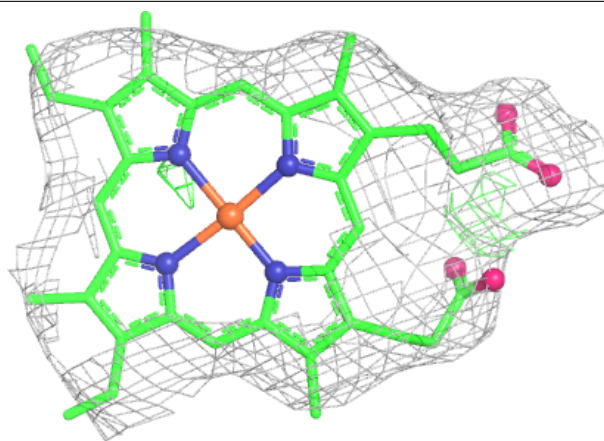
Electron density around HEM C 501:

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



Electron density around 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.