



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:05 PM UTC

PDB ID : 3S8F / pdb_00003s8f
Title : 1.8 Å structure of ba3 cytochrome c oxidase from *Thermus thermophilus* in lipid environment
Authors : Tiefenbrunn, T.; Liu, W.; Chen, Y.; Katritch, V.; Stout, C.D.; Fee, J.A.; Cherezov, V.
Deposited on : 2011-05-27
Resolution : 1.80 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

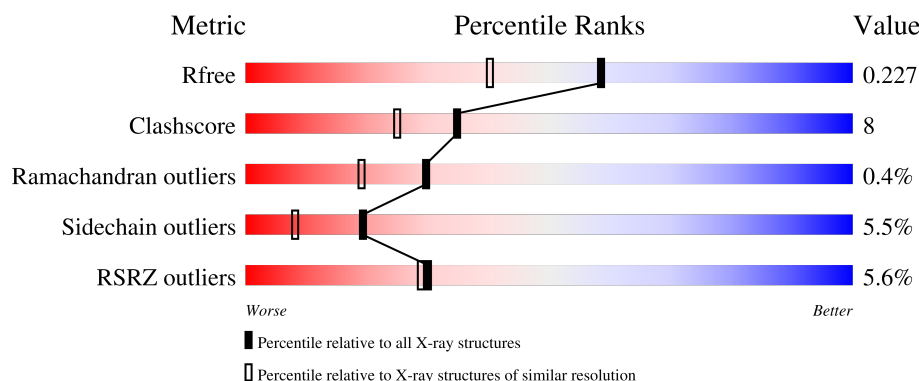
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	569	
2	B	168	
3	C	34	

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
6	HAS	A	801	X	-	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 6567 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 c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	5	0
			4389	2979	699	695	16			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	expression tag	UNP Q5SJ79
A	-5	HIS	-	expression tag	UNP Q5SJ79
A	-4	HIS	-	expression tag	UNP Q5SJ79
A	-3	HIS	-	expression tag	UNP Q5SJ79
A	-2	HIS	-	expression tag	UNP Q5SJ79
A	-1	HIS	-	expression tag	UNP Q5SJ79
A	0	HIS	-	expression tag	UNP Q5SJ79
A	1	HIS	-	expression tag	UNP Q5SJ79

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	166	Total	C	N	O	S	0	1	0
			1288	837	214	233	4			

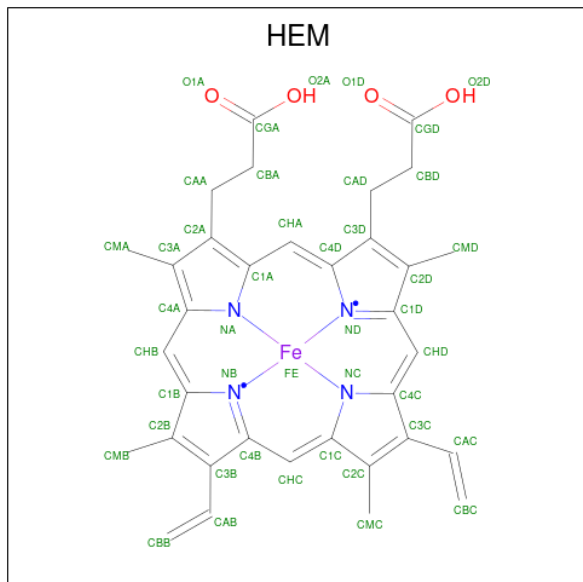
- Molecule 3 is a protein called Cytochrome c oxidase polypeptide 2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	31	Total	C	N	O	0	0	0
			241	169	37	35			

- Molecule 4 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

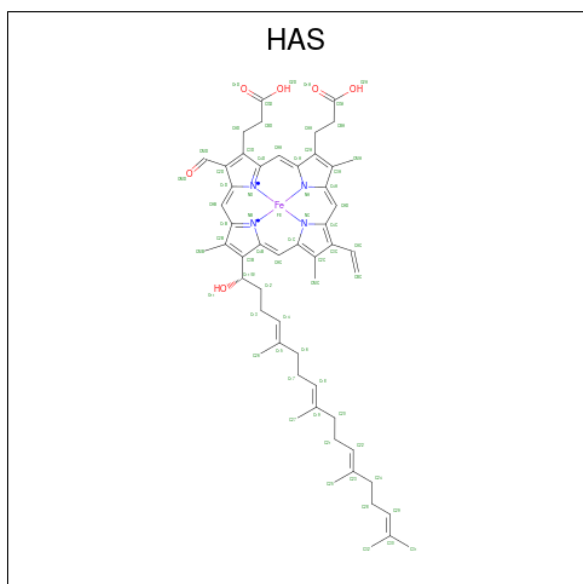
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



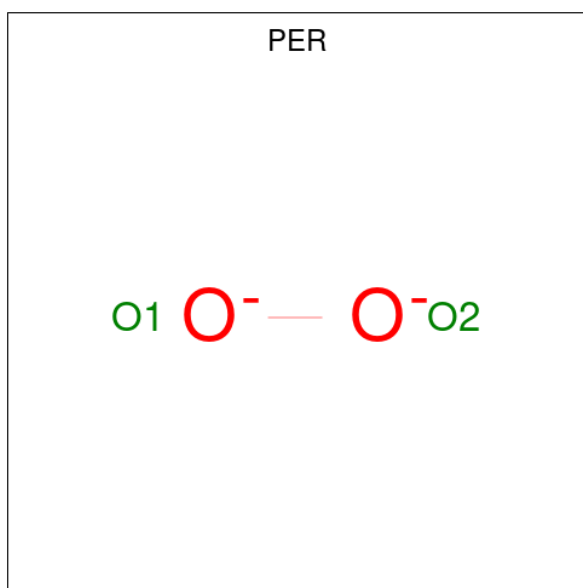
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 6 is HEME-AS (CCD ID: HAS) (formula: $C_{54}H_{64}FeN_4O_6$).



