



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 16, 2025 – 06:45 am GMT

PDB ID : 9GCX
Title : Crystal structure of bovine Cytochrome bc1 in complex with inhibitor F8
Authors : Pinthong, N.; Hong, W.; O'Neill, P.W.; Antonyuk, S.V.
Deposited on : 2024-08-03
Resolution : 3.52 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

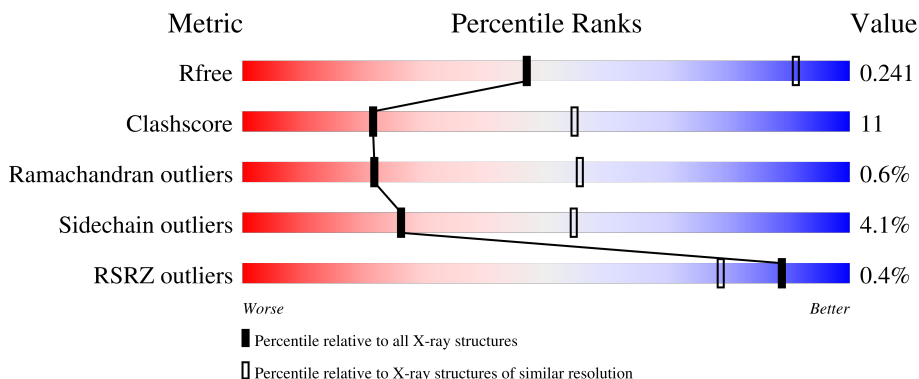
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.52 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}	164625	1089 (3.58-3.46)
Clashscore	180529	1165 (3.58-3.46)
Ramachandran outliers	177936	1150 (3.58-3.46)
Sidechain outliers	177891	1151 (3.58-3.46)
RSRZ outliers	164620	1088 (3.58-3.46)

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	 70% 20% • 8%
2	B	453	 67% 23% • 9%
3	C	379	 74% 24% •
4	D	325	 55% 17% • 26%
5	E	274	 % 48% 22% • 28%

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Mol	Chain	Length	Quality of chain
5	I	274	 5% . . . 90%
6	F	111	 75% 12% . 12%
7	G	82	 52% 28% 10% 10%
8	H	109	 44% 14% . 40%
9	J	64	 62% 23% . 12%
10	K	56	 4% 57% 12% 30%

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
12	CDL	A	502	-	-	X	-
14	A1IKG	C	505	X	-	-	-

2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 16707 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	440	3402	2129	600	653	20	0	0	0

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	414	3112	1952	552	601	7	0	1	0

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	378	3008	2019	470	500	19	0	2	0

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	240	1901	1213	326	347	15	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	E	196	1505	946	262	290	7	0	0	0
5	I	27	191	117	38	35	1	0	0	0

- 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	155	156	2			

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	74	Total	C	N	O	S	0	0	0
			620	405	116	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			

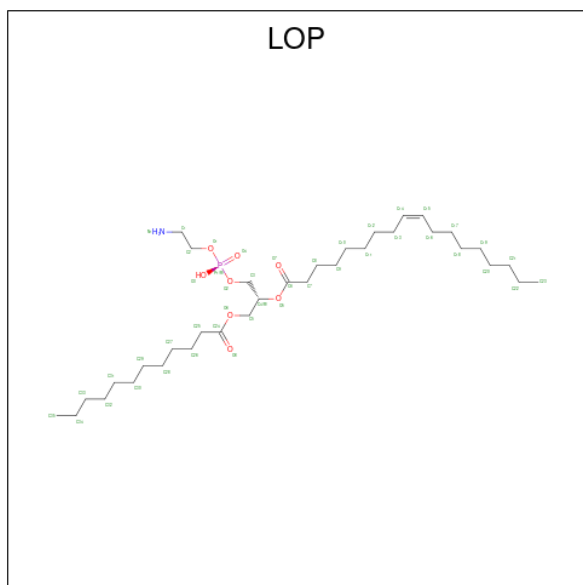
- Molecule 9 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	J	56	Total	C	N	O	0	0	0
			466	307	81	78			

- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 10.

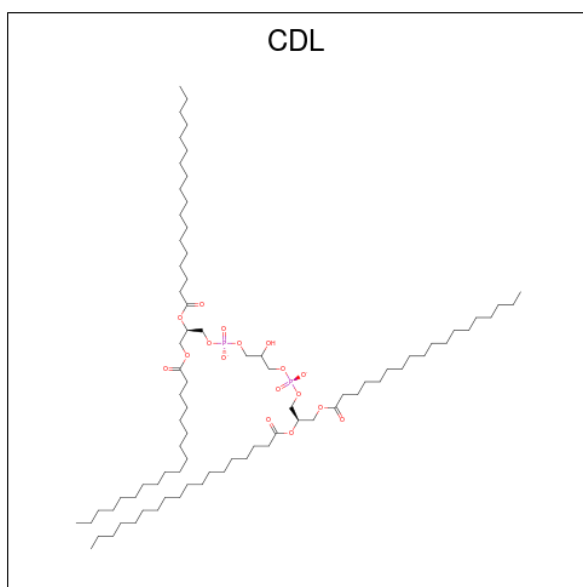
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	39	Total	C	N	O	0	0	0
			290	192	49	49			

- Molecule 11 is (1R)-2-[[[(R)-(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY]-1-[(DODECANOYLOXY)METHYL]ETHYL (9Z)-OCTADEC-9-ENOATE (three-letter code: LOP) (formula: C₃₅H₆₈NO₈P).



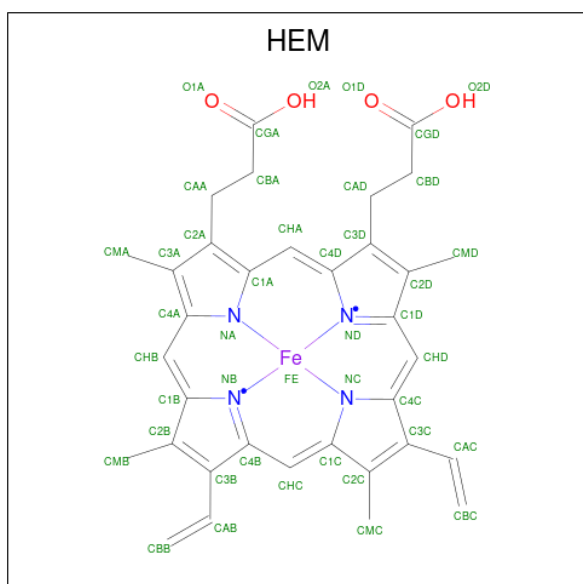
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
11	A	1	45	35	1	8	1	0	0
11	C	1	45	35	1	8	1	0	0
11	C	1	45	35	1	8	1	0	0
11	C	1	45	35	1	8	1	0	0
11	E	1	45	35	1	8	1	0	0
11	G	1	45	35	1	8	1	0	0

- Molecule 12 is CARDIOLIPIN (three-letter code: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



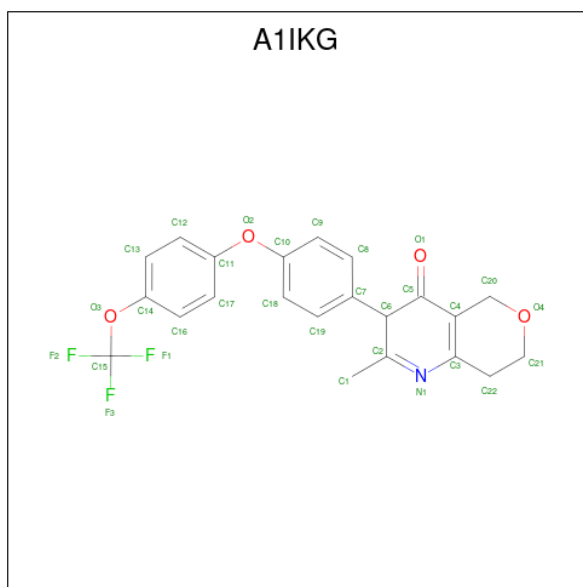
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
12	A	1	84	65	17	2	0	0
12	C	1	100	81	17	2	0	0
12	D	1	94	75	17	2	0	0

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



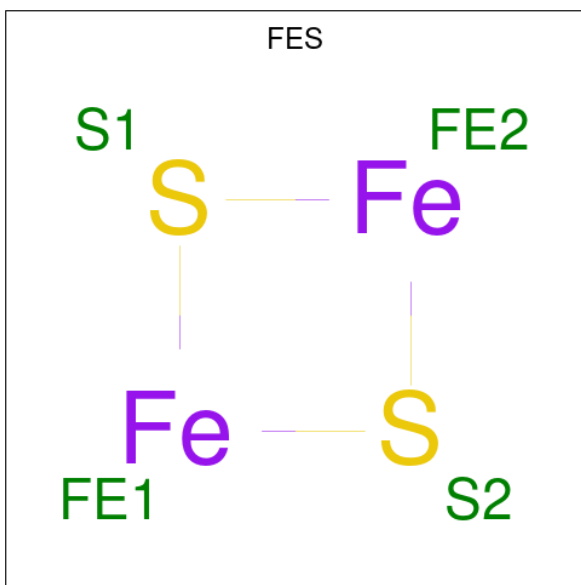
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
13	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
13	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 14 is 2-methyl-3-(4-(4-(trifluoromethoxy)phenoxy)phenoxy)phenyl)-1,5,7,8-tetrahydro-4H-pyrano[4,3-b]pyridin-4-one (three-letter code: A1IKG) (formula: C₂₂H₁₈F₃NO₄).



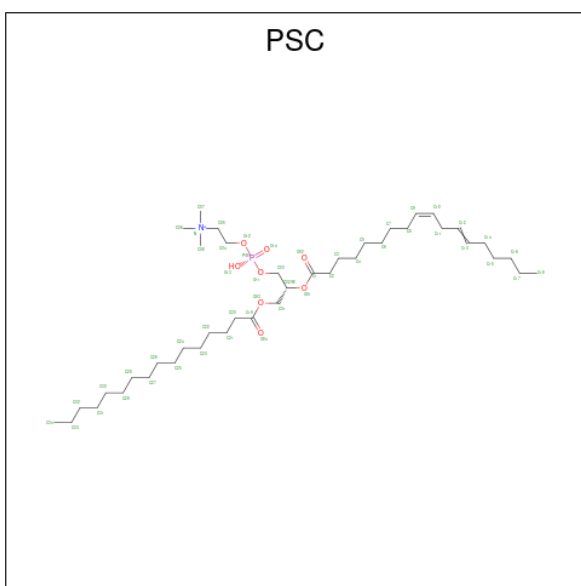
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
14	C	1	Total	C	F	N	O	0	0
			30	22	3	1	4		

- Molecule 15 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: C₂₄H₄₆O₁₁).



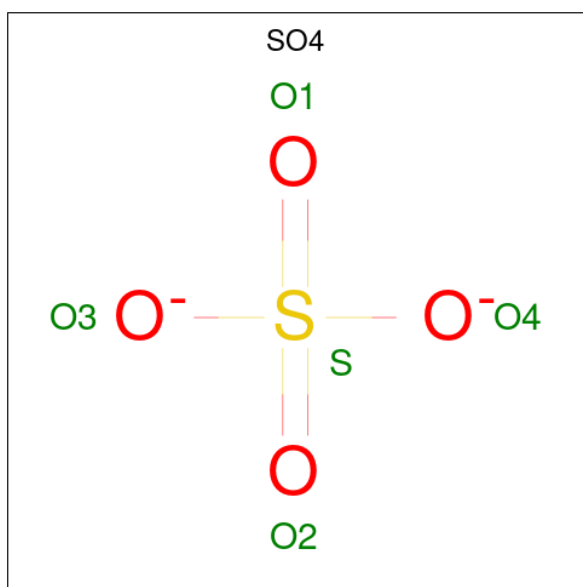
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	E	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 18 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C₄₂H₈₁NO₈P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
18	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 19 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	F	1	Total	O	S	0	0
			5	4	1		
19	G	1	Total	O	S	0	0
			5	4	1		
19	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 20 is water.

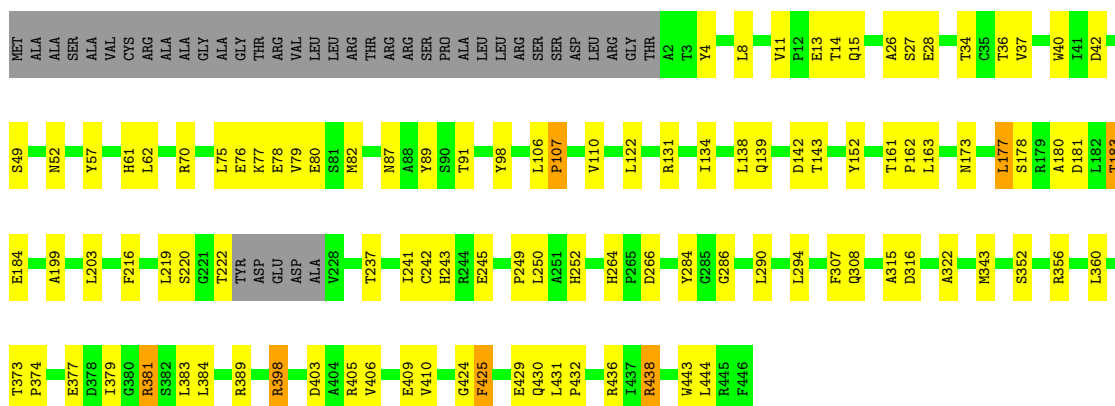
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	3	Total	O	0	0
			3	3		
20	B	1	Total	O	0	0
			1	1		
20	C	4	Total	O	0	0
			4	4		
20	E	1	Total	O	0	0
			1	1		
20	F	1	Total	O	0	0
			1	1		

3 Residue-property plots

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

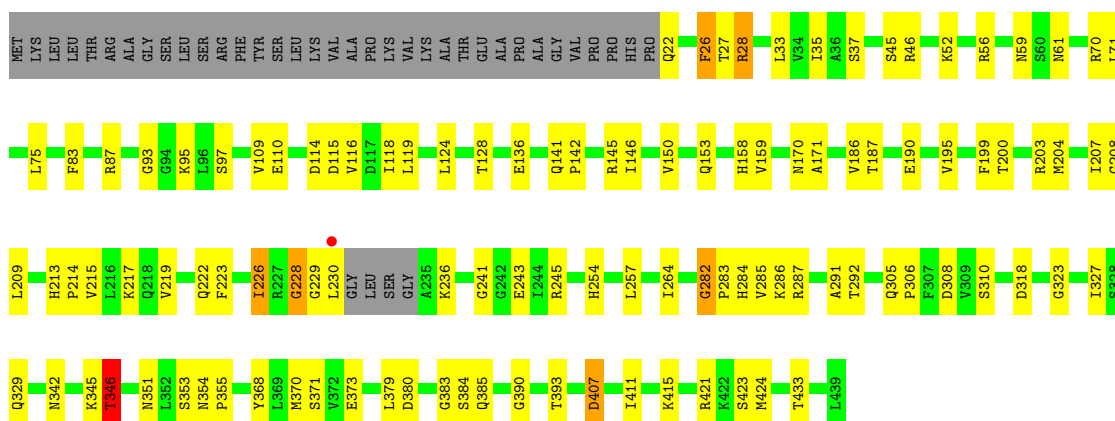
- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial

Chain A: 



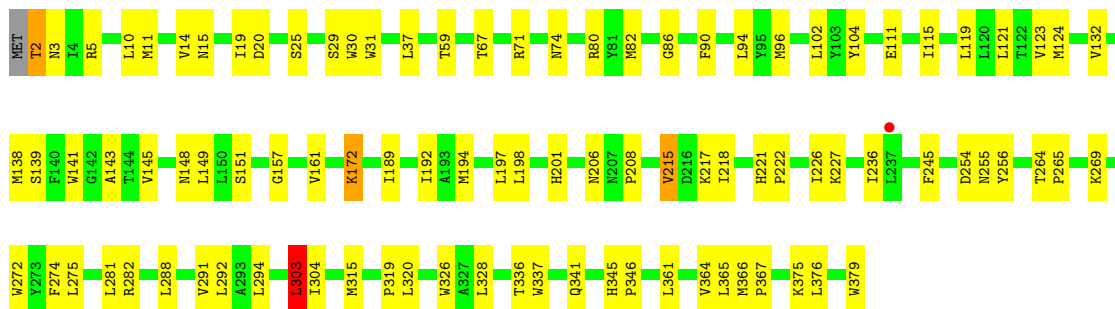
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial

Chain B: 



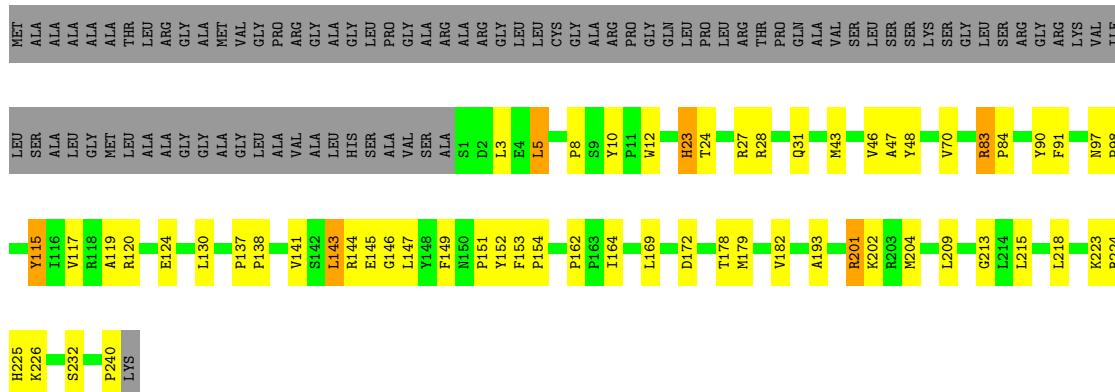
- Molecule 3: Cytochrome b

Chain C: 



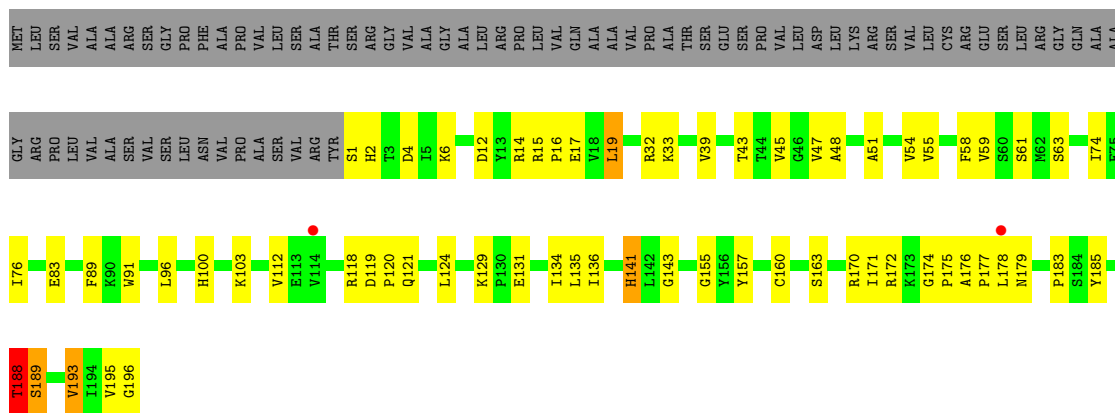
- Molecule 4: Cytochrome c1, heme protein, mitochondrial

Chain D: 55% 17% 26%



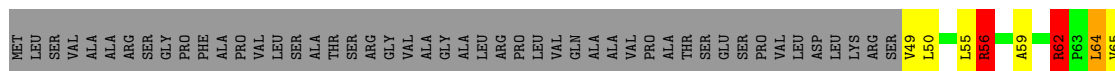
- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

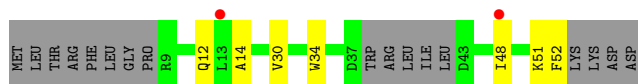
Chain E: 48% 22% 28%



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

Chain I: 5% 90%





4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	210.08Å 210.08Å 344.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 3.52 30.00 – 3.52	Depositor EDS
% Data completeness (in resolution range)	99.1 (30.00-3.52) 98.9 (30.00-3.52)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 3.48Å)	Xtrriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.188 , 0.241 0.188 , 0.241	Depositor DCC
R_{free} test set	2846 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	117.3	Xtrriage
Anisotropy	0.067	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 81.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16707	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, PSC, FES, LMT, HEC, SO4, A1IKG, LOP, CDL

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	0.40	0/3473	1.05	14/4713 (0.3%)
2	B	0.41	0/3167	1.03	7/4297 (0.2%)
3	C	0.38	0/3111	1.01	12/4259 (0.3%)
4	D	0.39	0/1960	1.01	5/2665 (0.2%)
5	E	0.39	0/1538	0.99	3/2082 (0.1%)
5	I	0.69	0/192	1.57	5/260 (1.9%)
6	F	0.40	0/879	1.16	5/1180 (0.4%)
7	G	0.45	0/641	1.27	7/869 (0.8%)
8	H	0.37	0/534	1.29	6/718 (0.8%)
9	J	0.42	0/478	1.08	3/644 (0.5%)
10	K	0.44	0/300	1.00	0/414
All	All	0.40	0/16273	1.06	67/22101 (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	2
2	B	0	2
4	D	0	2
5	E	0	1
5	I	0	1
6	F	0	2
7	G	0	3
9	J	0	1
All	All	0	14

There are no bond length outliers.