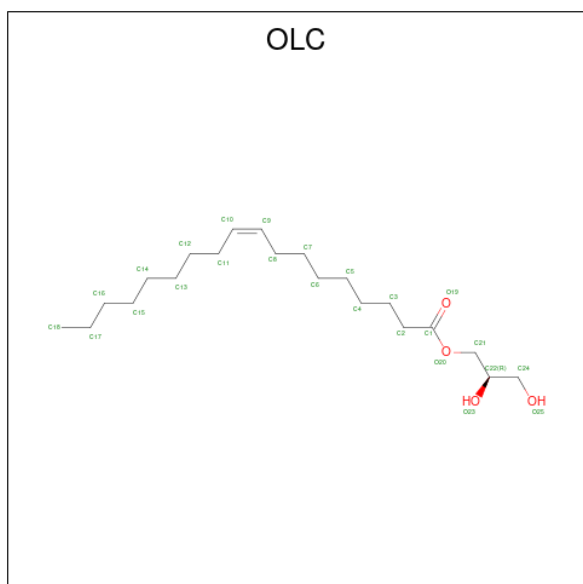
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	O	
			65	54	1	4	6	

- Molecule 7 is PEROXIDE ION (CCD ID: PER) (formula: O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O 2 2	0	0

- Molecule 8 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: $C_{21}H_{40}O_4$).



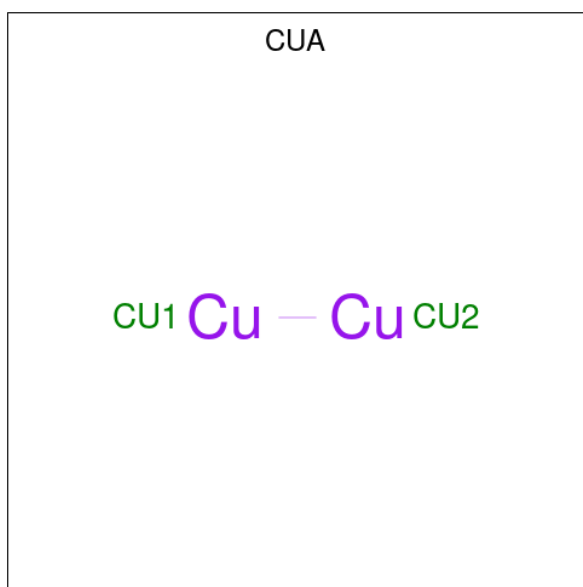
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			25	21	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			25	21	4		
8	A	1	Total	C	O	0	0
			23	19	4		
8	A	1	Total	C	O	0	0
			18	14	4		
8	A	1	Total	C	O	0	0
			17	13	4		
8	A	1	Total	C	O	0	0
			8	4	4		
8	A	1	Total	C	O	0	0
			15	11	4		
8	A	1	Total	C	O	0	0
			20	16	4		
8	A	1	Total	C	O	0	0
			25	21	4		
8	A	1	Total	C	O	0	0
			21	17	4		
8	A	1	Total	C	O	0	0
			25	21	4		
8	B	1	Total	C	O	0	0
			25	21	4		
8	B	1	Total	C	O	0	0
			25	21	4		
8	B	1	Total	C	O	0	0
			25	21	4		
8	B	1	Total	C	O	0	0
			21	19	2		
8	C	1	Total	C	O	0	0
			25	21	4		

- Molecule 9 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Cu 2 2	0	0

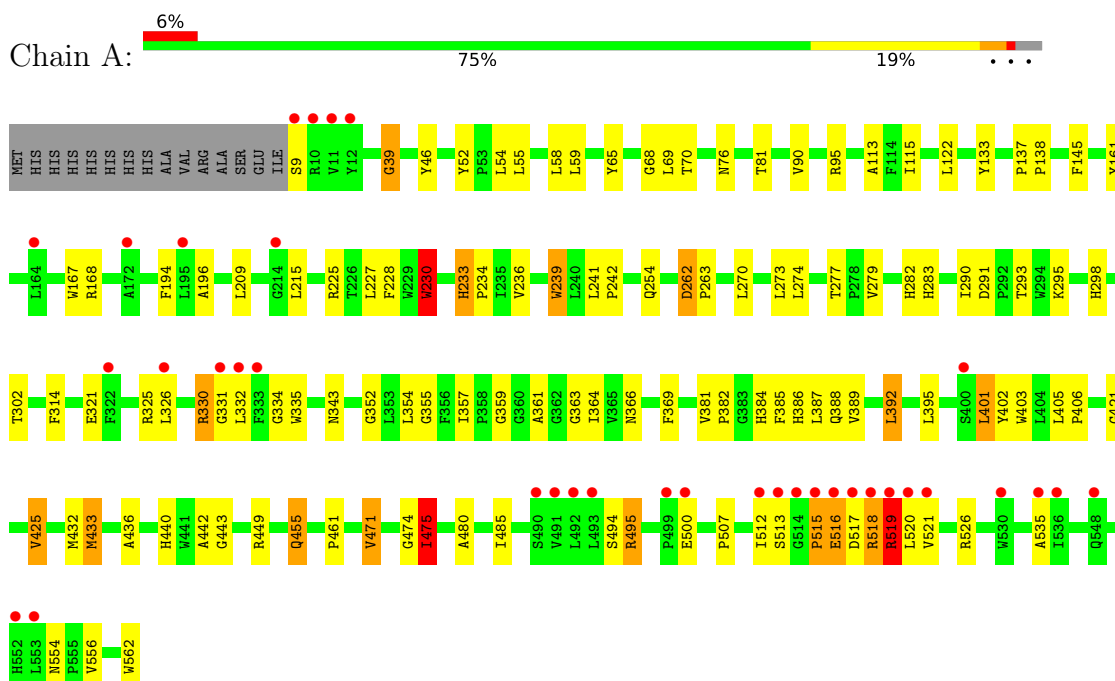
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	117	Total O 117 117	0	0
10	B	71	Total O 71 71	0	0
10	C	5	Total O 5 5	0	0

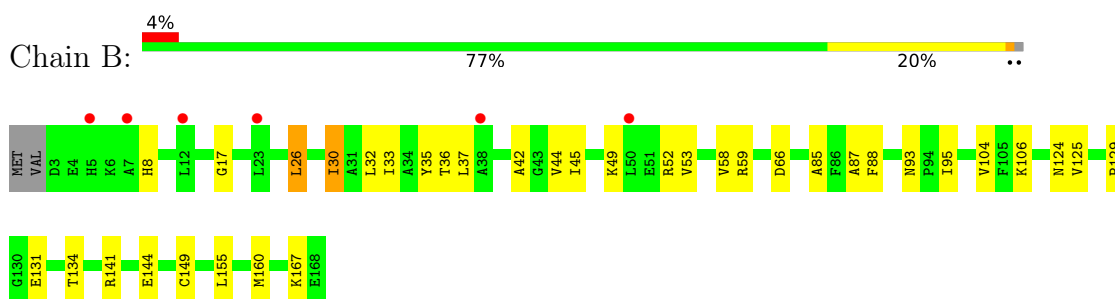
3 Residue-property plots

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.

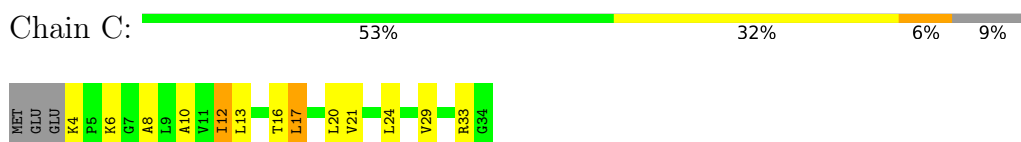
• Molecule 1: Cytochrome c oxidase subunit 1



• Molecule 2: Cytochrome c oxidase subunit 2



• Molecule 3: Cytochrome c oxidase polypeptide 2A



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.59Å 97.82Å 94.95Å 90.00° 128.30° 90.00°	Depositor
Resolution (Å)	37.26 – 1.80 37.26 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.2 (37.26-1.80) 97.2 (37.26-1.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 1.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.184 , 0.215 0.198 , 0.227	Depositor DCC
R_{free} test set	4656 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	27.5	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6567	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.08% 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: OLC, PER, CU, CUA, HEM, HAS

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	1.72	46/4562 (1.0%)	1.33	31/6263 (0.5%)
2	B	1.74	16/1330 (1.2%)	1.30	3/1817 (0.2%)
3	C	1.73	3/247 (1.2%)	1.35	1/335 (0.3%)
All	All	1.72	65/6139 (1.1%)	1.33	35/8415 (0.4%)