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	194[A]	MET	CG-SD-CE	12.18	119.69	100.20
3	C	194[B]	MET	CG-SD-CE	12.18	119.69	100.20
5	I	64	LEU	CB-CG-CD1	10.04	128.07	111.00
8	H	52	GLU	CB-CA-C	-8.43	93.53	110.40
7	G	2	ARG	CA-CB-CG	8.26	131.57	113.40
6	F	77	LYS	CB-CG-CD	8.15	132.78	111.60
2	B	346	THR	CA-CB-OG1	-7.60	93.03	109.00
9	J	8	ARG	CG-CD-NE	7.45	127.45	111.80
3	C	201	HIS	CB-CA-C	7.42	125.24	110.40
2	B	370	MET	CG-SD-CE	7.38	112.02	100.20
5	E	157	TYR	N-CA-CB	7.14	123.46	110.60
2	B	209	LEU	N-CA-CB	-6.94	96.53	110.40
8	H	29	LYS	N-CA-CB	-6.87	98.24	110.60
1	A	13	GLU	N-CA-CB	-6.79	98.37	110.60
8	H	29	LYS	CB-CA-C	6.75	123.91	110.40
7	G	3	GLN	CB-CA-C	-6.49	97.41	110.40
4	D	48	TYR	CB-CA-C	6.26	122.93	110.40
1	A	184	GLU	N-CA-CB	6.22	121.79	110.60
1	A	183	THR	CA-CB-OG1	-6.13	96.12	109.00
1	A	425	PHE	N-CA-CB	-6.13	99.56	110.60
3	C	303	LEU	CB-CG-CD2	-6.09	100.65	111.00
7	G	2	ARG	CD-NE-CZ	6.09	132.12	123.60
3	C	74	ASN	CB-CA-C	6.06	122.51	110.40
6	F	63	LYS	N-CA-CB	6.05	121.50	110.60
6	F	73	GLN	CB-CA-C	-6.03	98.34	110.40
9	J	8	ARG	CB-CA-C	5.89	122.18	110.40
7	G	16	TYR	N-CA-CB	5.87	121.17	110.60
1	A	438	ARG	NE-CZ-NH1	-5.85	117.38	120.30
1	A	143	THR	CA-CB-OG1	-5.82	96.78	109.00
3	C	375	LYS	CB-CG-CD	5.80	126.69	111.60
5	E	6	LYS	N-CA-CB	5.79	121.01	110.60
1	A	398	ARG	CB-CA-C	-5.70	99.00	110.40
5	E	17	GLU	CB-CA-C	5.63	121.66	110.40
1	A	131	ARG	NE-CZ-NH1	5.61	123.10	120.30
2	B	70	ARG	NE-CZ-NH2	-5.60	117.50	120.30
7	G	68	LYS	CA-CB-CG	5.56	125.63	113.40
5	I	56	ARG	CB-CG-CD	5.51	125.93	111.60
4	D	202	LYS	CB-CA-C	5.50	121.41	110.40
8	H	42	GLU	CB-CA-C	-5.50	99.41	110.40
5	I	56	ARG	CD-NE-CZ	5.48	131.27	123.60
3	C	255	ASN	CB-CA-C	5.46	121.32	110.40
8	H	29	LYS	CB-CG-CD	5.46	125.79	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	44	LYS	CG-CD-CE	5.43	128.19	111.90
7	G	16	TYR	CB-CA-C	-5.39	99.62	110.40
4	D	240	PRO	N-CA-C	5.36	126.03	112.10
7	G	40	ARG	NE-CZ-NH1	5.33	122.96	120.30
5	I	62	ARG	NE-CZ-NH1	5.31	122.96	120.30
6	F	77	LYS	CG-CD-CE	5.30	127.79	111.90
4	D	91	PHE	CB-CA-C	-5.24	99.91	110.40
3	C	328	LEU	CB-CG-CD2	-5.20	102.16	111.00
3	C	315	MET	CG-SD-CE	-5.18	91.91	100.20
4	D	201	ARG	CG-CD-NE	5.18	122.68	111.80
2	B	415	LYS	CB-CA-C	5.18	120.76	110.40
1	A	284	TYR	N-CA-CB	5.17	119.92	110.60
3	C	194[A]	MET	CB-CG-SD	5.17	127.92	112.40
3	C	194[B]	MET	CB-CG-SD	5.17	127.92	112.40
5	I	64	LEU	N-CA-CB	5.16	120.72	110.40
1	A	184	GLU	CB-CA-C	-5.14	100.11	110.40
2	B	52	LYS	CG-CD-CE	5.14	127.32	111.90
3	C	282	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	A	284	TYR	CB-CA-C	-5.13	100.13	110.40
9	J	8	ARG	CD-NE-CZ	5.13	130.79	123.60
2	B	26	PHE	N-CA-CB	-5.10	101.42	110.60
1	A	82	MET	CB-CA-C	-5.10	100.21	110.40
8	H	50	THR	N-CA-CB	5.08	119.95	110.30
1	A	14	THR	CA-CB-OG1	-5.05	98.40	109.00
1	A	383	LEU	CB-CG-CD2	-5.02	102.47	111.00

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	381	ARG	Sidechain
1	A	398	ARG	Sidechain
2	B	282	GLY	Peptide
2	B	421	ARG	Sidechain
4	D	201	ARG	Sidechain
4	D	83	ARG	Sidechain
5	E	172	ARG	Sidechain
6	F	61	ARG	Sidechain
6	F	99	ARG	Sidechain
7	G	11	ARG	Sidechain
7	G	2	ARG	Sidechain
7	G	42	ARG	Sidechain

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Mol	Chain	Res	Type	Group
5	I	62	ARG	Sidechain
9	J	16	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3402	0	3306	62	0
2	B	3112	0	3078	75	1
3	C	3008	0	3074	71	0
4	D	1901	0	1833	44	0
5	E	1505	0	1478	37	1
5	I	191	0	203	12	0
6	F	860	0	851	4	0
7	G	620	0	619	22	0
8	H	529	0	511	8	0
9	J	466	0	469	18	0
10	K	290	0	260	8	0
11	A	45	0	67	11	0
11	C	135	0	201	10	0
11	E	45	0	67	5	0
11	G	45	0	67	4	0
12	A	84	0	121	22	0
12	C	100	0	156	11	0
12	D	94	0	141	12	0
13	C	86	0	60	8	0
14	C	30	0	0	0	0
15	C	35	0	46	3	0
16	D	43	0	30	2	0
17	E	4	0	0	0	0
18	E	52	0	80	5	0
19	F	5	0	0	0	0
19	G	10	0	0	0	0
20	A	3	0	0	0	0
20	B	1	0	0	1	0
20	C	4	0	0	0	0
20	E	1	0	0	0	0
20	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	16707	0	16718	357	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 (357) 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)
12:A:502:CDL:H162	3:C:11:MET:HE1	1.48	0.95
12:A:502:CDL:HA22	12:A:502:CDL:H112	1.50	0.93
12:A:502:CDL:H422	12:A:502:CDL:H341	1.54	0.89
1:A:406:VAL:O	1:A:410:VAL:HG23	1.71	0.89
12:D:502:CDL:H342	12:D:502:CDL:H171	1.52	0.88
11:A:501:LOP:H352	18:E:203:PSC:H242	1.56	0.87
13:C:502:HEM:HBC2	13:C:502:HEM:HMC2	1.57	0.87
16:D:501:HEC:HMB1	16:D:501:HEC:HBB3	1.55	0.86
12:C:504:CDL:HA62	12:C:504:CDL:H351	1.57	0.86
1:A:444:LEU:HD11	11:A:501:LOP:H32	1.56	0.85
12:C:504:CDL:HB62	12:C:504:CDL:OB7	1.77	0.83
15:C:508:LMT:H61	15:C:508:LMT:H22	1.61	0.82
2:B:305:GLN:HB3	2:B:306:PRO:HD2	1.63	0.80
12:A:502:CDL:H872	12:A:502:CDL:H381	1.66	0.78
12:A:502:CDL:H422	12:A:502:CDL:C34	2.16	0.75
2:B:109:VAL:HB	2:B:119:LEU:HD23	1.69	0.75
3:C:141:TRP:CH2	3:C:264:THR:HG22	2.22	0.74
2:B:200:THR:HG21	2:B:229:GLY:H	1.53	0.73
11:E:202:LOP:H12	9:J:36:ASP:OD2	1.89	0.72
3:C:337:TRP:CH2	7:G:59:TYR:HA	2.24	0.72
2:B:385:GLN:HE22	2:B:393:THR:H	1.37	0.72
4:D:5:LEU:HD23	4:D:151:PRO:HB2	1.70	0.71
4:D:5:LEU:HG	4:D:152:TYR:CE1	2.25	0.71
11:A:501:LOP:H332	12:A:502:CDL:H792	1.72	0.71
3:C:141:TRP:O	3:C:145:VAL:HG23	1.92	0.70
9:J:13:LEU:O	9:J:19:THR:HG22	1.92	0.69
3:C:345:HIS:HB2	15:C:508:LMT:O3'	1.93	0.68
1:A:178:SER:HB3	1:A:181:ASP:OD2	1.94	0.68
12:D:502:CDL:H251	12:D:502:CDL:H591	1.76	0.68
3:C:15:ASN:HA	3:C:19:ILE:HD12	1.76	0.67
5:E:58:PHE:CZ	11:E:202:LOP:H352	2.30	0.66
1:A:444:LEU:HA	9:J:17:THR:HG21	1.78	0.66
1:A:360:LEU:HD23	2:B:93:GLY:HA2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:502:CDL:H341	12:A:502:CDL:C42	2.26	0.66
5:E:16:PRO:HA	5:E:19:LEU:HD12	1.78	0.66
3:C:320[A]:LEU:CD2	11:G:101:LOP:H251	2.26	0.65
2:B:229:GLY:O	2:B:230:LEU:HG	1.97	0.65
3:C:148:ASN:O	3:C:151:SER:OG	2.08	0.64
4:D:12:TRP:CZ2	4:D:124:GLU:HB3	2.33	0.64
4:D:232:SER:HB3	7:G:23:GLN:HE22	1.63	0.64
3:C:29:SER:OG	12:C:504:CDL:HA61	1.98	0.64
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.79	0.64
2:B:236:LYS:HE2	2:B:318:ASP:HB2	1.79	0.64
2:B:305:GLN:HB3	2:B:306:PRO:CD	2.26	0.64
2:B:327:ILE:HG21	5:I:55:LEU:HD11	1.81	0.63
5:E:1:SER:O	5:E:4:ASP:OD1	2.16	0.63
3:C:294:LEU:HD11	11:C:506:LOP:H12	1.80	0.63
2:B:215:VAL:O	2:B:219:VAL:HG23	1.99	0.63
7:G:50:PRO:HB2	7:G:51:PRO:HD3	1.79	0.63
2:B:222:GLN:HB2	2:B:223:PHE:HD1	1.63	0.63
11:A:501:LOP:H52	18:E:203:PSC:H012	1.80	0.62
11:G:101:LOP:H121	11:G:101:LOP:H321	1.81	0.62
7:G:28:HIS:HB2	7:G:32:LYS:HE2	1.82	0.61
12:D:502:CDL:HA32	7:G:37:VAL:HG23	1.82	0.61
6:F:101:ARG:O	6:F:105:GLU:HG3	2.00	0.61
3:C:217:LYS:HG3	7:G:7:LEU:HD13	1.83	0.61
11:A:501:LOP:H302	11:A:501:LOP:O6	2.00	0.61
12:D:502:CDL:H511	12:D:502:CDL:H132	1.83	0.61
3:C:138:MET:HE1	3:C:269:LYS:H	1.66	0.61
4:D:97:ASN:HB2	4:D:98:PRO:HD2	1.83	0.60
2:B:241:GLY:HA2	2:B:423:SER:OG	2.00	0.60
5:E:45:VAL:HG13	9:J:28:ALA:HA	1.83	0.60
1:A:80:GLU:HG2	2:B:284:HIS:HB2	1.82	0.60
8:H:47:ARG:HD3	8:H:48:SER:H	1.66	0.60
1:A:106:LEU:HB3	1:A:107:PRO:HD3	1.84	0.59
13:C:501:HEM:HMC1	13:C:501:HEM:HBC2	1.83	0.59
3:C:30:TRP:CH2	12:C:504:CDL:H312	2.37	0.59
8:H:16:PRO:O	8:H:20:VAL:HG23	2.02	0.59
5:I:72:VAL:HG13	5:I:73:PRO:HD2	1.84	0.59
12:A:502:CDL:H812	12:A:502:CDL:H232	1.85	0.58
2:B:37:SER:HA	2:B:208:GLY:O	2.03	0.58
2:B:145:ARG:NH2	20:B:501:HOH:O	2.35	0.58
3:C:361:LEU:HD23	3:C:365:LEU:HD12	1.84	0.58
2:B:380:ASP:O	2:B:384:SER:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:29:LEU:CD1	10:K:34:TRP:HB2	2.34	0.58
3:C:5:ARG:NH1	3:C:20:ASP:OD2	2.35	0.58
4:D:120:ARG:HG2	4:D:120:ARG:HH11	1.68	0.58
9:J:33:ARG:NH2	10:K:51:LYS:O	2.37	0.57
12:A:502:CDL:H232	12:A:502:CDL:C80	2.35	0.57
5:E:76:ILE:HB	5:E:193:VAL:HG12	1.87	0.57
2:B:56:ARG:HB2	2:B:171:ALA:HB1	1.86	0.56
4:D:204:MET:SD	11:E:202:LOP:H51	2.45	0.56
12:A:502:CDL:C16	3:C:11:MET:HE1	2.30	0.56
3:C:303:LEU:HD13	11:C:506:LOP:H233	1.86	0.56
4:D:24:THR:HG22	4:D:28:ARG:NH1	2.21	0.56
1:A:138:LEU:HB3	5:E:1:SER:HB2	1.87	0.56
2:B:236:LYS:CE	2:B:318:ASP:HB2	2.37	0.55
3:C:102:LEU:HD21	3:C:304:ILE:HD13	1.88	0.55
12:A:502:CDL:OA7	12:A:502:CDL:C51	2.55	0.55
12:A:502:CDL:H182	3:C:14:VAL:HG11	1.89	0.55
3:C:123:VAL:HG22	3:C:189:ILE:HD13	1.88	0.55
1:A:249:PRO:O	1:A:250:LEU:HD23	2.08	0.54
3:C:96:MET:CE	11:C:503:LOP:H14	2.37	0.54
3:C:132:VAL:HA	3:C:139:SER:HB3	1.89	0.54
5:E:48:ALA:HB1	10:K:34:TRP:CH2	2.42	0.54
2:B:200:THR:O	2:B:204:MET:HG3	2.08	0.54
5:E:129:LYS:HB3	5:E:131:GLU:OE1	2.08	0.54
7:G:72:LYS:HD3	8:H:56:GLU:OE2	2.08	0.54
11:A:501:LOP:H262	4:D:226:LYS:NZ	2.22	0.54
1:A:180:ALA:O	1:A:183:THR:HB	2.07	0.54
3:C:25:SER:HA	3:C:218:ILE:HD13	1.89	0.54
13:C:501:HEM:CMB	13:C:501:HEM:HBB2	2.38	0.54
12:C:504:CDL:H752	7:G:48:VAL:HG12	1.90	0.54
5:E:118:ARG:O	5:E:120:PRO:HD3	2.07	0.54
1:A:15:GLN:O	1:A:26:ALA:HA	2.08	0.54
12:A:502:CDL:H342	12:A:502:CDL:H432	1.88	0.53
4:D:164:ILE:HG22	4:D:179:MET:CG	2.39	0.53
5:E:141:HIS:CD2	5:E:175:PRO:HB2	2.43	0.53
1:A:403:ASP:OD1	1:A:406:VAL:HG23	2.08	0.53
2:B:213:HIS:N	2:B:214:PRO:CD	2.72	0.53
2:B:187:THR:OG1	2:B:190:GLU:HG3	2.08	0.53
9:J:33:ARG:HB2	10:K:48:ILE:HD13	1.91	0.53
4:D:225:HIS:CE1	7:G:20:PRO:HB2	2.44	0.53
3:C:320[A]:LEU:HD22	11:G:101:LOP:H251	1.89	0.53
4:D:213:GLY:HA2	12:D:502:CDL:H622	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:501:LOP:H92	12:A:502:CDL:H212	1.90	0.53
2:B:170:ASN:OD1	2:B:170:ASN:N	2.42	0.52
3:C:71:ARG:NH2	4:D:193:ALA:O	2.35	0.52
13:C:502:HEM:HBC2	13:C:502:HEM:CMC	2.35	0.52
5:E:51:ALA:O	5:E:55:VAL:HG23	2.08	0.52
3:C:326:TRP:NE1	7:G:48:VAL:HG22	2.24	0.52
1:A:430:GLN:O	1:A:430:GLN:HG2	2.09	0.52
5:E:83:GLU:HG2	5:E:100:HIS:CE1	2.44	0.52
7:G:9:ARG:HG3	7:G:9:ARG:HH11	1.74	0.52
1:A:4:TYR:HB3	2:B:114:ASP:OD2	2.10	0.52
12:A:502:CDL:OA7	12:A:502:CDL:CB5	2.57	0.52
3:C:149:LEU:HB3	3:C:291:VAL:CG2	2.40	0.52
12:D:502:CDL:H391	7:G:26:PHE:CE2	2.45	0.52
1:A:28:GLU:OE2	1:A:389:ARG:NH1	2.42	0.51
2:B:407:ASP:O	2:B:411:ILE:HG13	2.10	0.51
12:C:504:CDL:OB9	12:C:504:CDL:H731	2.10	0.51
3:C:236:ILE:HD13	11:E:202:LOP:H301	1.92	0.51
3:C:272:TRP:HA	3:C:275:LEU:HG	1.91	0.51
4:D:218:LEU:HD22	5:E:39:VAL:HG13	1.93	0.51
1:A:8:LEU:O	1:A:11:VAL:HG23	2.10	0.51
1:A:436:ARG:NH1	3:C:221:HIS:O	2.42	0.51
2:B:286:LYS:HG2	2:B:287:ARG:HG3	1.93	0.51
3:C:121:LEU:HB3	11:C:506:LOP:H251	1.92	0.51
5:E:121:GLN:O	5:E:170:ARG:HD3	2.11	0.51
2:B:45:SER:HB2	2:B:116:VAL:CG1	2.41	0.51
2:B:59:ASN:OD1	2:B:61:ASN:HB2	2.11	0.51
1:A:142:ASP:OD1	5:E:2:HIS:ND1	2.42	0.50
2:B:200:THR:HB	2:B:228:GLY:HA2	1.93	0.50
1:A:220:SER:OG	1:A:222:THR:HG22	2.11	0.50
11:A:501:LOP:H91	12:A:502:CDL:H732	1.92	0.50
3:C:124:MET:HG2	3:C:274:PHE:HE1	1.77	0.50
3:C:96:MET:HE2	11:C:503:LOP:H132	1.93	0.50
5:E:141:HIS:HB2	5:E:176:ALA:HA	1.94	0.50
9:J:29:LEU:HD12	10:K:34:TRP:CD1	2.47	0.50
16:D:501:HEC:HBB3	16:D:501:HEC:CMB	2.36	0.50
5:E:43:THR:O	5:E:47:VAL:HG23	2.11	0.50
2:B:354:ASN:N	2:B:355:PRO:HD2	2.27	0.50
4:D:120:ARG:HG2	4:D:120:ARG:NH1	2.27	0.50
2:B:346:THR:HG23	2:B:351:ASN:HB2	1.93	0.49
1:A:57:TYR:CE2	1:A:61:HIS:HE1	2.29	0.49
1:A:308:GLN:O	1:A:322:ALA:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:149:LEU:HB3	3:C:291:VAL:HG22	1.93	0.49
11:C:503:LOP:H291	12:C:504:CDL:H162	1.93	0.49
1:A:40:TRP:CZ2	1:A:377:GLU:HA	2.46	0.49
3:C:111:GLU:O	3:C:115:ILE:HG12	2.12	0.49
1:A:405:ARG:O	1:A:409:GLU:HB2	2.13	0.49
1:A:431:LEU:HD12	1:A:432:PRO:HD2	1.95	0.49
13:C:501:HEM:HBC2	13:C:501:HEM:CMC	2.43	0.49
18:E:203:PSC:H082	9:J:17:THR:OG1	2.12	0.49
9:J:13:LEU:O	9:J:19:THR:CG2	2.61	0.49
2:B:95:LYS:HE2	2:B:97:SER:HB3	1.95	0.49
4:D:224:ARG:HH21	7:G:26:PHE:HA	1.78	0.49
5:E:118:ARG:HH11	5:E:171:ILE:HG13	1.78	0.49
2:B:308:ASP:OD2	5:I:59:ALA:CB	2.61	0.48
1:A:106:LEU:O	1:A:110:VAL:HG23	2.14	0.48
3:C:366:MET:N	3:C:367:PRO:CD	2.76	0.48
3:C:31:TRP:CZ3	3:C:208:PRO:HG3	2.48	0.48
3:C:96:MET:CE	11:C:503:LOP:H132	2.44	0.48
2:B:115:ASP:HB3	2:B:118:ILE:HD12	1.94	0.48
1:A:139:GLN:HB2	5:I:50:LEU:HD12	1.95	0.48
5:E:55:VAL:O	5:E:59:VAL:HG23	2.13	0.48
7:G:34:ILE:HB	7:G:35:PRO:HD3	1.96	0.48
1:A:237:THR:HG21	5:E:14:ARG:NH2	2.28	0.48
3:C:226:ILE:HG12	4:D:223:LYS:HA	1.95	0.48
3:C:141:TRP:CZ3	3:C:264:THR:HG22	2.49	0.48
4:D:164:ILE:HD12	4:D:182:VAL:HG21	1.96	0.48
7:G:45:ILE:HG13	7:G:49:ALA:HB2	1.94	0.48
1:A:27:SER:HA	1:A:199:ALA:O	2.14	0.47
2:B:124:LEU:O	2:B:128:THR:HB	2.14	0.47
4:D:27:ARG:CZ	9:J:59:TYR:CE2	2.97	0.47
12:C:504:CDL:H581	12:D:502:CDL:H131	1.97	0.47
1:A:436:ARG:NH2	3:C:20:ASP:OD1	2.45	0.47
11:A:501:LOP:O8	3:C:221:HIS:HE1	1.97	0.47
2:B:159:VAL:HG21	2:B:254:HIS:HB3	1.95	0.47
1:A:286:GLY:HA3	1:A:290:LEU:HD21	1.97	0.47
2:B:33:LEU:HD23	2:B:204:MET:HB2	1.95	0.47
1:A:243:HIS:O	1:A:425:PHE:HA	2.15	0.47
3:C:206:ASN:HB3	13:C:502:HEM:O2D	2.15	0.47
3:C:67:THR:HG21	4:D:115:TYR:HE2	1.80	0.46
3:C:157:GLY:O	3:C:161:VAL:HG12	2.14	0.46
3:C:256:TYR:HB2	4:D:119:ALA:HB2	1.96	0.46
4:D:144:ARG:HH21	4:D:147:LEU:HD11	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:164:ILE:HG22	4:D:179:MET:HG2	1.97	0.46
10:K:51:LYS:O	10:K:52:PHE:C	2.53	0.46
3:C:275:LEU:HB2	3:C:336:THR:HG23	1.97	0.46
3:C:346:PRO:HG3	7:G:65:GLU:HB3	1.96	0.46
5:E:141:HIS:HA	5:E:177:PRO:HD2	1.97	0.46
1:A:152:TYR:HB3	1:A:241:ILE:HG21	1.96	0.46
2:B:200:THR:OG1	2:B:203:ARG:HG2	2.16	0.46
3:C:319:PRO:HB3	7:G:47:ARG:NH2	2.30	0.46
1:A:75:LEU:O	1:A:79:VAL:HG23	2.15	0.46
2:B:71:LEU:HD23	5:I:68:VAL:HG21	1.98	0.46
5:E:118:ARG:NH1	5:E:171:ILE:HG13	2.31	0.46
1:A:42:ASP:OD2	1:A:384:LEU:HD22	2.16	0.45
12:A:502:CDL:H232	12:A:502:CDL:C81	2.44	0.45
2:B:283:PRO:HG3	5:I:56:ARG:HD2	1.97	0.45
5:E:91:TRP:HZ2	5:E:196:GLY:HA2	1.81	0.45
12:A:502:CDL:H422	12:A:502:CDL:C35	2.45	0.45
1:A:249:PRO:HD2	1:A:250:LEU:H	1.81	0.45
1:A:252:HIS:O	1:A:424:GLY:HA2	2.17	0.45
2:B:150:VAL:O	2:B:153:GLN:HB2	2.17	0.45
5:E:54:VAL:HG22	11:E:202:LOP:H261	1.99	0.45
2:B:368:TYR:O	2:B:371:SER:OG	2.29	0.45
1:A:161:THR:HB	1:A:162:PRO:CD	2.47	0.45
2:B:282:GLY:HA2	5:I:56:ARG:CZ	2.47	0.45
12:D:502:CDL:HB62	12:D:502:CDL:H712	1.64	0.45
4:D:43:MET:HG2	4:D:46:VAL:HG23	1.97	0.44
8:H:44:VAL:HG22	8:H:52:GLU:HB2	1.97	0.44
1:A:61:HIS:CE1	1:A:134:ILE:HG12	2.52	0.44
3:C:104:TYR:CD1	3:C:208:PRO:HA	2.53	0.44
1:A:286:GLY:HA3	1:A:290:LEU:CD2	2.48	0.44
2:B:226:ILE:H	2:B:226:ILE:HG12	1.52	0.44
3:C:2:THR:HG23	3:C:3:ASN:H	1.82	0.44
3:C:215:VAL:O	6:F:63:LYS:HE2	2.17	0.44
11:C:506:LOP:H252	11:C:506:LOP:H281	1.56	0.44
12:D:502:CDL:H311	12:D:502:CDL:HA61	1.76	0.44
1:A:173:ASN:O	1:A:177:LEU:HB2	2.18	0.44
12:A:502:CDL:H172	12:A:502:CDL:H201	1.71	0.44
4:D:145:GLU:HG2	4:D:146:GLY:H	1.83	0.44
5:E:96:LEU:HD21	5:E:195:VAL:HG21	2.00	0.44
4:D:145:GLU:HG2	4:D:146:GLY:N	2.32	0.44
5:E:175:PRO:O	5:E:176:ALA:C	2.56	0.44
1:A:62:LEU:HD13	1:A:122:LEU:HD23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:CYS:O	7:G:14:ILE:HA	2.18	0.44
12:C:504:CDL:H462	12:C:504:CDL:H652	2.00	0.44
8:H:32:LYS:O	8:H:36:ARG:HG3	2.17	0.44
2:B:282:GLY:HA2	5:I:56:ARG:NH2	2.33	0.43
3:C:102:LEU:CD2	3:C:304:ILE:HD13	2.47	0.43
12:C:504:CDL:H522	7:G:40:ARG:NH2	2.33	0.43
2:B:207:ILE:HG13	2:B:383:GLY:HA2	2.00	0.43
3:C:197:LEU:HD23	3:C:197:LEU:HA	1.86	0.43
5:E:163:SER:HA	5:E:174:GLY:HA3	2.00	0.43
2:B:342:ASN:HA	2:B:345:LYS:HD3	2.00	0.43
2:B:346:THR:CG2	2:B:351:ASN:HB2	2.49	0.43
3:C:245:PHE:CE2	4:D:209:LEU:HD11	2.54	0.43
12:D:502:CDL:HA32	7:G:37:VAL:CG2	2.46	0.43
5:E:33:LYS:HE3	9:J:10:TYR:CE2	2.53	0.43
9:J:4:THR:O	9:J:8:ARG:HD3	2.18	0.43
2:B:245:ARG:NH2	2:B:433:THR:O	2.45	0.43
2:B:308:ASP:OD1	5:I:56:ARG:HD3	2.18	0.43
3:C:82:MET:O	3:C:86:GLY:N	2.41	0.43
4:D:137:PRO:HB3	4:D:141:VAL:CG1	2.48	0.43
4:D:164:ILE:HD12	4:D:182:VAL:CG2	2.49	0.43
2:B:195:VAL:O	2:B:199:PHE:HB2	2.19	0.43
3:C:198:LEU:O	3:C:198:LEU:HD12	2.18	0.43
4:D:23:HIS:HD2	9:J:52:TRP:HB2	1.83	0.43
12:A:502:CDL:H391	12:A:502:CDL:H861	2.01	0.43
12:C:504:CDL:H462	12:C:504:CDL:H672	2.01	0.43
4:D:31:GLN:HE22	4:D:172:ASP:CG	2.21	0.43
4:D:138:PRO:HG2	4:D:141:VAL:HG21	2.00	0.43
18:E:203:PSC:H081	9:J:14:PHE:O	2.18	0.43
1:A:429:GLU:O	1:A:429:GLU:HG2	2.18	0.43
4:D:8:PRO:HG3	8:H:66:ASP:HB3	2.01	0.43
2:B:46:ARG:HG2	2:B:379:LEU:HD22	2.00	0.43
1:A:76:GLU:HB2	2:B:285:VAL:HG21	2.01	0.43
2:B:159:VAL:HG21	2:B:254:HIS:CB	2.49	0.43
1:A:87:ASN:HB3	1:A:98:TYR:CZ	2.54	0.43
2:B:243:GLU:HA	2:B:424:MET:O	2.19	0.43
4:D:47:ALA:HA	4:D:90:TYR:HA	2.01	0.42
5:I:71:ASN:OD1	5:I:71:ASN:N	2.52	0.42
1:A:34:THR:HB	2:B:373:GLU:OE1	2.19	0.42
2:B:83:PHE:CZ	2:B:87:ARG:HG3	2.54	0.42
10:K:51:LYS:HD2	10:K:51:LYS:HA	1.75	0.42
11:A:501:LOP:H352	18:E:203:PSC:C24	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:143:LEU:HD11	4:D:149:PHE:HB2	2.01	0.42
2:B:254:HIS:CD2	2:B:327:ILE:HG12	2.54	0.42
2:B:385:GLN:NE2	2:B:393:THR:H	2.12	0.42
3:C:59:THR:HG23	3:C:172:LYS:HA	2.02	0.42
4:D:83:ARG:HB2	4:D:84:PRO:HD2	2.02	0.42
6:F:12:TRP:HA	6:F:12:TRP:CE3	2.54	0.42
2:B:141:GLN:NE2	2:B:186:VAL:O	2.52	0.42
2:B:286:LYS:O	2:B:287:ARG:HB2	2.20	0.42
1:A:106:LEU:HD22	1:A:203:LEU:HB3	2.02	0.42
1:A:237:THR:CG2	5:E:14:ARG:HH22	2.32	0.42
1:A:294:LEU:HG	1:A:307:PHE:CE2	2.55	0.42
1:A:379:ILE:HG12	1:A:389:ARG:HD2	2.02	0.42
2:B:27:THR:HG23	2:B:213:HIS:NE2	2.35	0.42
3:C:132:VAL:HG22	3:C:143:ALA:HB2	2.01	0.42
6:F:62:ILE:HG22	6:F:66:LEU:HD12	2.00	0.42
2:B:306:PRO:HG2	2:B:329:GLN:NE2	2.35	0.42
3:C:30:TRP:CE2	11:C:503:LOP:H82	2.54	0.42
4:D:215:LEU:HD23	4:D:215:LEU:HA	1.91	0.42
5:E:136:ILE:HD11	5:E:183:PRO:HB3	2.02	0.42
1:A:315:ALA:O	1:A:316:ASP:HB2	2.19	0.41
2:B:146:ILE:O	2:B:150:VAL:HG23	2.20	0.41
3:C:37:LEU:HD22	3:C:94:LEU:HD13	2.01	0.41
4:D:8:PRO:HG2	4:D:10:TYR:CZ	2.55	0.41
4:D:83:ARG:HB2	4:D:84:PRO:CD	2.50	0.41
4:D:164:ILE:HD13	4:D:164:ILE:HA	1.89	0.41
5:E:188:THR:OG1	5:E:189:SER:N	2.52	0.41
9:J:4:THR:N	9:J:8:ARG:NH1	2.68	0.41
2:B:35:ILE:HD13	2:B:217:LYS:HA	2.02	0.41
1:A:36:THR:HG21	1:A:373:THR:HA	2.02	0.41
11:A:501:LOP:H353	12:A:502:CDL:H822	2.03	0.41
3:C:141:TRP:CD1	3:C:265:PRO:HD3	2.56	0.41
13:C:502:HEM:HBB2	13:C:502:HEM:CMB	2.50	0.41
5:E:15:ARG:HD2	5:E:32:ARG:HG2	2.02	0.41
1:A:216:PHE:O	1:A:219:LEU:HB2	2.20	0.41
12:A:502:CDL:H872	12:A:502:CDL:C38	2.44	0.41
2:B:28:ARG:HH22	2:B:390:GLY:HA3	1.85	0.41
3:C:288:LEU:O	3:C:292:LEU:HG	2.21	0.41
3:C:337:TRP:O	3:C:341:GLN:HG2	2.20	0.41
8:H:32:LYS:HA	8:H:32:LYS:HE2	2.03	0.41
1:A:37:VAL:HG23	1:A:199:ALA:HB2	2.03	0.41
2:B:385:GLN:HE22	2:B:393:THR:N	2.10	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:153:PHE:CD1	4:D:154:PRO:HD2	2.56	0.41
12:D:502:CDL:H362	12:D:502:CDL:H392	1.59	0.41
1:A:163:LEU:HD23	1:A:163:LEU:HA	1.90	0.41
3:C:345:HIS:CE1	15:C:508:LMT:H31	2.55	0.41
5:E:103:LYS:HD2	5:E:103:LYS:HA	1.88	0.41
9:J:25:VAL:HG22	10:K:30:VAL:HG12	2.03	0.41
2:B:141:GLN:N	2:B:142:PRO:CD	2.84	0.41
13:C:502:HEM:HBB2	13:C:502:HEM:HMB1	2.03	0.41
2:B:95:LYS:HD3	2:B:110:GLU:OE1	2.21	0.41
3:C:119:LEU:CD2	3:C:192:ILE:HG22	2.51	0.41
3:C:215:VAL:H	3:C:215:VAL:HG13	1.52	0.41
4:D:144:ARG:HE	4:D:147:LEU:HD11	1.86	0.41
4:D:178:THR:O	4:D:182:VAL:HG13	2.21	0.41
8:H:41:ASP:O	8:H:45:SER:CB	2.69	0.41
1:A:70:ARG:HD3	1:A:78:GLU:OE2	2.21	0.41
4:D:138:PRO:HD3	4:D:149:PHE:CZ	2.56	0.41
5:E:76:ILE:HG23	5:E:89:PHE:CZ	2.56	0.41
7:G:53:VAL:O	7:G:57:LEU:HG	2.21	0.41
2:B:310:SER:HB2	5:I:56:ARG:HH22	1.86	0.40
5:E:33:LYS:HE3	9:J:10:TYR:CZ	2.57	0.40
1:A:77:LYS:HG2	2:B:291:ALA:HB3	2.02	0.40
1:A:343:MET:HB3	1:A:443:TRP:CE2	2.57	0.40
2:B:310:SER:HB3	5:I:59:ALA:HB1	2.04	0.40
1:A:49:SER:N	1:A:52:ASN:OD1	2.55	0.40
1:A:373:THR:N	1:A:374:PRO:HD2	2.37	0.40
2:B:207:ILE:HG13	2:B:383:GLY:CA	2.51	0.40
3:C:227:LYS:HE2	12:D:502:CDL:OB9	2.22	0.40
5:E:119:ASP:HB3	5:E:179:ASN:OD1	2.21	0.40
5:E:134:ILE:O	5:E:135:LEU:HD23	2.22	0.40
7:G:11:ARG:O	7:G:12:HIS:HB2	2.22	0.40
1:A:264:HIS:HD2	1:A:266:ASP:H	1.68	0.40
1:A:356:ARG:HH11	1:A:356:ARG:HD3	1.70	0.40
3:C:96:MET:HE2	11:C:503:LOP:C13	2.51	0.40
3:C:320[A]:LEU:HD22	11:G:101:LOP:H271	2.03	0.40
2:B:257:LEU:O	2:B:323:GLY:HA3	2.21	0.40
2:B:353:SER:HB2	2:B:355:PRO:HD2	2.03	0.40
3:C:138:MET:HA	3:C:138:MET:CE	2.52	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:305:GLN:NE2	5:E:112:VAL:O[5_555]	1.67	0.53

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	436/480 (91%)	423 (97%)	13 (3%)	0	100	100
2	B	411/453 (91%)	383 (93%)	26 (6%)	2 (0%)	25	59
3	C	378/379 (100%)	362 (96%)	16 (4%)	0	100	100
4	D	238/325 (73%)	227 (95%)	9 (4%)	2 (1%)	16	50
5	E	194/274 (71%)	174 (90%)	15 (8%)	5 (3%)	4	27
5	I	25/274 (9%)	21 (84%)	4 (16%)	0	100	100
6	F	96/111 (86%)	94 (98%)	2 (2%)	0	100	100
7	G	72/82 (88%)	66 (92%)	5 (7%)	1 (1%)	9	39
8	H	63/109 (58%)	61 (97%)	2 (3%)	0	100	100
9	J	54/64 (84%)	54 (100%)	0	0	100	100
10	K	35/56 (62%)	28 (80%)	5 (14%)	2 (6%)	1	13
All	All	2002/2607 (77%)	1893 (95%)	97 (5%)	12 (1%)	22	55

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	228	GLY
5	E	141	HIS
5	E	143	GLY
5	E	155	GLY
10	K	12	GLN
10	K	14	ALA
2	B	158	HIS
5	E	160	CYS

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Mol	Chain	Res	Type
4	D	5	LEU
4	D	162	PRO
5	E	188	THR
7	G	12	HIS

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	364/394 (92%)	356 (98%)	8 (2%)	47 69
2	B	324/355 (91%)	316 (98%)	8 (2%)	42 67
3	C	327/327 (100%)	314 (96%)	13 (4%)	27 55
4	D	203/257 (79%)	195 (96%)	8 (4%)	27 56
5	E	165/228 (72%)	154 (93%)	11 (7%)	13 40
5	I	21/228 (9%)	14 (67%)	7 (33%)	0 1
6	F	90/99 (91%)	85 (94%)	5 (6%)	17 45
7	G	65/72 (90%)	60 (92%)	5 (8%)	10 34
8	H	62/99 (63%)	59 (95%)	3 (5%)	21 50
9	J	47/54 (87%)	46 (98%)	1 (2%)	48 70
10	K	25/46 (54%)	25 (100%)	0	100 100
All	All	1693/2159 (78%)	1624 (96%)	69 (4%)	26 54

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	TYR
1	A	91	THR
1	A	107	PRO
1	A	177	LEU
1	A	245	GLU
1	A	352	SER
1	A	381	ARG

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Mol	Chain	Res	Type
1	A	438	ARG
2	B	22	GLN
2	B	26	PHE
2	B	28	ARG
2	B	226	ILE
2	B	264	ILE
2	B	292	THR
2	B	346	THR
2	B	407	ASP
3	C	2	THR
3	C	10	LEU
3	C	80	ARG
3	C	90	PHE
3	C	172	LYS
3	C	215	VAL
3	C	222	PRO
3	C	254	ASP
3	C	281	LEU
3	C	303	LEU
3	C	364	VAL
3	C	376	LEU
3	C	379	TRP
4	D	3	LEU
4	D	23	HIS
4	D	70	VAL
4	D	115	TYR
4	D	117	VAL
4	D	130	LEU
4	D	143	LEU
4	D	169	LEU
5	E	12	ASP
5	E	19	LEU
5	E	61	SER
5	E	63	SER
5	E	74	ILE
5	E	124	LEU
5	E	178	LEU
5	E	185	TYR
5	E	188	THR
5	E	189	SER
5	E	193	VAL
6	F	38	HIS

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Mol	Chain	Res	Type
6	F	59	VAL
6	F	77	LYS
6	F	95	LYS
6	F	106	GLU
7	G	3	GLN
7	G	6	HIS
7	G	42	ARG
7	G	45	ILE
7	G	72	LYS
8	H	29	LYS
8	H	35	GLU
8	H	38	GLU
5	I	49	VAL
5	I	56	ARG
5	I	62	ARG
5	I	64	LEU
5	I	65	VAL
5	I	67	SER
5	I	68	VAL
9	J	12	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	136	GLN
1	A	264	HIS
1	A	308	GLN
2	B	277	HIS
2	B	297	GLN
2	B	329	GLN
2	B	385	GLN
3	C	201	HIS
3	C	267	HIS
4	D	23	HIS
4	D	71	GLN
4	D	198	HIS
4	D	225	HIS
5	E	164	HIS
7	G	23	GLN
7	G	28	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](#)