All (65) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	381	VAL	CA-CB	11.61	1.60	1.54
3	C	8	ALA	CA-CB	-8.34	1.40	1.53
1	A	352	GLY	CA-C	8.07	1.61	1.52
1	A	65	TYR	CA-C	7.98	1.63	1.52
1	A	480	ALA	CA-CB	7.74	1.65	1.53
2	B	134	THR	CA-CB	7.69	1.65	1.53
1	A	364	ILE	N-CA	7.38	1.55	1.46
1	A	39	GLY	N-CA	7.38	1.54	1.44
3	C	29	VAL	CA-CB	7.10	1.62	1.54
1	A	442	ALA	CA-CB	7.04	1.64	1.53
1	A	449	ARG	CZ-NH1	6.98	1.42	1.32
2	B	85	ALA	N-CA	6.82	1.54	1.46
1	A	230	TRP	N-CA	6.82	1.54	1.46
2	B	36	THR	CA-CB	6.78	1.63	1.53
1	A	277	THR	CA-C	6.73	1.61	1.52
2	B	58	VAL	CA-C	6.71	1.61	1.52
2	B	66	ASP	N-CA	6.66	1.54	1.46
1	A	461	PRO	N-CA	6.65	1.56	1.47
1	A	386	HIS	N-CA	6.50	1.54	1.46
2	B	131	GLU	N-CA	-6.41	1.37	1.45
1	A	90	VAL	CA-CB	6.40	1.61	1.55
1	A	443	GLY	N-CA	6.39	1.53	1.45
1	A	363	GLY	CA-C	6.37	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	298	HIS	N-CA	6.36	1.54	1.46
2	B	44	VAL	N-CA	6.19	1.53	1.46
1	A	535	ALA	CA-C	6.11	1.60	1.52
1	A	228	PHE	N-CA	6.10	1.53	1.46
1	A	137	PRO	C-O	-6.10	1.19	1.25
1	A	535	ALA	CA-CB	-6.09	1.43	1.53
1	A	384	HIS	CA-CB	6.08	1.62	1.53
1	A	239	TRP	N-CA	6.03	1.53	1.46
2	B	106	LYS	CA-C	-5.95	1.45	1.53
1	A	113	ALA	CA-CB	5.93	1.62	1.53
1	A	395	LEU	N-CA	5.88	1.53	1.46
1	A	388	GLN	CA-C	5.86	1.60	1.52
1	A	440	HIS	N-CA	5.86	1.53	1.46
1	A	115	ILE	CA-CB	5.74	1.61	1.54
1	A	68	GLY	CA-C	5.70	1.58	1.52
2	B	95	ILE	N-CA	5.70	1.53	1.46
2	B	33	ILE	C-O	5.66	1.30	1.24
1	A	279	VAL	CA-C	5.65	1.59	1.52
1	A	137	PRO	CA-CB	5.65	1.59	1.53
2	B	53	VAL	CA-C	-5.58	1.46	1.52
1	A	273	LEU	CA-C	5.56	1.60	1.52
1	A	381	VAL	N-CA	-5.51	1.40	1.46
2	B	160	MET	CA-CB	5.49	1.60	1.53
1	A	194	PHE	C-O	-5.46	1.17	1.24
1	A	270	LEU	C-O	-5.46	1.17	1.24
1	A	425	VAL	N-CA	5.43	1.52	1.46
1	A	70	THR	N-CA	5.43	1.52	1.46
1	A	471	VAL	C-O	5.41	1.30	1.24
1	A	262	ASP	CA-C	5.40	1.58	1.52
1	A	421	GLY	N-CA	5.39	1.52	1.45
1	A	433	MET	N-CA	5.35	1.52	1.46
3	C	16	THR	CA-CB	5.31	1.61	1.53
2	B	30	ILE	CA-CB	-5.30	1.47	1.54
1	A	357	ILE	CA-C	5.25	1.58	1.52
1	A	361	ALA	CA-CB	5.24	1.61	1.53
2	B	125	VAL	CA-CB	5.23	1.62	1.54
2	B	124	ASN	CA-C	-5.20	1.48	1.53
1	A	209	LEU	C-O	-5.15	1.19	1.24
1	A	432	MET	N-CA	5.09	1.52	1.46
1	A	507	PRO	CA-C	5.09	1.58	1.53
2	B	149	CYS	C-O	5.04	1.30	1.24
1	A	69	LEU	CA-C	5.01	1.59	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	HIS	N-CA-CB	11.17	121.00	110.39
1	A	227	LEU	N-CA-C	-8.11	102.01	112.23
1	A	331	GLY	N-CA-C	-7.41	104.07	111.56
1	A	359	GLY	N-CA-C	-7.37	103.95	112.50
1	A	270	LEU	N-CA-C	-7.23	103.48	111.36
1	A	474	GLY	N-CA-C	-7.05	103.74	112.77
1	A	475	ILE	CB-CG1-CD1	-6.62	99.90	113.80
1	A	425	VAL	N-CA-CB	-6.43	100.93	110.58
1	A	389	VAL	N-CA-C	-6.09	106.57	111.81
2	B	59	ARG	NE-CZ-NH1	-6.08	115.42	121.50
1	A	352	GLY	N-CA-C	-6.04	105.49	112.73
1	A	233	HIS	CA-CB-CG	-5.92	107.88	113.80
1	A	515	PRO	N-CA-C	5.85	124.52	112.47
1	A	302	THR	N-CA-C	-5.79	104.57	111.69
1	A	52	TYR	CA-CB-CG	-5.77	103.51	113.90
1	A	314	PHE	N-CA-C	5.72	117.59	111.36
1	A	425	VAL	CG1-CB-CG2	5.68	123.30	110.80
1	A	425	VAL	CA-CB-CG1	5.63	119.98	110.40
1	A	145	PHE	N-CA-C	-5.59	105.10	111.14
1	A	137	PRO	CB-CA-C	-5.57	106.15	111.39
1	A	95	ARG	NE-CZ-NH2	5.53	124.18	119.20
1	A	436	ALA	N-CA-C	-5.53	105.15	111.07
3	C	10	ALA	N-CA-C	-5.30	105.41	111.14
1	A	392[A]	LEU	N-CA-C	5.27	116.71	111.07
1	A	392[B]	LEU	N-CA-C	5.27	116.71	111.07
1	A	355	GLY	N-CA-C	-5.25	107.80	114.16
1	A	46	TYR	CA-CB-CG	-5.23	104.48	113.90
2	B	149	CYS	CA-CB-SG	-5.18	102.48	114.40
1	A	421	GLY	N-CA-C	-5.14	106.20	112.77
1	A	521	VAL	N-CA-C	5.13	115.74	110.36
2	B	104	VAL	N-CA-C	-5.13	99.78	107.37
1	A	556	VAL	CA-C-N	5.11	125.01	119.85
1	A	556	VAL	C-N-CA	5.11	125.01	119.85
1	A	485	ILE	N-CA-C	-5.08	105.54	110.42
1	A	401	LEU	N-CA-C	-5.03	105.93	111.71

There are no chirality outliers.

There are no planarity outliers.

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	4389	0	4484	59	0
2	B	1288	0	1260	20	0
3	C	241	0	267	7	0
4	A	1	0	0	0	0
5	A	43	0	30	3	0
6	A	65	0	62	3	0
7	A	2	0	0	1	0
8	A	222	0	320	21	0
8	B	96	0	153	16	0
8	C	25	0	40	1	0
9	B	2	0	0	0	0
10	A	117	0	0	5	0
10	B	71	0	0	1	1
10	C	5	0	0	0	0
All	All	6567	0	6616	98	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 8.