19 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
16	HEC	D	501	4	32,50,50	2.05	9 (28%)	24,82,82	2.51	11 (45%)
13	HEM	C	502	3	41,50,50	1.59	6 (14%)	45,82,82	1.66	10 (22%)
12	CDL	A	502	-	83,83,99	0.52	0	89,95,111	0.87	3 (3%)
11	LOP	C	506	-	44,44,44	0.62	0	47,49,49	0.90	1 (2%)
15	LMT	C	508	-	36,36,36	0.52	0	47,47,47	0.84	2 (4%)
18	PSC	E	203	-	51,51,51	0.56	0	57,59,59	1.28	4 (7%)
11	LOP	G	101	-	44,44,44	0.44	0	47,49,49	1.25	3 (6%)
11	LOP	C	503	-	44,44,44	0.56	0	47,49,49	0.95	3 (6%)
12	CDL	C	504	-	99,99,99	0.43	0	105,111,111	0.79	2 (1%)
11	LOP	E	202	-	44,44,44	0.45	0	47,49,49	0.92	2 (4%)
14	A1IKG	C	505	-	32,33,33	1.57	6 (18%)	40,48,48	1.46	7 (17%)
11	LOP	C	507	-	44,44,44	0.56	0	47,49,49	0.76	2 (4%)
19	SO4	G	102	-	4,4,4	0.34	0	6,6,6	0.12	0
11	LOP	A	501	-	44,44,44	0.49	0	47,49,49	0.80	0
12	CDL	D	502	-	93,93,99	0.44	0	99,105,111	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	HEM	C	501	3	41,50,50	1.51	7 (17%)	45,82,82	2.11	14 (31%)
19	SO4	F	201	-	4,4,4	0.30	0	6,6,6	0.17	0
19	SO4	G	103	-	4,4,4	0.28	0	6,6,6	0.11	0
17	FES	E	201	5	0,4,4	-	-	-	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	LOP	A	501	-	-	22/48/48/48	-
11	LOP	C	506	-	-	21/48/48/48	-
12	CDL	D	502	-	-	49/104/104/110	-
15	LMT	C	508	-	-	7/21/61/61	0/2/2/2
16	HEC	D	501	4	-	2/10/54/54	-
13	HEM	C	501	3	-	4/12/54/54	-
14	A1IKG	C	505	-	1/1/6/6	0/13/40/40	0/4/4/4
18	PSC	E	203	-	-	28/55/55/55	-
13	HEM	C	502	3	-	4/12/54/54	-
11	LOP	C	507	-	-	33/48/48/48	-
12	CDL	A	502	-	-	52/93/93/110	-
11	LOP	G	101	-	-	27/48/48/48	-
17	FES	E	201	5	-	-	0/1/1/1
11	LOP	C	503	-	-	17/48/48/48	-
12	CDL	C	504	-	-	54/110/110/110	-
11	LOP	E	202	-	-	23/48/48/48	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	D	501	HEC	C3C-C2C	7.01	1.48	1.40
14	C	505	A1IKG	C6-C2	-6.04	1.42	1.52
13	C	502	HEM	C1B-NB	-5.33	1.31	1.40
16	D	501	HEC	C2B-C3B	3.61	1.44	1.40
14	C	505	A1IKG	C5-C4	-3.58	1.39	1.47
13	C	501	HEM	C1B-NB	-3.53	1.34	1.40
13	C	502	HEM	C4B-NB	-3.35	1.31	1.38
16	D	501	HEC	C2A-C3A	3.34	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	502	HEM	C4D-ND	-3.28	1.34	1.40
16	D	501	HEC	C3D-C2D	3.27	1.47	1.37
13	C	501	HEM	C4D-ND	-3.27	1.34	1.40
13	C	501	HEM	C1D-ND	-3.18	1.32	1.38
13	C	501	HEM	C4B-NB	-2.98	1.32	1.38
14	C	505	A1IKG	C7-C6	-2.93	1.49	1.53
16	D	501	HEC	C2A-C1A	2.87	1.49	1.42
14	C	505	A1IKG	C4-C3	2.50	1.42	1.37
13	C	502	HEM	O1A-CGA	2.44	1.30	1.22
13	C	501	HEM	FE-NB	2.43	2.08	1.96
14	C	505	A1IKG	C6-C5	-2.40	1.42	1.50
16	D	501	HEC	C3A-C4A	2.39	1.48	1.42
13	C	501	HEM	C4D-C3D	2.36	1.49	1.45
16	D	501	HEC	C1C-CHC	2.30	1.47	1.41
13	C	502	HEM	C1D-ND	-2.29	1.34	1.38
16	D	501	HEC	C4B-C3B	2.24	1.47	1.43
14	C	505	A1IKG	O1-C5	2.12	1.26	1.22
16	D	501	HEC	C3C-C4C	2.04	1.46	1.43
13	C	501	HEM	FE-ND	-2.02	1.86	1.96
13	C	502	HEM	FE-NB	2.00	2.06	1.96

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	D	501	HEC	C1D-C2D-C3D	-7.22	101.98	107.00
18	E	203	PSC	O01-C1-C2	6.49	125.50	111.50
11	G	101	LOP	O5-C6-C7	6.29	125.06	111.50
13	C	501	HEM	CBA-CAA-C2A	-5.87	102.60	112.62
14	C	505	A1IKG	C7-C6-C2	5.26	123.16	111.45
16	D	501	HEC	CMC-C2C-C3C	5.19	131.92	125.82
13	C	502	HEM	CHC-C4B-NB	4.69	129.52	124.43
13	C	501	HEM	CHC-C4B-NB	4.65	129.48	124.43
13	C	501	HEM	CAD-C3D-C4D	4.43	132.39	124.66
14	C	505	A1IKG	C7-C6-C5	4.35	117.98	111.37
13	C	502	HEM	C1B-NB-C4B	4.23	109.44	105.07
11	E	202	LOP	O5-C4-C5	-3.92	94.20	108.40
13	C	501	HEM	CHB-C1B-NB	3.78	129.05	124.38
13	C	501	HEM	CMD-C2D-C1D	3.70	130.68	125.04
12	C	504	CDL	OB6-CB5-C51	-3.68	103.57	111.50
13	C	501	HEM	C1B-NB-C4B	3.62	108.82	105.07
13	C	502	HEM	CBA-CAA-C2A	-3.61	106.45	112.62
11	E	202	LOP	O5-C4-C3	3.57	121.33	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	502	CDL	CB4-OB6-CB5	3.51	124.43	117.90
11	C	506	LOP	O5-C6-C7	3.45	118.94	111.50
12	C	504	CDL	OB6-CB4-CB3	-3.22	96.74	108.40
18	E	203	PSC	O01-C1-O02	-3.17	116.03	123.70
16	D	501	HEC	CAA-CBA-CGA	-3.02	105.31	113.76
11	C	503	LOP	C5-C4-C3	2.93	118.72	111.79
16	D	501	HEC	CMB-C2B-C3B	2.90	129.23	125.82
12	A	502	CDL	OB6-CB5-C51	2.76	116.17	111.09
13	C	501	HEM	CHB-C1B-C2B	-2.74	119.14	126.72
11	C	503	LOP	O5-C6-C7	2.72	117.36	111.50
18	E	203	PSC	O11-P-O14	2.71	119.66	109.07
11	C	507	LOP	O5-C6-C7	2.67	117.26	111.50
16	D	501	HEC	CBD-CAD-C3D	-2.59	108.21	112.62
15	C	508	LMT	O1'-C1'-C2'	2.58	112.34	108.30
13	C	501	HEM	O2D-CGD-CBD	2.51	122.09	114.03
11	G	101	LOP	O5-C6-O7	-2.48	117.70	123.70
13	C	501	HEM	O2D-CGD-O1D	-2.48	117.12	123.30
13	C	502	HEM	CHD-C1D-ND	2.46	127.10	124.43
13	C	502	HEM	CHB-C1B-NB	2.44	127.40	124.38
14	C	505	A1IKG	C1-C2-N1	-2.43	116.23	119.71
11	C	507	LOP	O6-C5-C4	2.41	115.44	108.43
16	D	501	HEC	CMA-C3A-C2A	2.35	129.38	124.94
13	C	502	HEM	CHA-C4D-C3D	-2.33	120.95	125.33
16	D	501	HEC	O2A-CGA-CBA	2.32	121.48	114.03
14	C	505	A1IKG	C4-C3-N1	-2.32	120.31	123.68
14	C	505	A1IKG	O1-C5-C4	-2.32	118.59	122.59
15	C	508	LMT	C1-O1'-C1'	2.32	117.68	113.84
11	G	101	LOP	C4-O5-C6	2.31	123.47	117.79
16	D	501	HEC	C3B-C4B-NB	2.29	115.28	110.94
13	C	502	HEM	C4B-C3B-C2B	-2.27	105.31	107.11
13	C	502	HEM	CHD-C1D-C2D	-2.25	121.46	124.98
16	D	501	HEC	CBA-CAA-C2A	2.25	116.40	112.60
13	C	502	HEM	CAD-C3D-C4D	2.23	128.56	124.66
16	D	501	HEC	O2D-CGD-CBD	2.19	121.06	114.03
13	C	501	HEM	CHA-C4D-C3D	-2.18	121.24	125.33
13	C	501	HEM	C4D-C3D-C2D	-2.18	103.72	106.90
14	C	505	A1IKG	C6-C5-C4	2.16	120.18	112.24
13	C	501	HEM	CAD-C3D-C2D	-2.15	123.87	127.88
13	C	501	HEM	O2A-CGA-CBA	2.14	120.92	114.03
16	D	501	HEC	C4C-C3C-C2C	2.10	108.62	106.35
11	C	503	LOP	O6-C5-C4	-2.07	102.41	108.43
12	A	502	CDL	OB7-CB5-C51	-2.06	117.30	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	C	501	HEM	CMC-C2C-C3C	2.06	128.53	124.68
14	C	505	A1IKG	C5-C4-C3	-2.04	118.98	120.65
18	E	203	PSC	O13-P-O11	-2.01	98.41	107.75
13	C	502	HEM	C4A-C3A-C2A	-2.01	105.60	107.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	C	505	A1IKG	C6

All (343) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	501	LOP	N1-C1-C2-O1
11	A	501	LOP	C2-O1-P1-O4
11	C	507	LOP	N1-C1-C2-O1
11	C	507	LOP	C2-O1-P1-O2
11	C	507	LOP	C2-O1-P1-O3
11	C	507	LOP	C2-O1-P1-O4
11	C	507	LOP	C3-O2-P1-O1
11	C	507	LOP	C3-O2-P1-O3
11	C	507	LOP	C3-O2-P1-O4
11	E	202	LOP	O2-C3-C4-O5
11	G	101	LOP	C3-O2-P1-O4
11	G	101	LOP	O7-C6-O5-C4
11	G	101	LOP	C7-C6-O5-C4
12	A	502	CDL	OA6-CA4-CA6-OA8
12	C	504	CDL	CA2-OA2-PA1-OA3
12	D	502	CDL	CB2-OB2-PB2-OB4
15	C	508	LMT	C2-C1-O1'-C1'
18	E	203	PSC	O02-C1-O01-C02
18	E	203	PSC	C2-C1-O01-C02
11	A	501	LOP	O8-C24-O6-C5
12	D	502	CDL	OA9-CA7-OA8-CA6
12	D	502	CDL	OB9-CB7-OB8-CB6
11	A	501	LOP	C25-C24-O6-C5
12	D	502	CDL	C31-CA7-OA8-CA6
12	D	502	CDL	C71-CB7-OB8-CB6
12	A	502	CDL	OA9-CA7-OA8-CA6
12	A	502	CDL	C31-CA7-OA8-CA6
11	A	501	LOP	C18-C19-C20-C21
12	D	502	CDL	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
15	C	508	LMT	O5B-C5B-C6B-O6B
12	C	504	CDL	CA7-C31-C32-C33
12	C	504	CDL	C63-C64-C65-C66
11	C	506	LOP	C25-C26-C27-C28
11	A	501	LOP	C30-C31-C32-C33
18	E	203	PSC	C1-C2-C3-C4
15	C	508	LMT	C2'-C1'-O1'-C1
11	A	501	LOP	O5-C4-C5-O6
11	C	507	LOP	C6-C7-C8-C9
12	C	504	CDL	CB5-C51-C52-C53
11	C	503	LOP	C24-C25-C26-C27
11	C	507	LOP	C24-C25-C26-C27
12	D	502	CDL	CB5-C51-C52-C53
12	A	502	CDL	CA7-C31-C32-C33
12	C	504	CDL	CA5-C11-C12-C13
18	E	203	PSC	C19-C20-C21-C22
12	A	502	CDL	C17-C18-C19-C20
12	D	502	CDL	CA7-C31-C32-C33
15	C	508	LMT	O1'-C1-C2-C3
15	C	508	LMT	C4B-C5B-C6B-O6B
12	D	502	CDL	CB2-OB2-PB2-OB5
18	E	203	PSC	C04-O12-P-O11
11	A	501	LOP	C27-C28-C29-C30
11	C	503	LOP	C18-C19-C20-C21
11	C	507	LOP	C26-C27-C28-C29
12	A	502	CDL	C36-C37-C38-C39
12	D	502	CDL	C22-C23-C24-C25
11	C	507	LOP	C19-C20-C21-C22
12	A	502	CDL	C23-C24-C25-C26
12	A	502	CDL	C41-C42-C43-C44
12	D	502	CDL	C12-C13-C14-C15
12	C	504	CDL	CB6-CB4-OB6-CB5
12	D	502	CDL	C74-C75-C76-C77
12	D	502	CDL	C83-C84-C85-C86
12	C	504	CDL	C36-C37-C38-C39
12	C	504	CDL	C55-C56-C57-C58
12	C	504	CDL	C56-C57-C58-C59
11	A	501	LOP	C29-C30-C31-C32
11	C	506	LOP	C30-C31-C32-C33
11	C	507	LOP	C25-C26-C27-C28
12	C	504	CDL	C15-C16-C17-C18
12	D	502	CDL	C37-C38-C39-C40

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Mol	Chain	Res	Type	Atoms
18	E	203	PSC	C5-C6-C7-C8
18	E	203	PSC	C26-C27-C28-C29
11	C	503	LOP	C7-C8-C9-C10
11	C	506	LOP	C11-C10-C9-C8
11	G	101	LOP	C19-C20-C21-C22
12	A	502	CDL	C39-C40-C41-C42
12	C	504	CDL	C23-C24-C25-C26
12	C	504	CDL	C73-C74-C75-C76
12	C	504	CDL	C82-C83-C84-C85
18	E	203	PSC	C22-C23-C24-C25
11	C	503	LOP	C27-C28-C29-C30
11	C	506	LOP	C10-C11-C12-C13
12	A	502	CDL	C11-CA5-OA6-CA4
12	A	502	CDL	C16-C17-C18-C19
11	G	101	LOP	C25-C26-C27-C28
11	G	101	LOP	C29-C30-C31-C32
12	A	502	CDL	C11-C12-C13-C14
12	C	504	CDL	C14-C15-C16-C17
12	C	504	CDL	C16-C17-C18-C19
12	C	504	CDL	C19-C20-C21-C22
12	C	504	CDL	C41-C42-C43-C44
12	C	504	CDL	C83-C84-C85-C86
12	D	502	CDL	C61-C62-C63-C64
11	G	101	LOP	C11-C10-C9-C8
12	A	502	CDL	C15-C16-C17-C18
15	C	508	LMT	C5-C6-C7-C8
11	C	506	LOP	N1-C1-C2-O1
11	C	503	LOP	C16-C17-C18-C19
11	C	503	LOP	C28-C29-C30-C31
11	G	101	LOP	C7-C8-C9-C10
12	A	502	CDL	C34-C35-C36-C37
12	A	502	CDL	C74-C75-C76-C77
12	A	502	CDL	C83-C84-C85-C86
12	C	504	CDL	C61-C62-C63-C64
12	C	504	CDL	C80-C81-C82-C83
12	C	504	CDL	C35-C36-C37-C38
12	C	504	CDL	C77-C78-C79-C80
11	C	506	LOP	C26-C27-C28-C29
11	C	503	LOP	C29-C30-C31-C32
11	C	507	LOP	C3-C4-C5-O6
11	A	501	LOP	C31-C32-C33-C34
12	C	504	CDL	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
12	C	504	CDL	C43-C44-C45-C46
11	A	501	LOP	C26-C27-C28-C29
12	D	502	CDL	C54-C55-C56-C57
12	D	502	CDL	C55-C56-C57-C58
18	E	203	PSC	C3-C4-C5-C6
11	A	501	LOP	C16-C17-C18-C19
11	C	503	LOP	C30-C31-C32-C33
11	C	507	LOP	C17-C18-C19-C20
11	E	202	LOP	C26-C27-C28-C29
12	C	504	CDL	C32-C33-C34-C35
12	A	502	CDL	C24-C25-C26-C27
11	C	503	LOP	C15-C16-C17-C18
11	C	506	LOP	C15-C16-C17-C18
11	E	202	LOP	C28-C29-C30-C31
12	C	504	CDL	C22-C23-C24-C25
11	E	202	LOP	C30-C31-C32-C33
12	A	502	CDL	C38-C39-C40-C41
11	E	202	LOP	C7-C6-O5-C4
12	D	502	CDL	C51-CB5-OB6-CB4
11	A	501	LOP	C19-C20-C21-C22
12	A	502	CDL	OB6-CB4-CB6-OB8
11	G	101	LOP	C25-C24-O6-C5
11	E	202	LOP	C17-C18-C19-C20
11	E	202	LOP	C11-C12-C13-C14
11	C	506	LOP	C19-C20-C21-C22
12	A	502	CDL	C12-C13-C14-C15
18	E	203	PSC	C2-C3-C4-C5
11	A	501	LOP	C2-O1-P1-O2
11	G	101	LOP	C3-O2-P1-O1
12	A	502	CDL	CB2-OB2-PB2-OB5
12	A	502	CDL	CB3-OB5-PB2-OB2
12	C	504	CDL	CA2-OA2-PA1-OA5
12	A	502	CDL	CA5-C11-C12-C13
11	E	202	LOP	O2-C3-C4-C5
12	D	502	CDL	CA5-C11-C12-C13
12	D	502	CDL	C53-C54-C55-C56
18	E	203	PSC	C6-C7-C8-C9
12	A	502	CDL	C20-C21-C22-C23
12	D	502	CDL	C34-C35-C36-C37
18	E	203	PSC	C24-C25-C26-C27
11	C	503	LOP	C10-C11-C12-C13
12	A	502	CDL	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
18	E	203	PSC	C29-C30-C31-C32
12	A	502	CDL	C33-C34-C35-C36
12	D	502	CDL	C16-C17-C18-C19
12	C	504	CDL	CB3-CB4-CB6-OB8
12	C	504	CDL	C52-C53-C54-C55
12	D	502	CDL	C33-C34-C35-C36
12	D	502	CDL	C84-C85-C86-C87
12	C	504	CDL	C44-C45-C46-C47
11	C	507	LOP	C11-C10-C9-C8
11	C	507	LOP	C30-C31-C32-C33
18	E	203	PSC	C27-C28-C29-C30
11	A	501	LOP	C15-C16-C17-C18
11	C	507	LOP	C25-C24-O6-C5
11	C	506	LOP	C27-C28-C29-C30
15	C	508	LMT	C9-C10-C11-C12
12	C	504	CDL	C31-CA7-OA8-CA6
12	C	504	CDL	OB5-CB3-CB4-OB6
12	A	502	CDL	C43-C44-C45-C46
12	D	502	CDL	C17-C18-C19-C20
12	D	502	CDL	C80-C81-C82-C83
11	C	506	LOP	C29-C30-C31-C32
11	C	506	LOP	C31-C32-C33-C34
12	C	504	CDL	C54-C55-C56-C57
11	C	507	LOP	O2-C3-C4-C5
11	E	202	LOP	C24-C25-C26-C27
12	A	502	CDL	C75-C76-C77-C78
12	A	502	CDL	OA7-CA5-OA6-CA4
11	C	507	LOP	C10-C11-C12-C13
12	A	502	CDL	C71-CB7-OB8-CB6
11	G	101	LOP	C9-C10-C11-C12
12	C	504	CDL	C81-C82-C83-C84
11	A	501	LOP	C3-C4-C5-O6
12	A	502	CDL	CA3-CA4-CA6-OA8
12	A	502	CDL	CB3-CB4-CB6-OB8
18	E	203	PSC	O03-C01-C02-C03
12	D	502	CDL	C32-C33-C34-C35
11	C	507	LOP	C9-C10-C11-C12
11	G	101	LOP	C2-O1-P1-O2
12	C	504	CDL	CB2-OB2-PB2-OB5
18	E	203	PSC	C21-C22-C23-C24
11	C	507	LOP	O2-C3-C4-O5
12	C	504	CDL	C57-C58-C59-C60

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Mol	Chain	Res	Type	Atoms
11	E	202	LOP	C6-C7-C8-C9
11	G	101	LOP	C27-C28-C29-C30
12	C	504	CDL	C74-C75-C76-C77
11	G	101	LOP	O5-C4-C5-O6
12	D	502	CDL	C24-C25-C26-C27
11	E	202	LOP	C18-C19-C20-C21
11	E	202	LOP	C19-C20-C21-C22
11	G	101	LOP	C31-C32-C33-C34
12	D	502	CDL	C63-C64-C65-C66
11	E	202	LOP	C14-C15-C16-C17
18	E	203	PSC	C7-C8-C9-C10
12	D	502	CDL	C81-C82-C83-C84
12	D	502	CDL	OB7-CB5-OB6-CB4
11	C	507	LOP	C7-C6-O5-C4
12	C	504	CDL	C51-CB5-OB6-CB4
12	C	504	CDL	OB5-CB3-CB4-CB6
12	D	502	CDL	OB5-CB3-CB4-CB6
11	C	507	LOP	C12-C13-C14-C15
11	G	101	LOP	C15-C16-C17-C18
12	A	502	CDL	C77-C78-C79-C80
12	A	502	CDL	C21-C22-C23-C24
11	C	507	LOP	C7-C8-C9-C10
12	A	502	CDL	C44-C45-C46-C47
12	C	504	CDL	C51-C52-C53-C54
12	C	504	CDL	CA4-CA3-OA5-PA1
11	G	101	LOP	O8-C24-O6-C5
11	C	507	LOP	O5-C4-C5-O6
18	E	203	PSC	O03-C01-C02-O01
18	E	203	PSC	C15-C16-C17-C18
11	E	202	LOP	C16-C17-C18-C19
12	C	504	CDL	C71-C72-C73-C74
11	E	202	LOP	C9-C10-C11-C12
11	A	501	LOP	C32-C33-C34-C35
12	A	502	CDL	C79-C80-C81-C82
11	C	506	LOP	C2-O1-P1-O2
12	A	502	CDL	CA2-OA2-PA1-OA5
12	D	502	CDL	C72-C73-C74-C75
11	E	202	LOP	C2-O1-P1-O3
11	G	101	LOP	C3-O2-P1-O3
12	A	502	CDL	CB3-OB5-PB2-OB3
12	A	502	CDL	CB3-OB5-PB2-OB4
12	C	504	CDL	CA2-OA2-PA1-OA4

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Mol	Chain	Res	Type	Atoms
18	E	203	PSC	C04-O12-P-O14
11	C	503	LOP	C26-C27-C28-C29
12	D	502	CDL	C23-C24-C25-C26
11	C	507	LOP	C15-C16-C17-C18
12	D	502	CDL	C76-C77-C78-C79
12	D	502	CDL	CA2-C1-CB2-OB2
18	E	203	PSC	C25-C26-C27-C28
12	D	502	CDL	OB5-CB3-CB4-OB6
18	E	203	PSC	O01-C02-C03-O11
12	D	502	CDL	C79-C80-C81-C82
12	A	502	CDL	C73-C74-C75-C76
11	G	101	LOP	C3-C4-C5-O6
12	C	504	CDL	OB6-CB4-CB6-OB8
11	C	507	LOP	C31-C32-C33-C34
11	E	202	LOP	C32-C33-C34-C35
11	C	507	LOP	O8-C24-O6-C5
11	G	101	LOP	C24-C25-C26-C27
11	G	101	LOP	C28-C29-C30-C31
12	C	504	CDL	C21-C22-C23-C24
18	E	203	PSC	C4-C5-C6-C7
11	C	503	LOP	C12-C13-C14-C15
12	D	502	CDL	C18-C19-C20-C21
11	C	506	LOP	C17-C18-C19-C20
11	C	506	LOP	C3-O2-P1-O1
12	A	502	CDL	CA3-OA5-PA1-OA2
12	D	502	CDL	CA3-OA5-PA1-OA2
11	C	503	LOP	C25-C26-C27-C28
12	A	502	CDL	C13-C14-C15-C16
11	E	202	LOP	O7-C6-O5-C4
12	D	502	CDL	C52-C53-C54-C55
11	G	101	LOP	C4-C3-O2-P1
12	A	502	CDL	C35-C36-C37-C38
12	C	504	CDL	C31-C32-C33-C34
12	D	502	CDL	C35-C36-C37-C38
11	C	506	LOP	O2-C3-C4-C5
11	E	202	LOP	C10-C11-C12-C13
11	A	501	LOP	C11-C12-C13-C14
11	C	503	LOP	C3-C4-C5-O6
12	C	504	CDL	CA3-CA4-CA6-OA8
12	C	504	CDL	C42-C43-C44-C45
11	C	507	LOP	C18-C19-C20-C21
11	C	507	LOP	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
12	A	502	CDL	C78-C79-C80-C81
13	C	502	HEM	CAA-CBA-CGA-O1A
11	C	503	LOP	O2-C3-C4-C5
11	E	202	LOP	C11-C10-C9-C8
13	C	501	HEM	CAA-CBA-CGA-O2A
12	D	502	CDL	OA6-CA4-CA6-OA8
13	C	502	HEM	CAA-CBA-CGA-O2A
12	A	502	CDL	CB2-C1-CA2-OA2
12	A	502	CDL	CA2-C1-CB2-OB2
12	D	502	CDL	C58-C59-C60-C61
12	C	504	CDL	OA9-CA7-OA8-CA6
13	C	501	HEM	CAA-CBA-CGA-O1A
11	A	501	LOP	C12-C13-C14-C15
18	E	203	PSC	C01-C02-C03-O11
11	E	202	LOP	C27-C28-C29-C30
18	E	203	PSC	C23-C24-C25-C26
11	C	507	LOP	C14-C15-C16-C17
12	D	502	CDL	C52-C51-CB5-OB6
12	D	502	CDL	C77-C78-C79-C80
12	A	502	CDL	C72-C71-CB7-OB8
13	C	501	HEM	CAD-CBD-CGD-O2D
11	G	101	LOP	C14-C15-C16-C17
18	E	203	PSC	C04-C05-N-C06
11	C	503	LOP	C20-C21-C22-C23
12	D	502	CDL	C15-C16-C17-C18
11	C	506	LOP	O6-C24-C25-C26
11	E	202	LOP	O5-C4-C5-O6
11	G	101	LOP	O5-C6-C7-C8
18	E	203	PSC	C04-C05-N-C07
12	D	502	CDL	C13-C14-C15-C16
11	C	506	LOP	C16-C17-C18-C19
11	A	501	LOP	C25-C26-C27-C28
13	C	501	HEM	CAD-CBD-CGD-O1D
12	A	502	CDL	C71-C72-C73-C74
12	C	504	CDL	C20-C21-C22-C23
12	A	502	CDL	C72-C71-CB7-OB9
12	D	502	CDL	C52-C51-CB5-OB7
12	C	504	CDL	C59-C60-C61-C62
11	C	506	LOP	O5-C6-C7-C8
11	A	501	LOP	C14-C15-C16-C17
11	C	506	LOP	C3-O2-P1-O4
11	E	202	LOP	C2-O1-P1-O4

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Mol	Chain	Res	Type	Atoms
11	G	101	LOP	C2-O1-P1-O4
12	A	502	CDL	CA2-OA2-PA1-OA4
18	E	203	PSC	C04-C05-N-C08
12	C	504	CDL	C52-C51-CB5-OB7
12	C	504	CDL	C53-C54-C55-C56
16	D	501	HEC	CAD-CBD-CGD-O2D
11	G	101	LOP	O7-C6-C7-C8
16	D	501	HEC	CAD-CBD-CGD-O1D
12	A	502	CDL	OB9-CB7-OB8-CB6
11	A	501	LOP	O6-C24-C25-C26
13	C	502	HEM	CAD-CBD-CGD-O2D
12	A	502	CDL	C12-C11-CA5-OA7
11	C	503	LOP	C13-C14-C15-C16
11	C	507	LOP	O5-C6-C7-C8
11	C	506	LOP	O8-C24-C25-C26
13	C	502	HEM	CAD-CBD-CGD-O1D
11	G	101	LOP	O6-C24-C25-C26
12	C	504	CDL	C32-C31-CA7-OA8
11	C	507	LOP	C32-C33-C34-C35
11	C	506	LOP	O7-C6-C7-C8

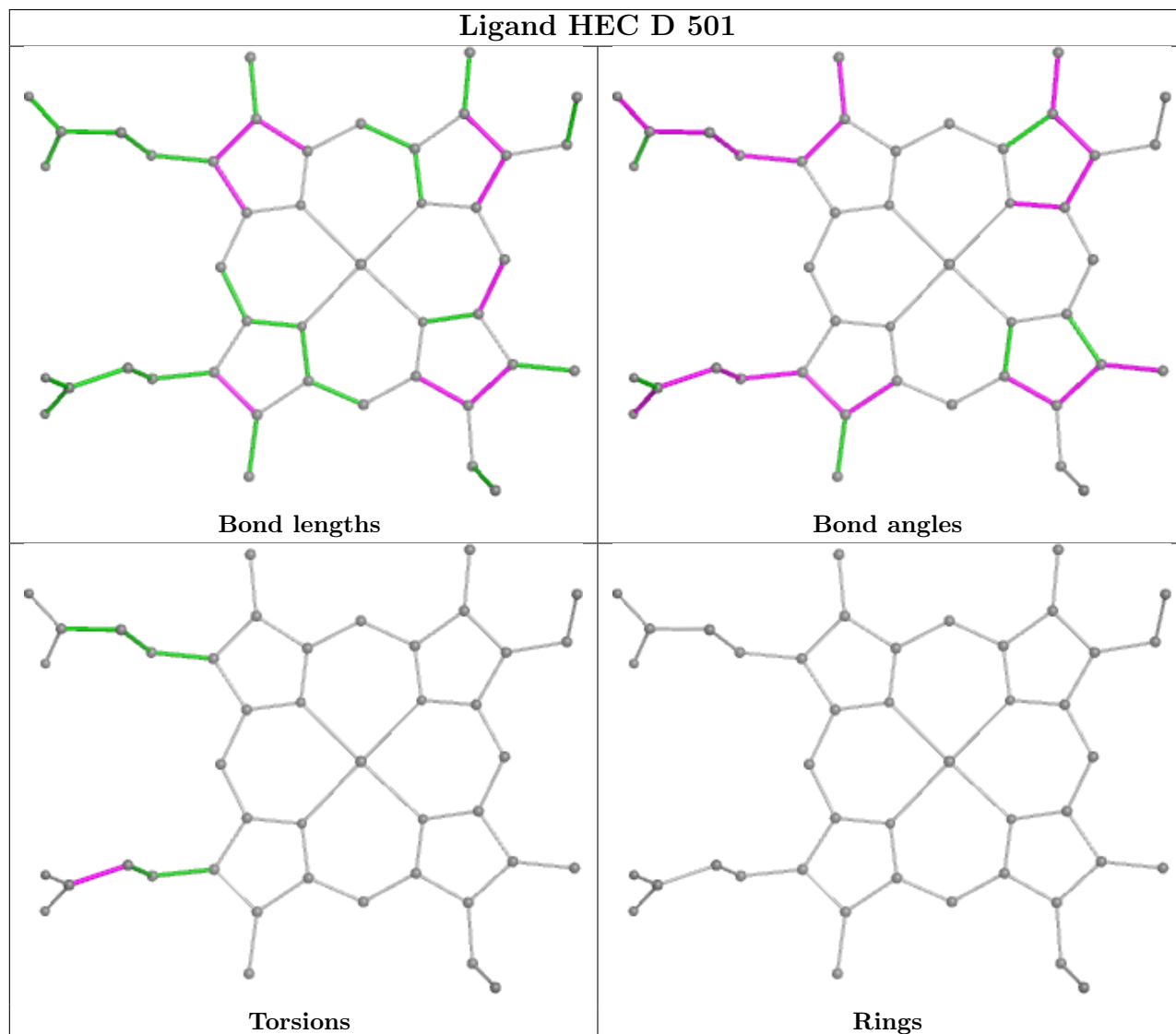
There are no ring outliers.

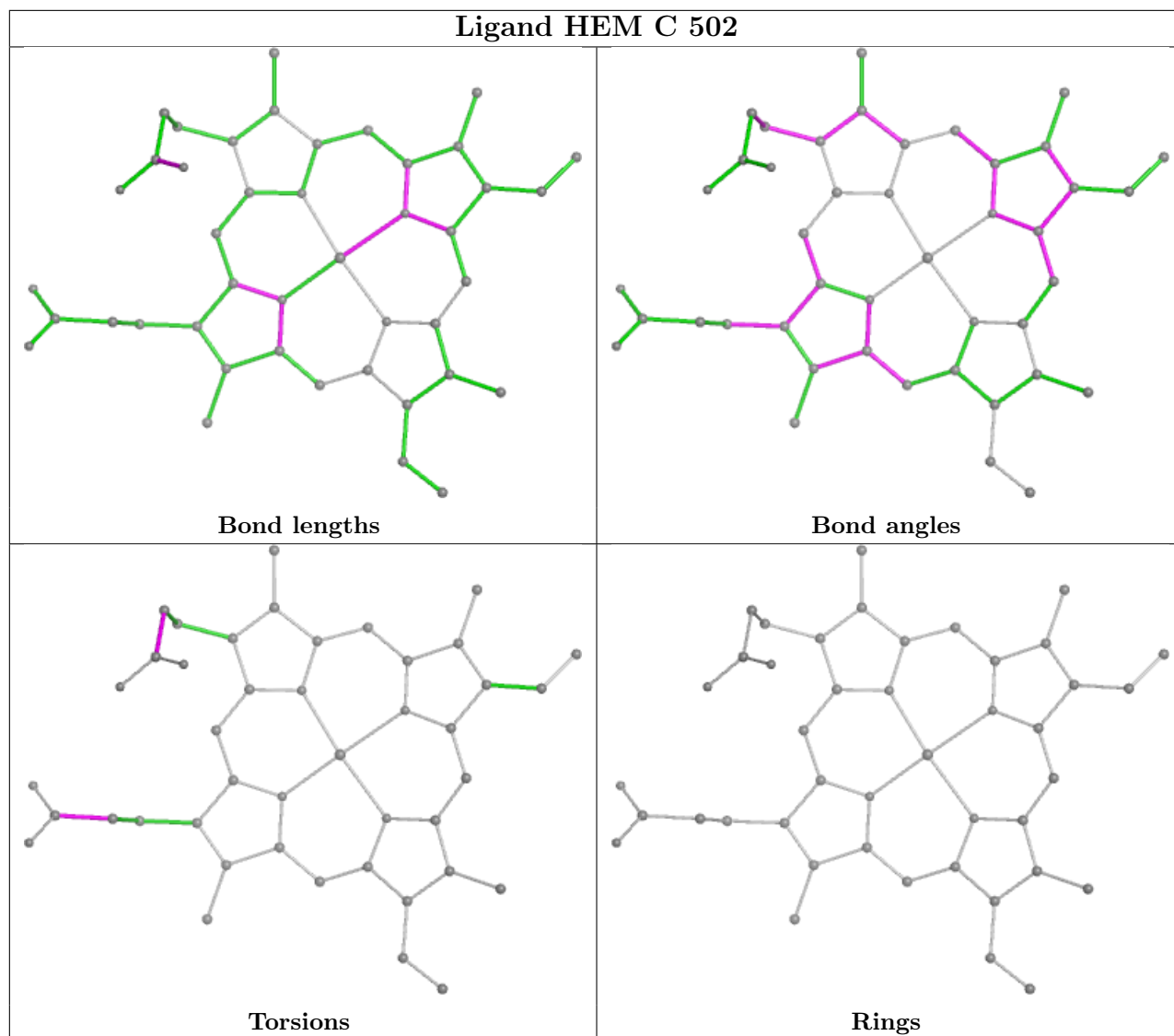
13 monomers are involved in 84 short contacts:

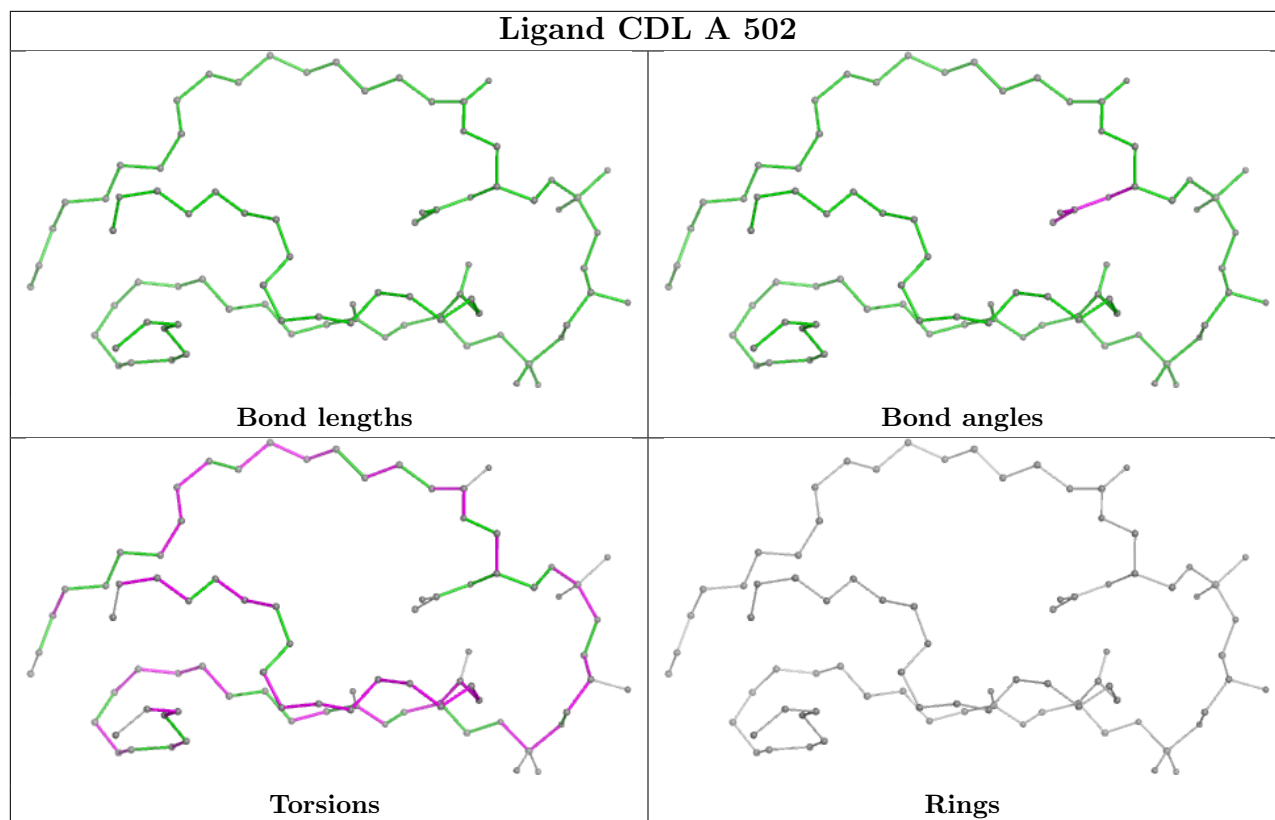
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	D	501	HEC	2	0
13	C	502	HEM	5	0
12	A	502	CDL	22	0
11	C	506	LOP	4	0
15	C	508	LMT	3	0
18	E	203	PSC	5	0
11	G	101	LOP	4	0
11	C	503	LOP	6	0
12	C	504	CDL	11	0
11	E	202	LOP	5	0
11	A	501	LOP	11	0
12	D	502	CDL	12	0
13	C	501	HEM	3	0

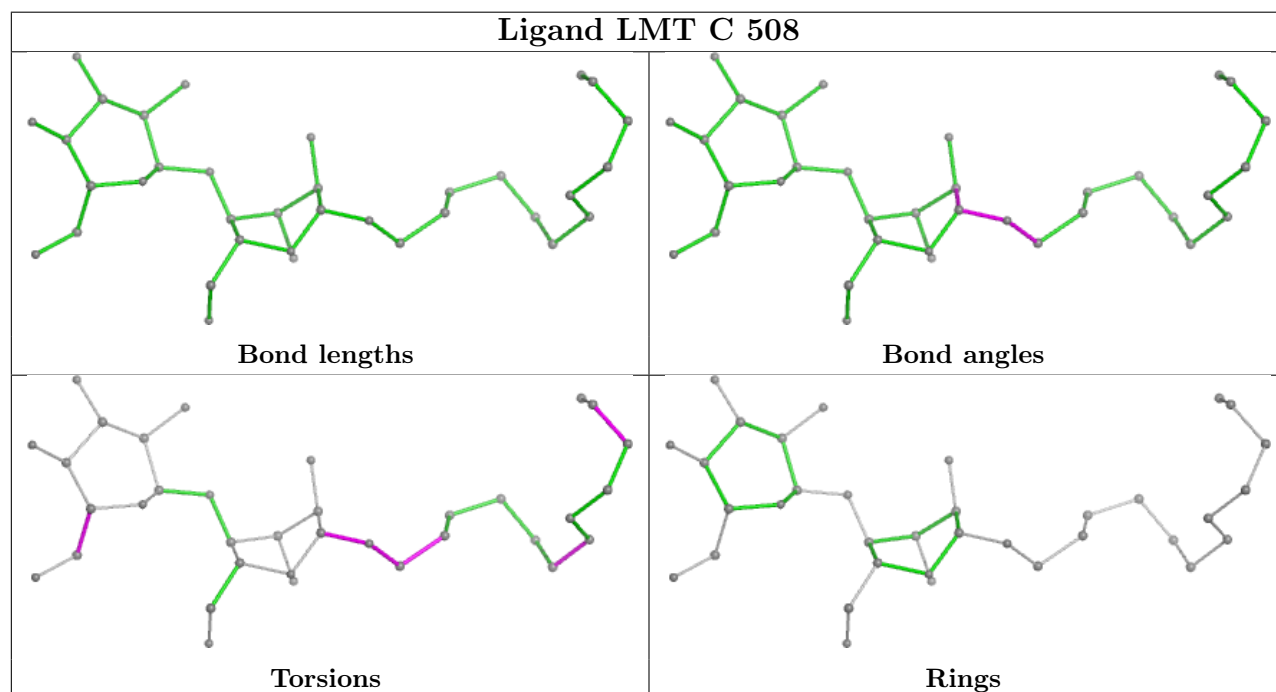
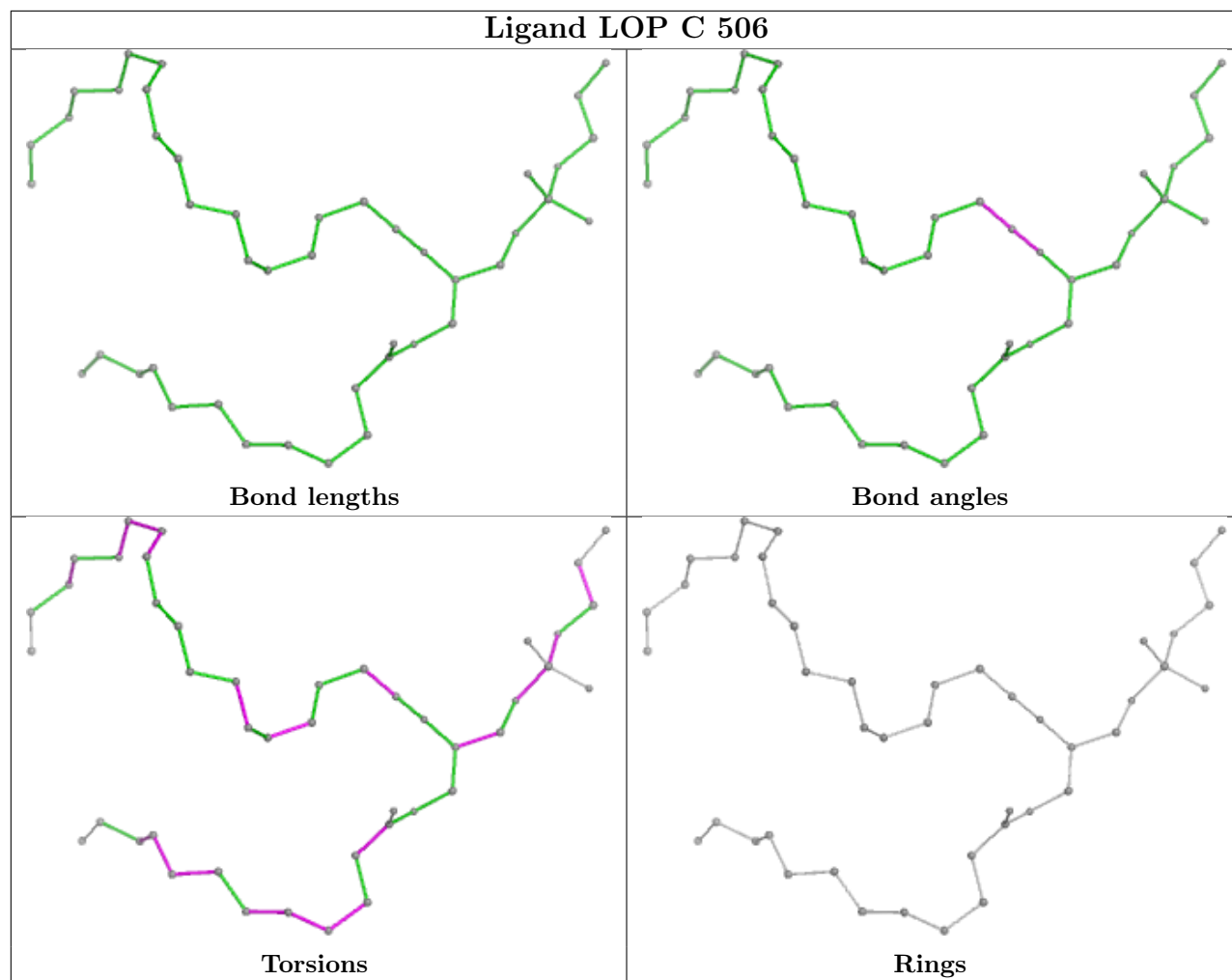
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