All (98) 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)
7:A:563:PER:O1	7:A:563:PER:O2	1.54	1.23
1:A:330[B]:ARG:HH11	1:A:330[B]:ARG:CG	1.49	1.21
1:A:330[B]:ARG:HG2	1:A:330[B]:ARG:NH1	1.41	1.13
1:A:516[A]:GLU:HG3	1:A:517:ASP:H	1.08	1.12
1:A:516[A]:GLU:HG3	1:A:517:ASP:N	1.55	1.11
2:B:141:ARG:HH12	8:B:170:OLC:H24A	1.28	0.98
1:A:263:PRO:HG2	1:A:516[A]:GLU:HG2	1.42	0.98
1:A:554:ASN:HB2	2:B:52:ARG:HD2	1.45	0.96
2:B:141:ARG:NH1	8:B:170:OLC:H24A	1.82	0.94
1:A:495:ARG:HH21	1:A:495:ARG:HA	1.32	0.94
8:A:565:OLC:H12	8:A:572:OLC:H14A	1.48	0.92
1:A:516[A]:GLU:CG	1:A:517:ASP:H	1.86	0.89
1:A:168:ARG:HH22	8:A:570:OLC:C6	1.90	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:ARG:O	1:A:519:ARG:HB3	1.82	0.79
2:B:141:ARG:HH12	8:B:170:OLC:C24	1.96	0.78
1:A:330[B]:ARG:CG	1:A:330[B]:ARG:NH1	2.20	0.78
2:B:35:TYR:OH	8:B:169:OLC:H24A	1.84	0.76
2:B:93:ASN:O	10:B:201:HOH:O	2.06	0.74
1:A:168:ARG:HH22	8:A:570:OLC:H6A	1.54	0.71
1:A:495:ARG:HA	1:A:495:ARG:NH2	2.07	0.69
8:B:170:OLC:H6	3:C:33:ARG:HE	1.59	0.67
8:A:565:OLC:C12	8:A:572:OLC:H14A	2.22	0.65
2:B:17:GLY:HA3	8:B:171:OLC:H3	1.79	0.64
1:A:330[B]:ARG:HH11	1:A:330[B]:ARG:HG2	0.59	0.63
8:A:569:OLC:O19	8:A:570:OLC:C8	2.48	0.62
1:A:168:ARG:HH22	8:A:570:OLC:H6	1.62	0.61
1:A:518:ARG:O	1:A:519:ARG:CB	2.49	0.61
1:A:321:GLU:HA	1:A:335:TRP:CE3	2.36	0.60
1:A:282:HIS:CD2	1:A:283:HIS:CD2	2.88	0.60
8:A:564:OLC:O25	8:B:170:OLC:H7A	2.03	0.58
8:B:170:OLC:H4	3:C:33:ARG:HG2	1.86	0.57
8:A:572:OLC:C8	8:A:572:OLC:H13A	2.36	0.56
1:A:161:TYR:CE2	8:A:569:OLC:H21	2.42	0.55
2:B:32:LEU:HD21	8:B:169:OLC:H7A	1.90	0.54
1:A:39:GLY:C	5:A:800:HEM:HMB3	2.33	0.53
2:B:141:ARG:HH12	8:B:170:OLC:C22	2.21	0.52
3:C:21:VAL:HG11	8:C:35:OLC:H9	1.90	0.52
2:B:141:ARG:NH1	8:B:170:OLC:C24	2.62	0.52
1:A:475:ILE:CG1	8:A:565:OLC:H13A	2.41	0.50
1:A:516[B]:GLU:OE1	1:A:517:ASP:N	2.44	0.50
10:A:583:HOH:O	8:B:170:OLC:H4A	2.10	0.50
1:A:241:LEU:N	1:A:242:PRO:CD	2.75	0.50
1:A:233:HIS:O	1:A:236:VAL:HG22	2.12	0.49
10:A:592:HOH:O	2:B:8:HIS:HE1	1.96	0.48
1:A:290:ILE:HB	1:A:295:LYS:HE3	1.95	0.48
1:A:168:ARG:HH11	8:A:569:OLC:C22	2.27	0.47
2:B:52:ARG:HG3	2:B:52:ARG:HH11	1.80	0.47
2:B:32:LEU:CD2	8:B:169:OLC:H7A	2.45	0.47
3:C:4:LYS:HG3	3:C:6:LYS:HG2	1.96	0.46
8:A:566:OLC:H13A	8:A:572:OLC:H12	1.97	0.46
8:A:572:OLC:H13A	8:A:572:OLC:H8A	1.97	0.46
3:C:12:ILE:C	3:C:12:ILE:HD12	2.40	0.46
1:A:168:ARG:HD2	8:A:569:OLC:O23	2.15	0.46
1:A:138:PRO:HG2	2:B:129:PRO:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ARG:HG3	10:A:609:HOH:O	2.16	0.45
1:A:526:ARG:NH2	10:A:658:HOH:O	2.42	0.45
1:A:455:GLN:NE2	10:A:580:HOH:O	2.50	0.45
1:A:167:TRP:CH2	8:A:570:OLC:H22	2.51	0.45
3:C:13:LEU:HD13	3:C:17:LEU:HD22	1.98	0.45
2:B:35:TYR:HE2	8:B:169:OLC:H21A	1.82	0.44
2:B:26:LEU:O	2:B:30:ILE:HG13	2.16	0.44
1:A:230:TRP:C	1:A:230:TRP:CD1	2.95	0.44
1:A:233:HIS:CD2	1:A:233:HIS:C	2.96	0.44
2:B:141:ARG:HH12	8:B:170:OLC:H22	1.82	0.44
8:B:172:OLC:H14A	8:B:172:OLC:H11A	1.90	0.44
1:A:405:LEU:HB3	1:A:406:PRO:HD3	2.00	0.44
1:A:168:ARG:NH2	8:A:570:OLC:H6A	2.28	0.43
2:B:42:ALA:HB1	2:B:45:ILE:HD12	2.00	0.43
1:A:387:LEU:CD2	1:A:433:MET:HE1	2.48	0.43
1:A:562:TRP:HA	2:B:155:LEU:HG	2.01	0.43
1:A:366:ASN:HB3	6:A:801:HAS:C2D	2.48	0.43
1:A:168:ARG:NH2	8:A:570:OLC:H3A	2.34	0.43
1:A:475:ILE:HG12	8:A:565:OLC:H13A	2.00	0.43
1:A:122:LEU:HD23	1:A:122:LEU:HA	1.81	0.43
1:A:516[A]:GLU:CG	1:A:517:ASP:N	2.41	0.43
1:A:55:LEU:HD11	1:A:59:LEU:HD12	2.01	0.42
1:A:196:ALA:CB	1:A:234:PRO:HB2	2.49	0.42
1:A:236:VAL:HG12	1:A:239:TRP:CZ3	2.54	0.42
2:B:87:ALA:HA	2:B:88:PHE:HA	1.80	0.42
1:A:196:ALA:HB1	1:A:234:PRO:HB2	2.02	0.41
8:A:571:OLC:O19	8:A:572:OLC:O23	2.38	0.41
1:A:325:ARG:HH21	1:A:325:ARG:HG2	1.84	0.41
6:A:801:HAS:HAA2	6:A:801:HAS:HHA	1.81	0.41
1:A:291:ASP:OD2	1:A:293:THR:HB	2.19	0.41
1:A:254:GLN:HE22	1:A:403:TRP:CD1	2.39	0.41
5:A:800:HEM:CMC	5:A:800:HEM:HBC2	2.51	0.41
3:C:17:LEU:HD12	3:C:17:LEU:HA	1.91	0.41
1:A:471:VAL:O	1:A:475:ILE:HG23	2.20	0.41
1:A:343:ASN:OD1	1:A:402[B]:TYR:CE2	2.74	0.41
1:A:354:LEU:HD21	6:A:801:HAS:H323	2.02	0.41
1:A:76:ASN:HB3	5:A:800:HEM:CAC	2.52	0.40
8:A:566:OLC:H15	8:A:571:OLC:H12	2.01	0.40
1:A:81:THR:HB	1:A:239:TRP:CD1	2.57	0.40
8:A:574:OLC:H10	8:A:574:OLC:H13	1.57	0.40
1:A:382:PRO:HA	1:A:385:PHE:CE2	2.56	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)
10:B:175:HOH:O	10:B:201:HOH:O[2_556]	2.08	0.12