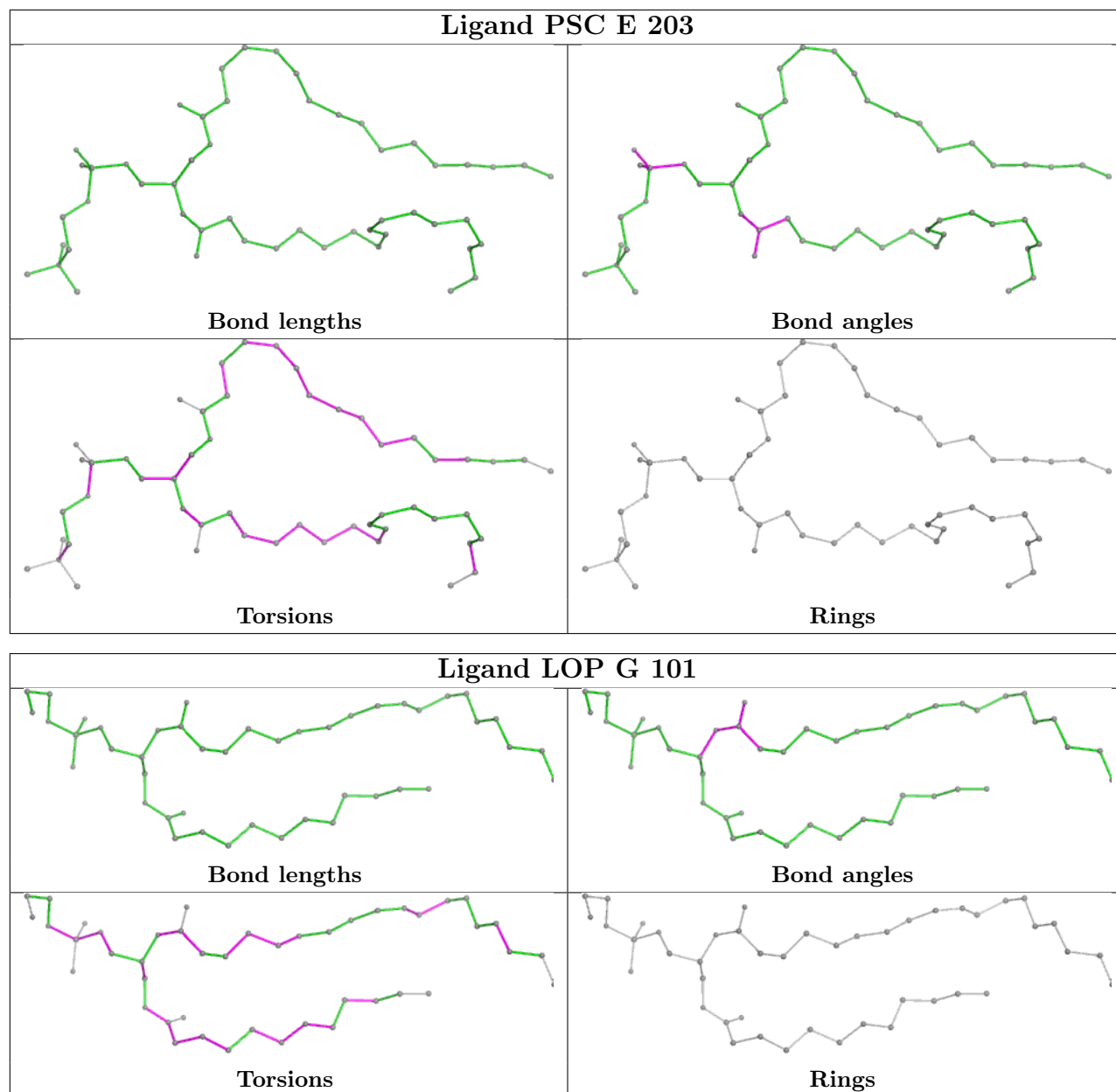
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

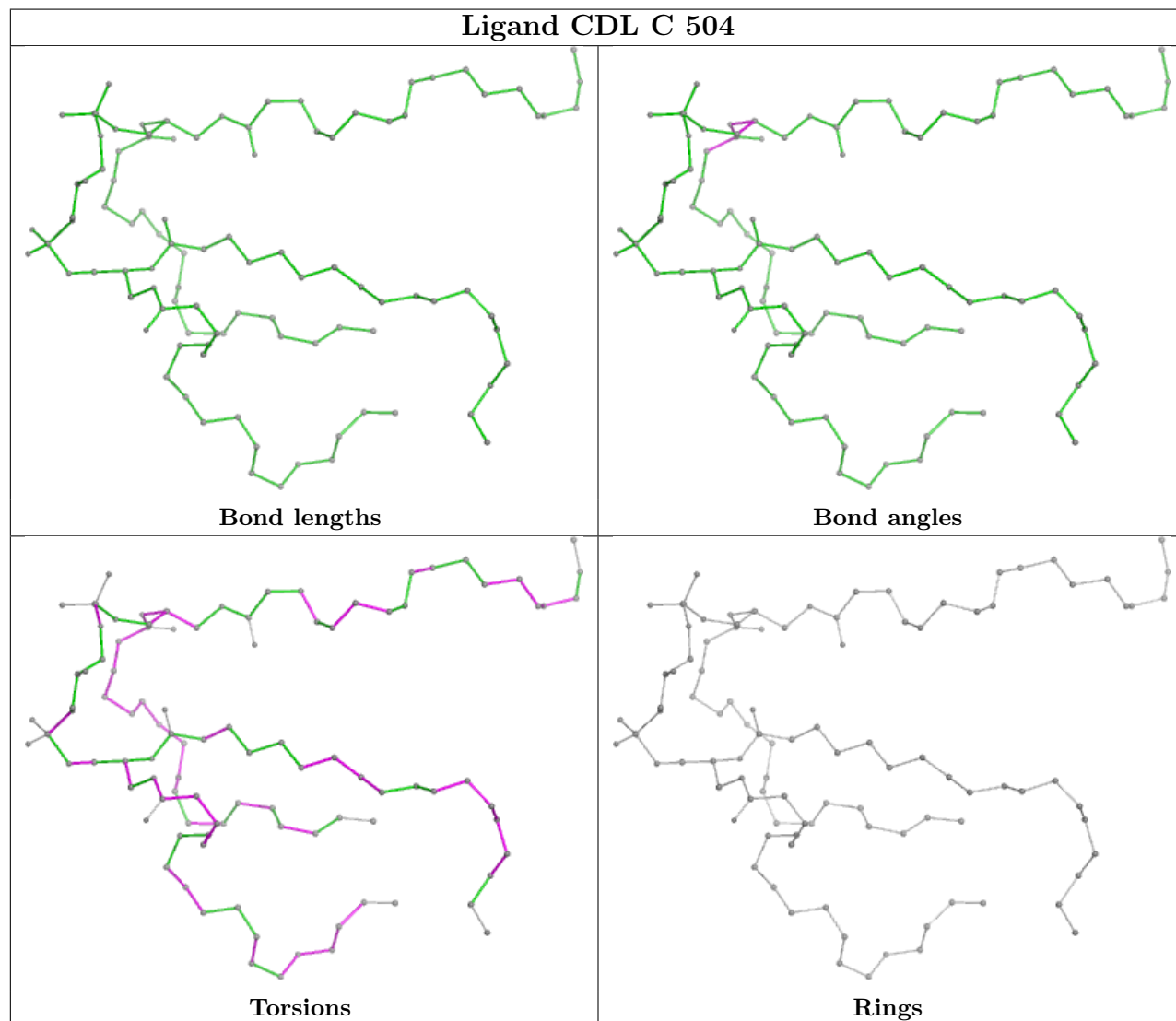
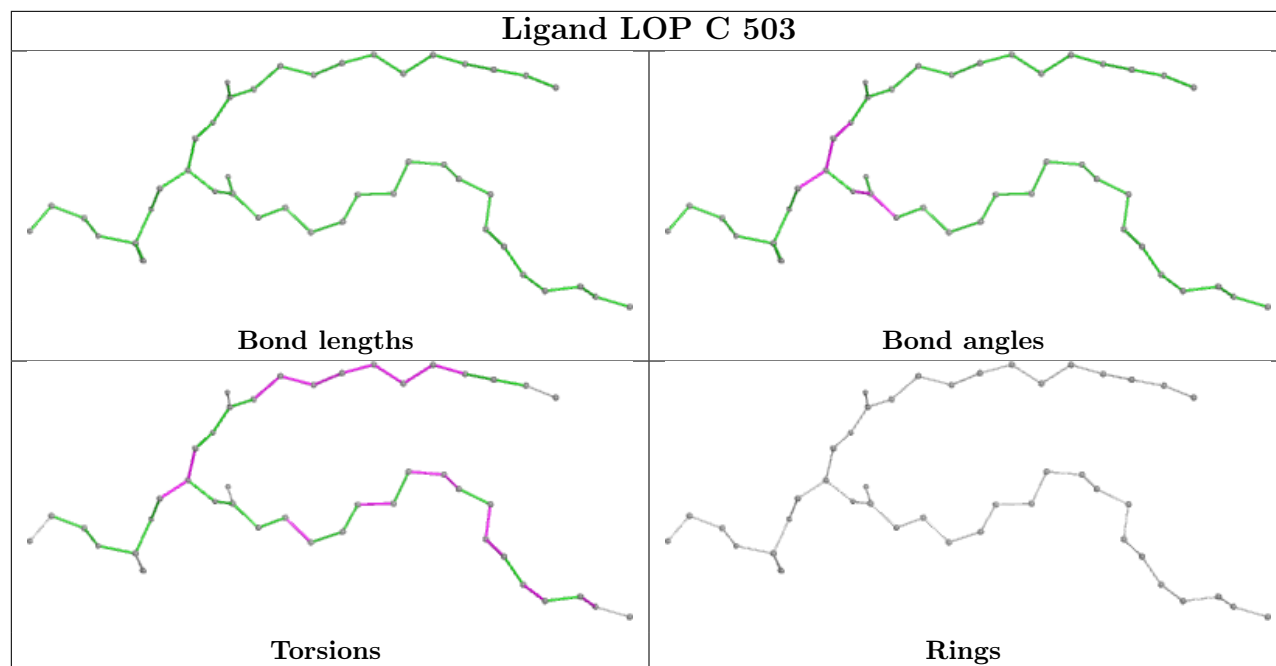


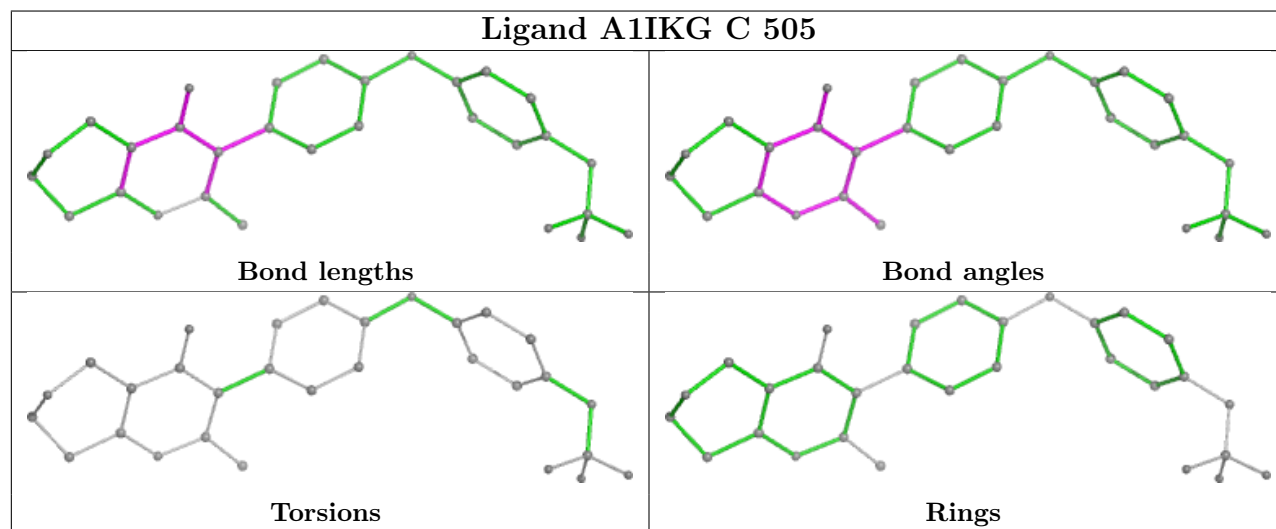
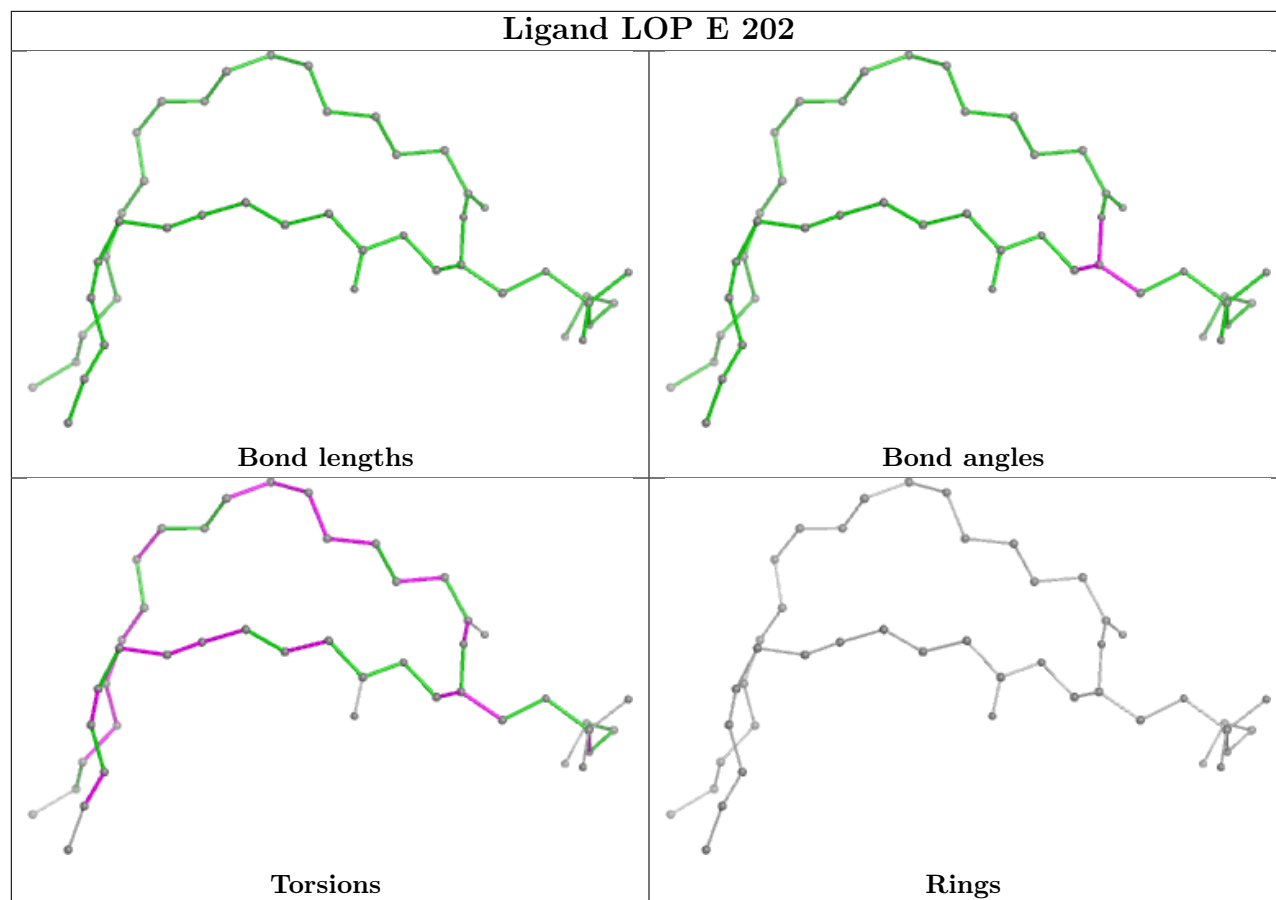


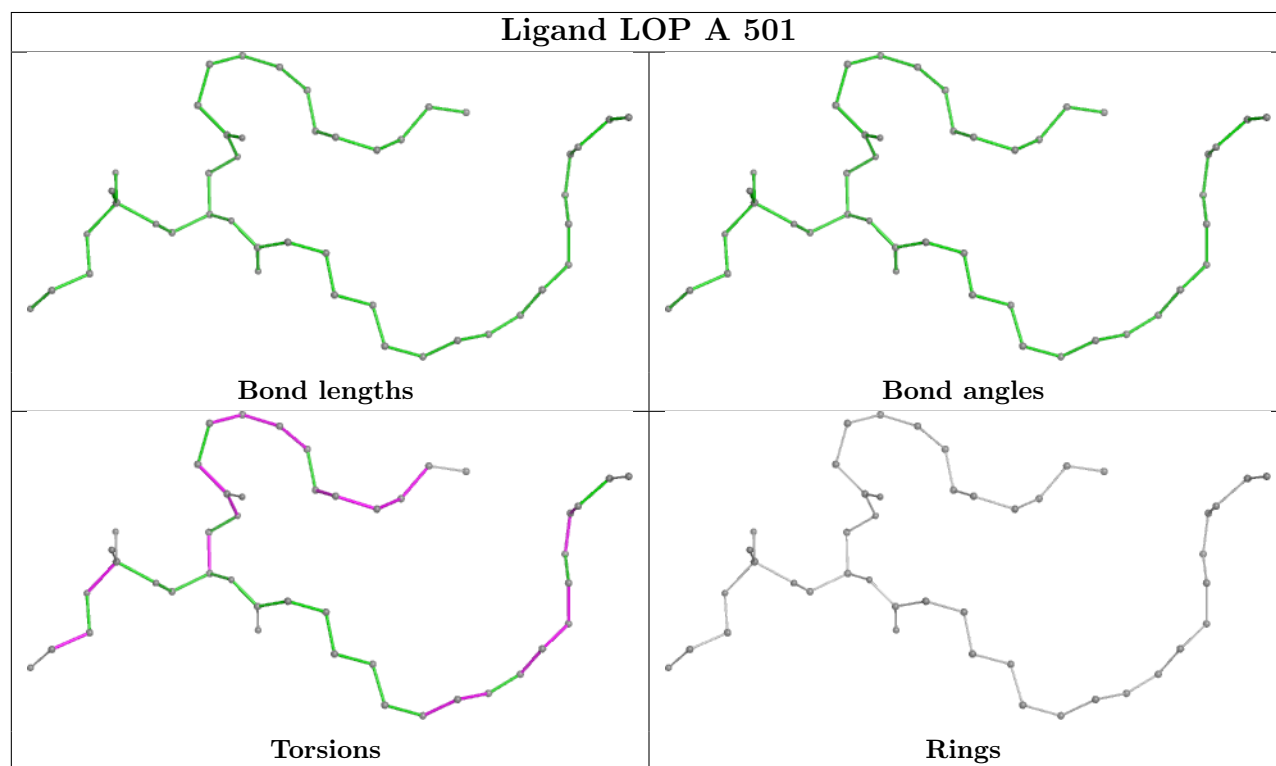
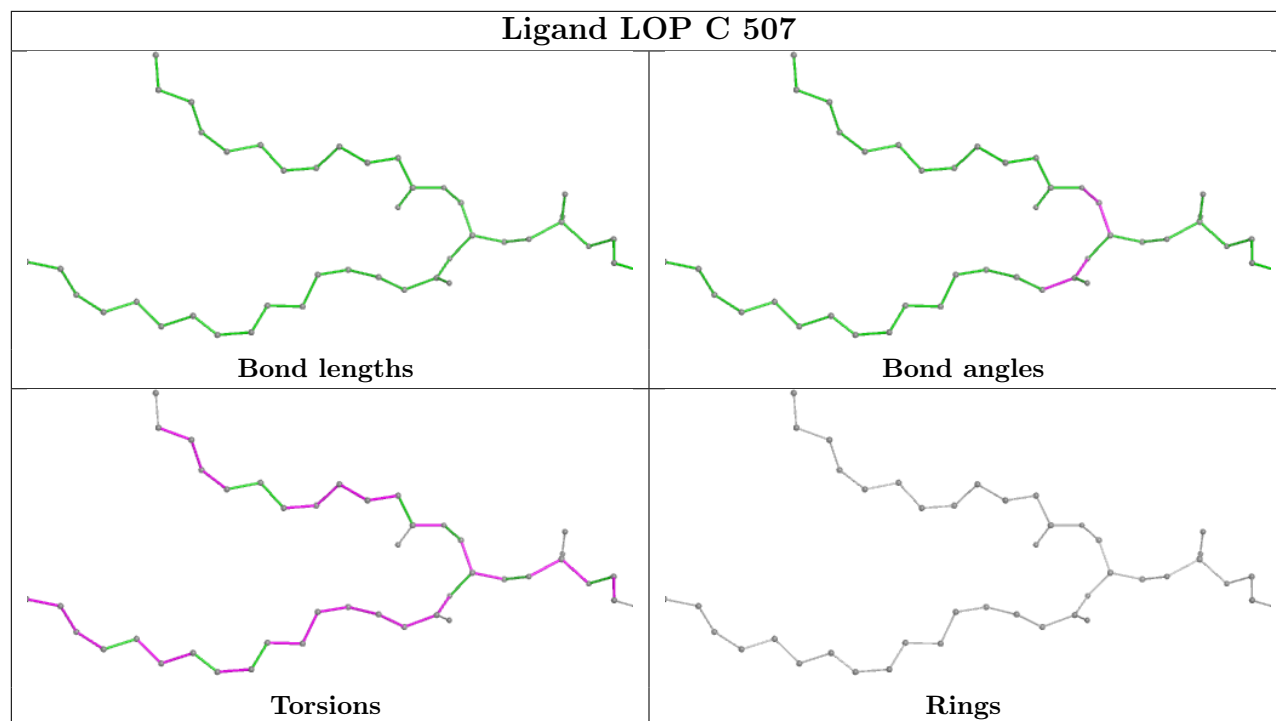


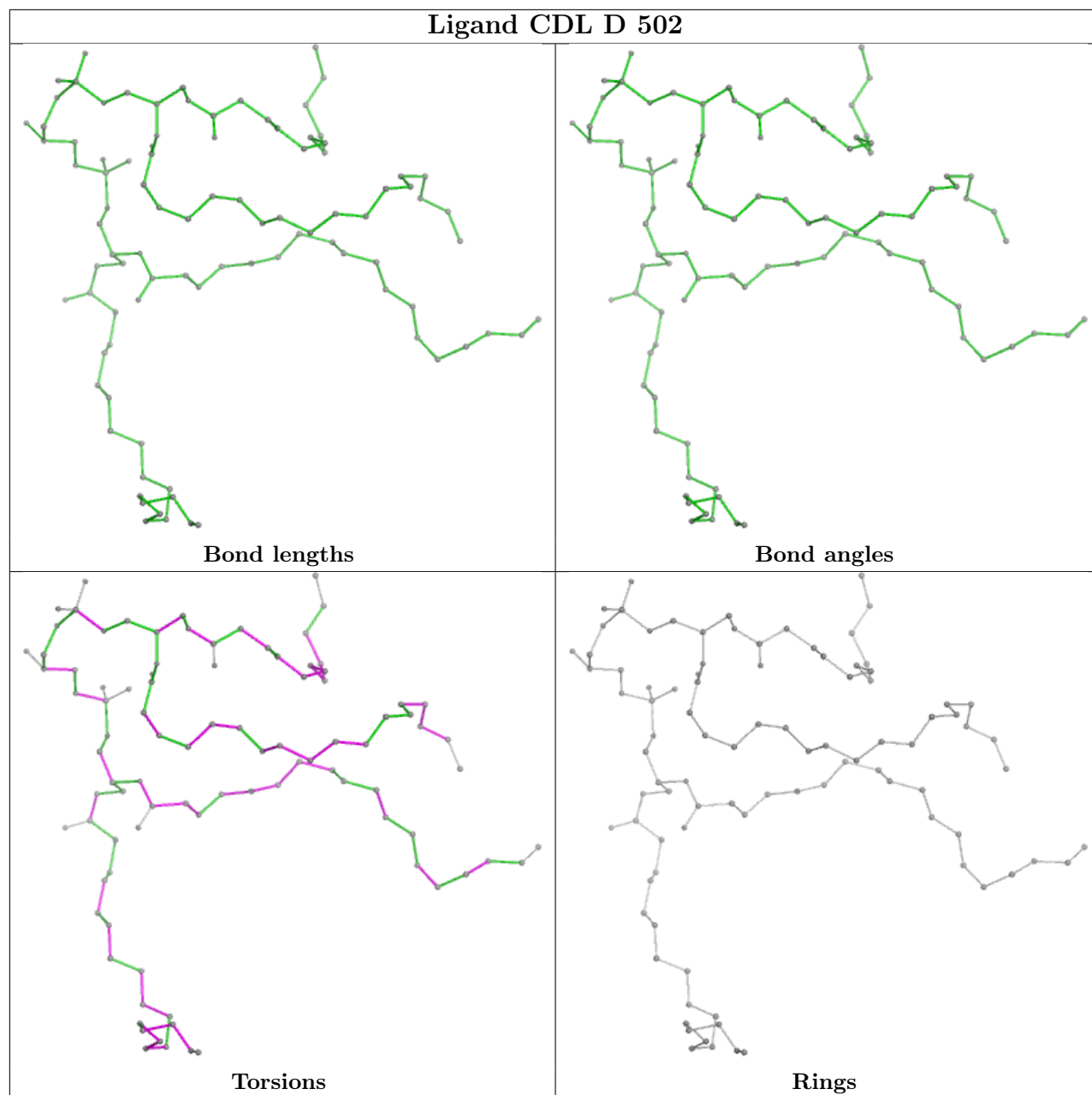


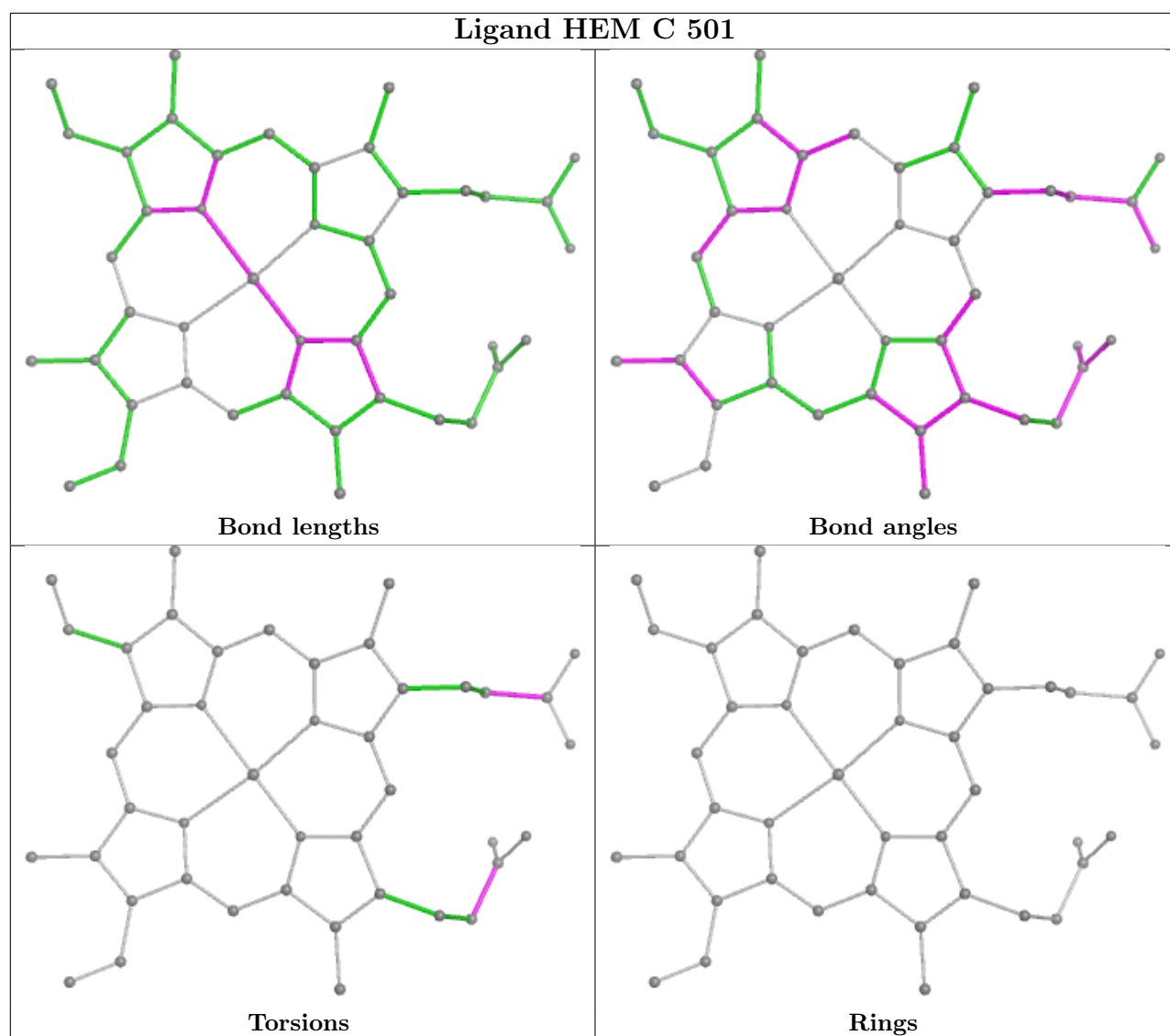












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	440/480 (91%)	-0.94	0 100 100	70, 111, 146, 195	0
2	B	414/453 (91%)	-0.86	1 (0%) 92 86	47, 112, 148, 230	1 (0%)
3	C	378/379 (99%)	-0.80	1 (0%) 90 82	28, 104, 140, 195	3 (0%)
4	D	240/325 (73%)	-0.69	0 100 100	91, 140, 171, 199	0
5	E	196/274 (71%)	-0.48	2 (1%) 79 60	88, 156, 199, 240	0
5	I	27/274 (9%)	0.16	2 (7%) 22 16	101, 143, 177, 188	0
6	F	98/111 (88%)	-0.72	0 100 100	82, 107, 149, 167	0
7	G	74/82 (90%)	-0.78	0 100 100	80, 115, 155, 176	0
8	H	65/109 (59%)	-0.52	0 100 100	126, 164, 182, 200	0
9	J	56/64 (87%)	-0.76	0 100 100	101, 121, 149, 167	0
10	K	39/56 (69%)	0.45	2 (5%) 34 24	152, 185, 233, 265	0
All	All	2027/2607 (77%)	-0.75	8 (0%) 89 79	28, 116, 177, 265	4 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	230	LEU	4.0
5	E	114	VAL	2.9
3	C	237	LEU	2.6
5	E	178	LEU	2.5
10	K	13	LEU	2.4
5	I	70	LEU	2.4
5	I	71	ASN	2.3
10	K	48	ILE	2.1

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](#)

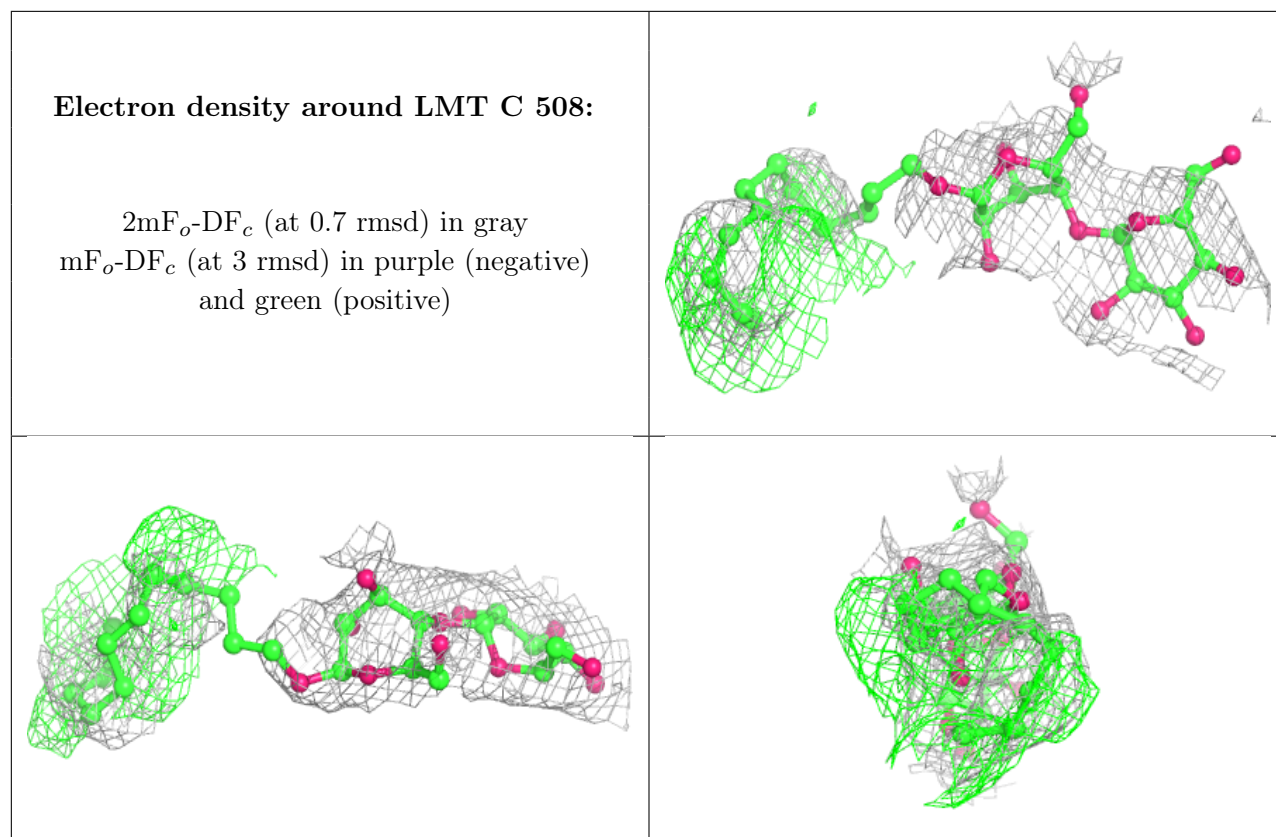
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

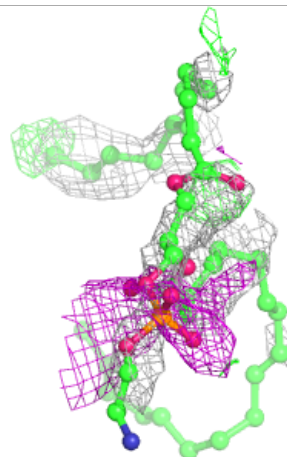
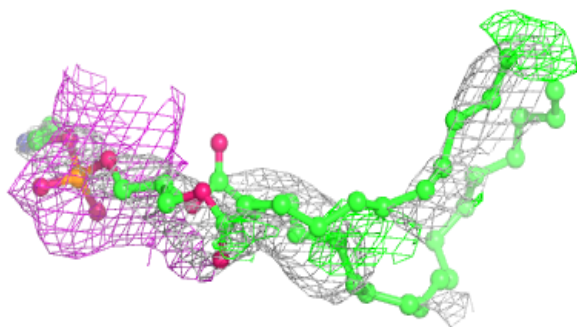
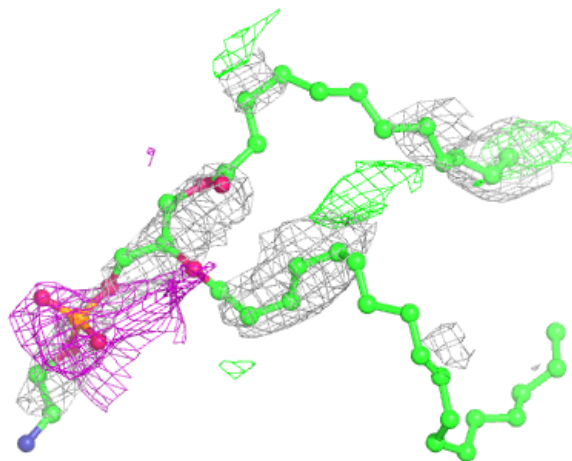
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	LMT	C	508	35/35	0.55	0.15	127,200,240,296	0
11	LOP	C	506	45/45	0.77	0.27	66,143,208,276	0
19	SO4	G	102	5/5	0.77	0.07	160,182,202,241	0
19	SO4	F	201	5/5	0.85	0.16	145,161,171,183	0
11	LOP	G	101	45/45	0.86	0.23	105,180,215,234	0
19	SO4	G	103	5/5	0.88	0.09	139,145,164,170	0
11	LOP	C	507	45/45	0.90	0.20	76,140,205,246	0
11	LOP	A	501	45/45	0.90	0.18	81,186,233,251	0
12	CDL	A	502	84/100	0.91	0.15	109,172,285,348	0
12	CDL	D	502	94/100	0.91	0.16	88,156,187,215	0
18	PSC	E	203	52/52	0.92	0.17	99,147,207,260	0
14	A1IKG	C	505	30/30	0.93	0.12	98,134,186,196	0
12	CDL	C	504	100/100	0.93	0.14	94,149,200,240	0
11	LOP	E	202	45/45	0.96	0.11	93,113,175,262	0
11	LOP	C	503	45/45	0.98	0.09	80,106,125,172	0
17	FES	E	201	4/4	0.98	0.06	220,233,252,274	0
16	HEC	D	501	43/43	0.99	0.07	116,138,150,162	0
13	HEM	C	501	43/43	0.99	0.05	86,94,105,128	0
13	HEM	C	502	43/43	0.99	0.06	62,96,111,124	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.