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	556/569 (98%)	536 (96%)	17 (3%)	3 (0%)	24	14
2	B	165/168 (98%)	162 (98%)	3 (2%)	0	100	100
3	C	29/34 (85%)	29 (100%)	0	0	100	100
All	All	750/771 (97%)	727 (97%)	20 (3%)	3 (0%)	30	19

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	515	PRO
1	A	519	ARG
1	A	369	PHE

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	450/463 (97%)	424 (94%)	26 (6%)	18	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	134/138 (97%)	129 (96%)	5 (4%)	30	18
3	C	24/27 (89%)	20 (83%)	4 (17%)	2	0
All	All	608/628 (97%)	573 (94%)	35 (6%)	19	7

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	54	LEU
1	A	58	LEU
1	A	133	TYR
1	A	215	LEU
1	A	230	TRP
1	A	262	ASP
1	A	274	LEU
1	A	326	LEU
1	A	330[A]	ARG
1	A	330[B]	ARG
1	A	332	LEU
1	A	401	LEU
1	A	425	VAL
1	A	455	GLN
1	A	475	ILE
1	A	494	SER
1	A	495	ARG
1	A	500	GLU
1	A	512	ILE
1	A	513	SER
1	A	516[A]	GLU
1	A	516[B]	GLU
1	A	518	ARG
1	A	519	ARG
1	A	520	LEU
2	B	26	LEU
2	B	37	LEU
2	B	49	LYS
2	B	144	GLU
2	B	167	LYS
3	C	12	ILE
3	C	17	LEU
3	C	20	LEU

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Mol	Chain	Res	Type
3	C	24	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	407	ASN
1	A	455	GLN
2	B	40	HIS
2	B	91	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 for Mogul analysis.