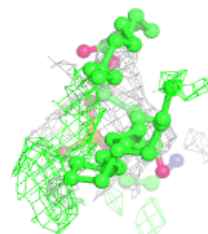
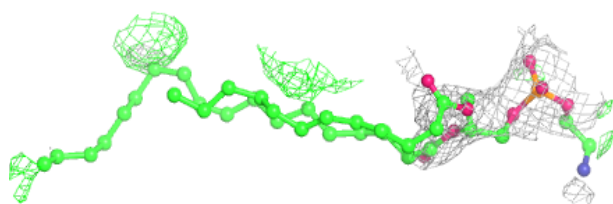
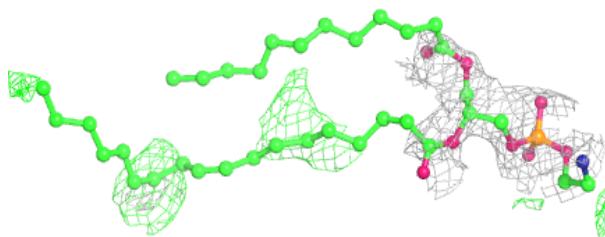
Electron density around LOP C 506:

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

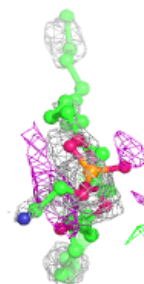
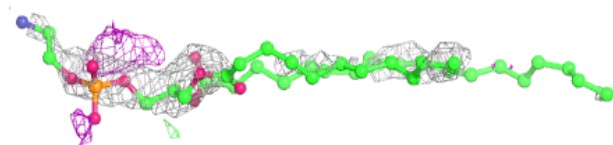
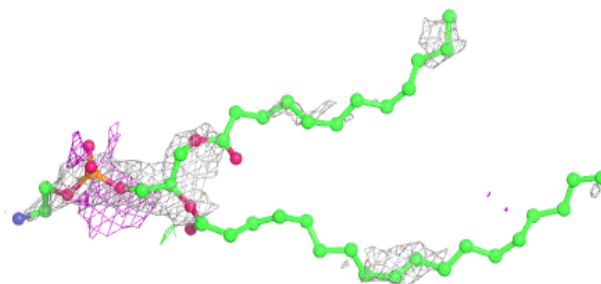


Electron density around LOP G 101:

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

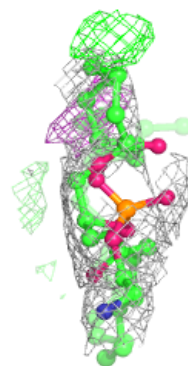
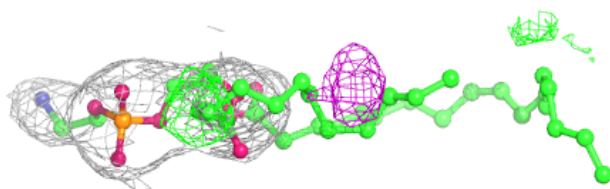
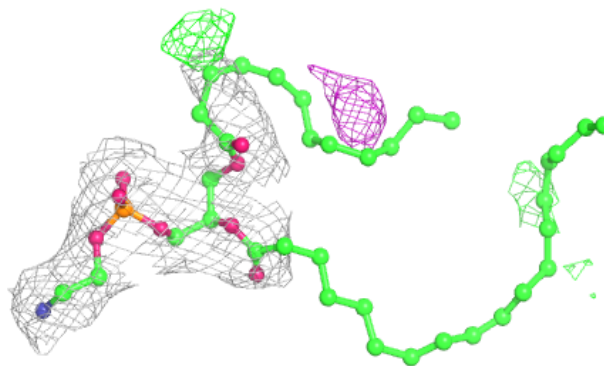
**Electron density around LOP C 507:**

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

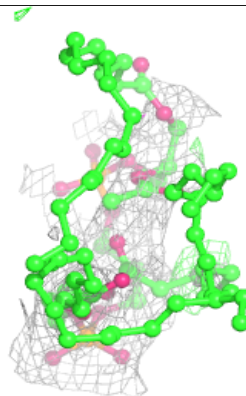
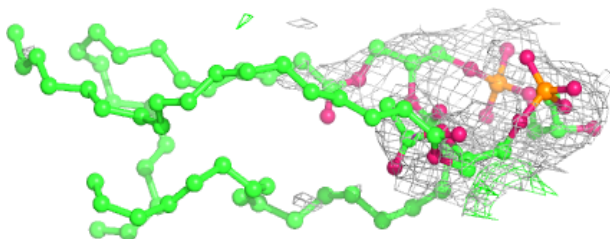
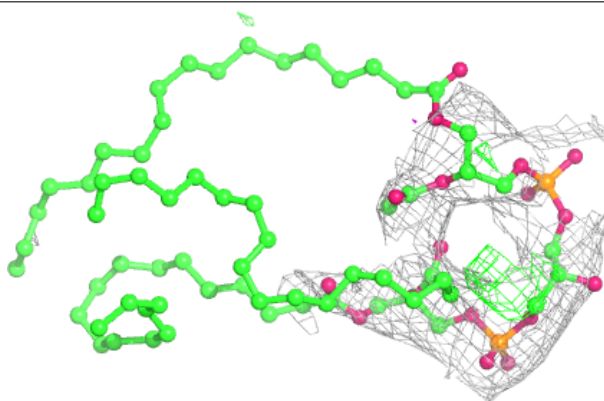


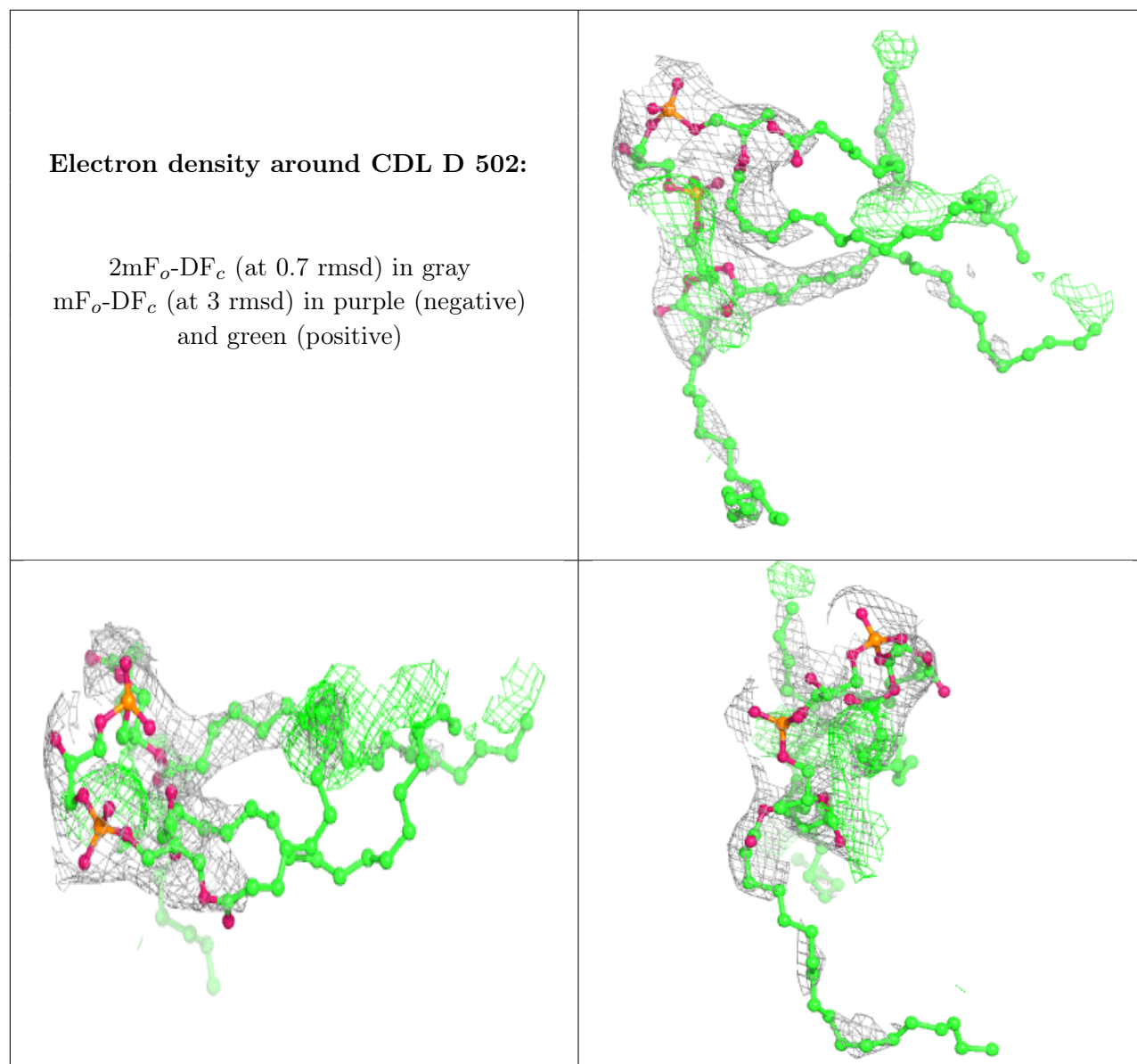
Electron density around LOP A 501:

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

**Electron density around CDL A 502:**

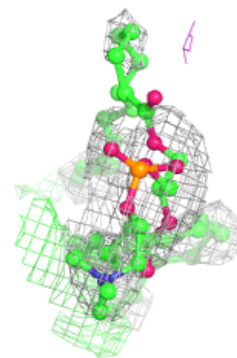
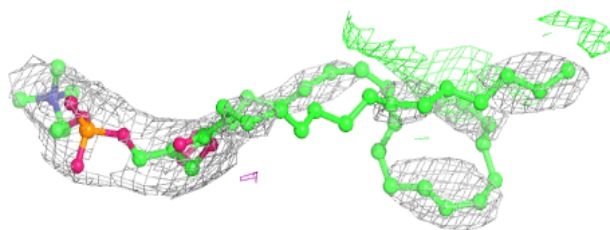
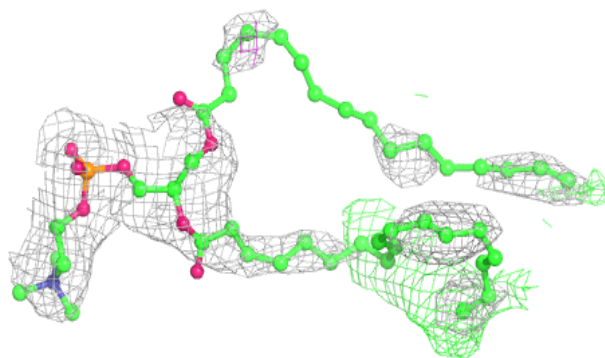
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



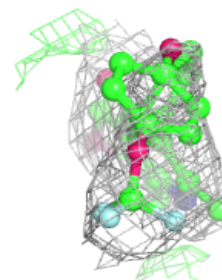
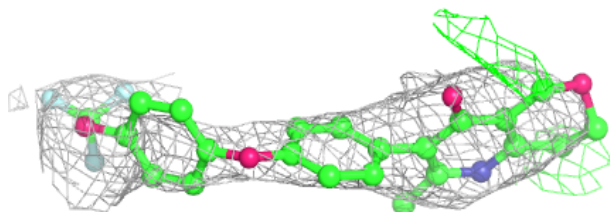
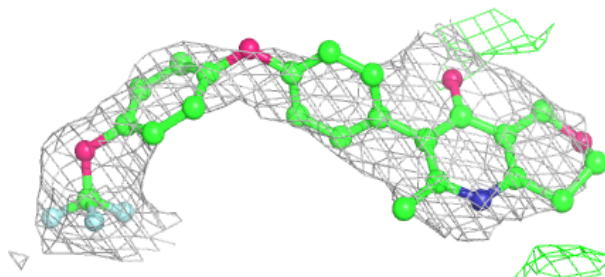


Electron density around PSC E 203:

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

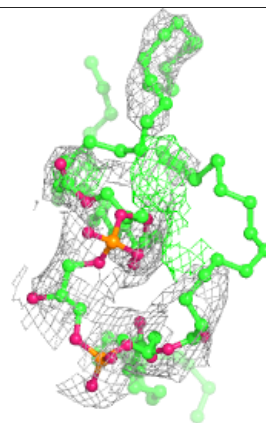
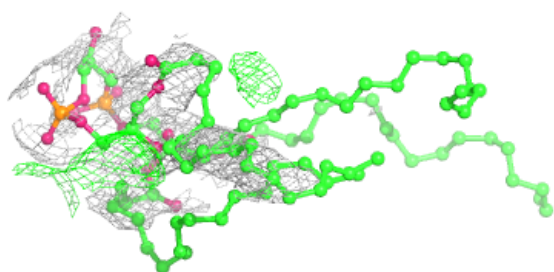
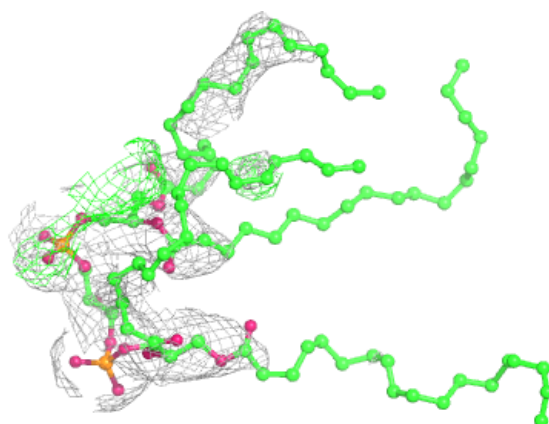
**Electron density around A1IKG C 505:**

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

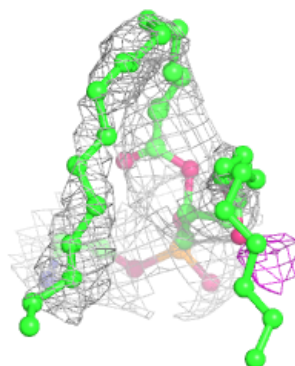
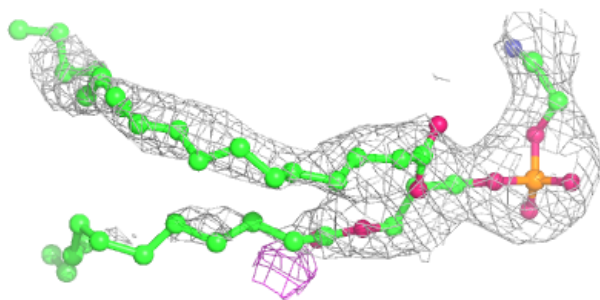
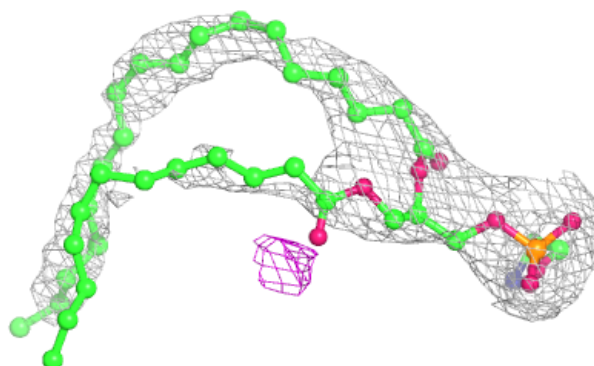


Electron density around CDL C 504:

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

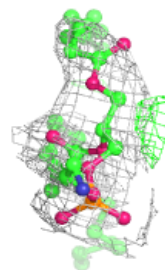
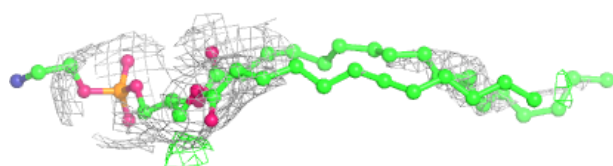
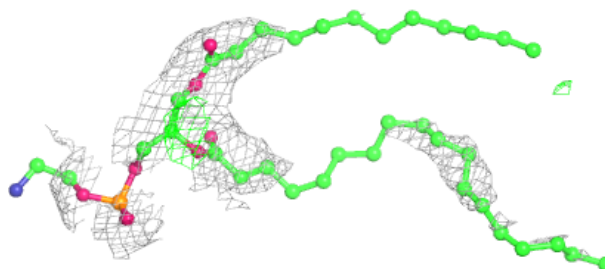
**Electron density around LOP E 202:**

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

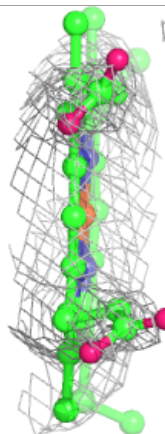
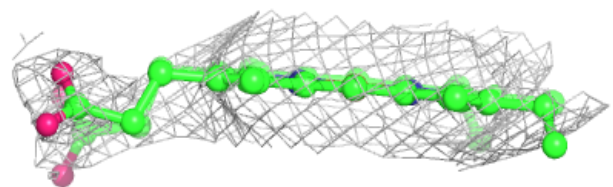
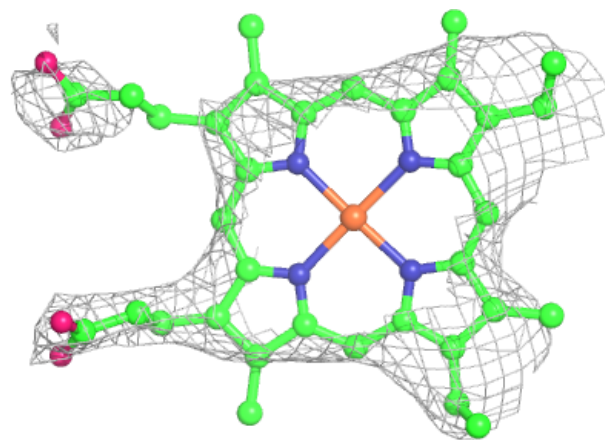


Electron density around LOP C 503:

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

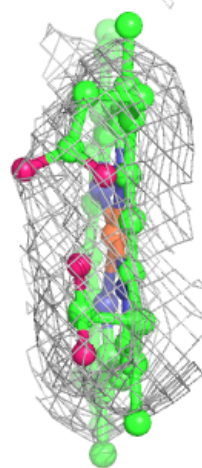
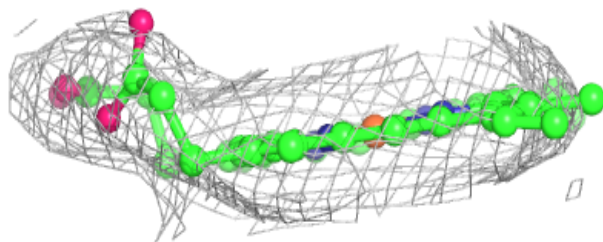
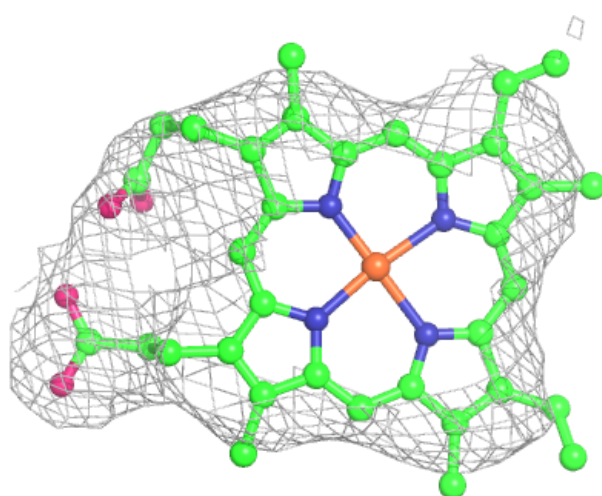
**Electron density around HEC D 501:**

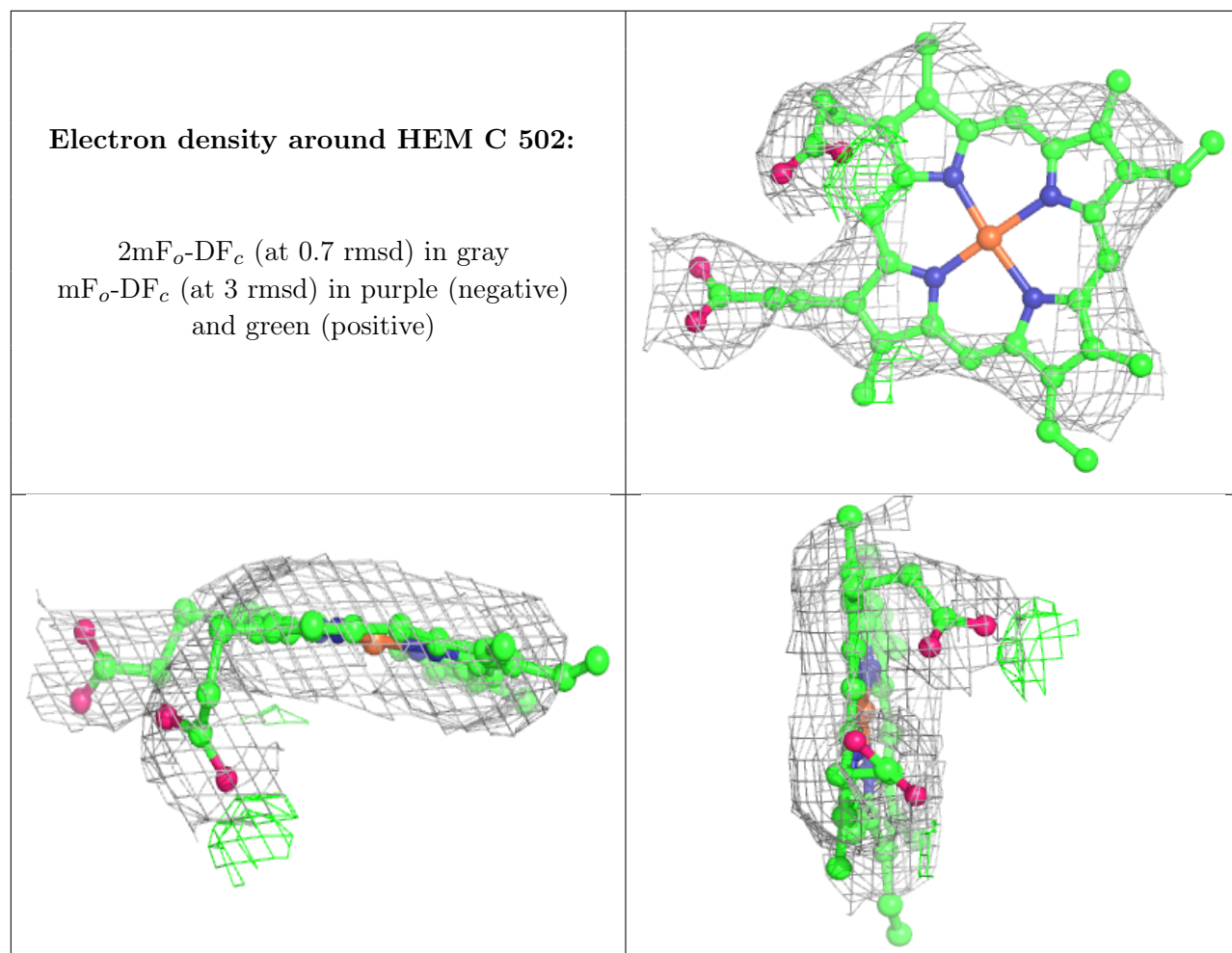
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM 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)





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

There are no such residues in this entry.