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	$\# Z > 2$
8	OLC	A	574	-	24,24,24	0.49	0	25,25,25	0.94	2 (8%)
8	OLC	A	572	-	24,24,24	0.70	1 (4%)	25,25,25	0.96	1 (4%)
8	OLC	B	171	-	24,24,24	0.51	0	25,25,25	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	OLC	B	169	-	24,24,24	0.51	0	25,25,25	0.82	0
8	OLC	A	566	-	22,22,24	0.54	0	23,23,25	1.26	4 (17%)
6	HAS	A	801	1,7	72,72,72	2.33	26 (36%)	87,109,109	2.34	34 (39%)
9	CUA	B	802	2	0,1,1	-	-	-	-	-
8	OLC	A	564	-	24,24,24	0.53	0	25,25,25	0.72	0
8	OLC	B	170	-	24,24,24	0.85	1 (4%)	25,25,25	1.10	2 (8%)
8	OLC	A	565	-	24,24,24	0.47	0	25,25,25	0.83	0
7	PER	A	563	4,6	1,1,1	0.85	0	-	-	-
8	OLC	A	570	-	14,14,24	0.70	1 (7%)	15,15,25	0.58	0
8	OLC	A	573	-	20,20,24	0.54	0	21,21,25	0.87	1 (4%)
5	HEM	A	800	1	50,50,50	2.85	22 (44%)	67,82,82	3.64	33 (49%)
8	OLC	A	571	-	19,19,24	0.51	0	20,20,25	1.09	2 (10%)
8	OLC	B	172	-	20,20,24	0.65	1 (5%)	20,20,25	0.73	1 (5%)
8	OLC	C	35	-	24,24,24	0.52	0	25,25,25	0.51	0
8	OLC	A	567	-	17,17,24	0.58	0	18,18,25	0.66	0
8	OLC	A	569	-	7,7,24	0.42	0	6,7,25	0.92	0
8	OLC	A	568	-	16,16,24	0.75	0	17,17,25	0.70	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
8	OLC	B	169	-	-	11/24/24/24	-
8	OLC	A	566	-	-	10/22/22/24	-
6	HAS	A	801	1,7	1/1/8/18	6/42/82/82	-
8	OLC	A	570	-	-	5/14/14/24	-
8	OLC	A	572	-	-	15/24/24/24	-
8	OLC	A	574	-	-	8/24/24/24	-
8	OLC	A	573	-	-	10/20/20/24	-
8	OLC	A	564	-	-	13/24/24/24	-
8	OLC	A	571	-	-	7/19/19/24	-
8	OLC	B	170	-	-	10/24/24/24	-
8	OLC	B	172	-	-	9/19/19/24	-
8	OLC	C	35	-	-	12/24/24/24	-
8	OLC	A	567	-	-	6/17/17/24	-
8	OLC	B	171	-	-	10/24/24/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	HEM	A	800	1	-	0/14/54/54	-
8	OLC	A	565	-	-	11/24/24/24	-
8	OLC	A	569	-	-	4/6/6/24	-
8	OLC	A	568	-	-	6/16/16/24	-

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	800	HEM	C3C-C4C	-8.19	1.31	1.46
5	A	800	HEM	C1C-C2C	-7.00	1.31	1.45
5	A	800	HEM	CHC-C1C	6.45	1.51	1.38
6	A	801	HAS	CHC-C1C	6.19	1.53	1.39
5	A	800	HEM	CHA-C1A	5.29	1.51	1.39
6	A	801	HAS	C4C-NC	4.77	1.48	1.39
6	A	801	HAS	C4D-C3D	4.67	1.53	1.45
6	A	801	HAS	C4B-C3B	4.41	1.52	1.44
5	A	800	HEM	CHD-C4C	4.40	1.47	1.38
6	A	801	HAS	C4D-ND	4.36	1.47	1.38
6	A	801	HAS	C1D-ND	4.33	1.47	1.40
6	A	801	HAS	CHB-C1D	4.27	1.47	1.38
5	A	800	HEM	CHB-C1B	4.22	1.46	1.38
6	A	801	HAS	C4A-NA	-4.19	1.31	1.39
5	A	800	HEM	CBB-CAB	4.12	1.50	1.30
6	A	801	HAS	CMD-C2D	3.96	1.54	1.45
5	A	800	HEM	CAB-C3B	-3.91	1.37	1.47
6	A	801	HAS	FE-NA	3.89	2.08	1.95
6	A	801	HAS	CBC-CAC	3.88	1.49	1.30
6	A	801	HAS	C4B-NB	-3.86	1.33	1.40
5	A	800	HEM	O2A-CGA	3.80	1.43	1.30
6	A	801	HAS	CHA-C4D	3.62	1.47	1.39
5	A	800	HEM	C4D-ND	-3.52	1.34	1.40
6	A	801	HAS	CHD-C4C	3.46	1.47	1.39
5	A	800	HEM	C1A-NA	3.40	1.46	1.39
6	A	801	HAS	C1C-C2C	-3.37	1.35	1.43
5	A	800	HEM	C1B-NB	-3.34	1.34	1.40
5	A	800	HEM	C4B-NB	-3.33	1.32	1.38
6	A	801	HAS	FE-NB	3.20	2.04	1.94
6	A	801	HAS	C1C-NC	-3.06	1.33	1.39
5	A	800	HEM	C3C-C2C	2.83	1.42	1.37
5	A	800	HEM	FE-ND	2.79	2.03	1.94
6	A	801	HAS	C1B-NB	-2.77	1.33	1.38
6	A	801	HAS	CMA-C3A	2.76	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	801	HAS	C2D-C1D	2.71	1.50	1.44
6	A	801	HAS	CHD-C4A	-2.70	1.33	1.38
8	B	170	OLC	O20-C1	2.68	1.41	1.33
5	A	800	HEM	C1D-ND	-2.62	1.33	1.38
6	A	801	HAS	CMB-C2B	2.62	1.56	1.50
5	A	800	HEM	C4C-NC	2.60	1.44	1.39
5	A	800	HEM	CHC-C4B	-2.48	1.33	1.39
6	A	801	HAS	CAC-C3C	-2.48	1.40	1.47
5	A	800	HEM	C1B-C2B	-2.42	1.39	1.44
5	A	800	HEM	C4A-NA	2.37	1.44	1.39
6	A	801	HAS	C3C-C2C	2.34	1.49	1.41
5	A	800	HEM	FE-NB	2.28	2.01	1.94
8	B	172	OLC	O20-C1	2.25	1.40	1.33
6	A	801	HAS	O2D-CGD	-2.17	1.23	1.30
8	A	572	OLC	O20-C1	2.14	1.39	1.33
5	A	800	HEM	CHD-C1D	-2.10	1.34	1.39
6	A	801	HAS	C1A-NA	-2.09	1.35	1.39
8	A	570	OLC	O20-C1	2.07	1.39	1.33

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	800	HEM	CHD-C1D-ND	9.71	134.87	124.42
5	A	800	HEM	C4C-C3C-C2C	-9.50	98.58	106.81
5	A	800	HEM	CHA-C4D-ND	9.28	135.84	124.37
5	A	800	HEM	C4D-ND-C1D	8.87	115.71	105.21
5	A	800	HEM	CHC-C4B-NB	8.60	133.67	124.42
6	A	801	HAS	C4C-C3C-C2C	-7.31	98.21	107.30
5	A	800	HEM	C2D-C1D-ND	-6.77	102.07	109.90
5	A	800	HEM	CHC-C1C-NC	-6.27	117.63	124.45
5	A	800	HEM	C4C-NC-C1C	-6.16	95.79	105.82
6	A	801	HAS	C3C-C4C-NC	5.90	114.77	109.80
5	A	800	HEM	C1A-CHA-C4D	-5.71	112.81	126.25
5	A	800	HEM	CHB-C1B-NB	4.91	130.44	124.37
6	A	801	HAS	CHC-C4B-NB	4.89	130.42	124.37
6	A	801	HAS	C2C-C1C-NC	4.75	117.76	110.14
6	A	801	HAS	CAA-C2A-C3A	4.38	136.07	127.87
6	A	801	HAS	C2D-C3D-C4D	4.35	109.58	106.43
6	A	801	HAS	CHA-C1A-NA	4.17	129.00	124.45
5	A	800	HEM	C4B-C3B-C2B	-4.17	103.44	107.28
5	A	800	HEM	O2D-CGD-O1D	-4.15	112.67	123.33
6	A	801	HAS	CMA-C3A-C4A	4.10	131.94	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	800	HEM	C1D-C2D-C3D	4.07	111.26	106.98
5	A	800	HEM	C4A-NA-C1A	-3.98	99.33	105.82
6	A	801	HAS	O11-C11-C12	3.96	119.65	109.14
6	A	801	HAS	C4C-NC-C1C	-3.96	99.36	105.82
5	A	800	HEM	C1C-CHC-C4B	-3.94	117.66	126.02
5	A	800	HEM	CHC-C4B-C3B	-3.91	117.26	125.07
5	A	800	HEM	CHA-C4D-C3D	-3.90	118.03	125.23
5	A	800	HEM	C3D-C4D-ND	-3.71	106.11	110.17
6	A	801	HAS	CHC-C1C-NC	-3.62	117.30	123.86
5	A	800	HEM	C1B-NB-C4B	3.54	109.40	105.21
5	A	800	HEM	CHD-C4C-NC	-3.49	120.65	124.45
6	A	801	HAS	CAA-CBA-CGA	-3.49	104.41	113.67
6	A	801	HAS	C27-C19-C20	3.46	121.23	115.23
5	A	800	HEM	O2A-CGA-O1A	-3.46	114.44	123.33
8	A	571	OLC	C4-C3-C2	-3.30	100.99	113.13
5	A	800	HEM	CAC-C3C-C4C	3.28	132.65	124.82
6	A	801	HAS	CMB-C2B-C3B	-3.18	124.12	130.28
6	A	801	HAS	CHB-C1D-ND	-3.16	120.46	124.37
8	A	566	OLC	O20-C21-C22	-3.15	91.03	105.85
6	A	801	HAS	C1D-ND-C4D	-2.92	101.75	105.21
6	A	801	HAS	CAA-C2A-C1A	-2.88	118.99	124.85
5	A	800	HEM	O2D-CGD-CBD	2.87	123.08	114.00
6	A	801	HAS	CHA-C1A-C2A	-2.85	120.36	124.86
5	A	800	HEM	C3B-C2B-C1B	2.82	108.53	106.41
8	B	170	OLC	C21-O20-C1	2.78	127.29	117.12
6	A	801	HAS	C1A-CHA-C4D	-2.78	120.12	126.02
6	A	801	HAS	O2D-CGD-CBD	2.76	122.72	114.00
6	A	801	HAS	CHD-C4A-C3A	-2.76	119.75	125.49
6	A	801	HAS	OMD-CMD-C2D	-2.73	119.45	125.62
6	A	801	HAS	O2A-CGA-CBA	2.66	122.40	114.00
5	A	800	HEM	CHD-C4C-C3C	-2.62	120.79	125.21
6	A	801	HAS	C20-C19-C18	-2.60	115.33	121.17
5	A	800	HEM	CMC-C2C-C3C	-2.58	122.19	128.43
8	B	170	OLC	O20-C21-C22	2.57	117.92	105.85
6	A	801	HAS	C12-C13-C14	2.54	118.84	112.16
6	A	801	HAS	CHC-C4B-C3B	-2.53	119.42	125.80
5	A	800	HEM	C4A-CHB-C1B	-2.48	120.41	126.25
8	B	172	OLC	C21-O20-C1	2.47	123.97	116.07
8	A	566	OLC	C21-C22-C24	2.46	120.06	111.77
5	A	800	HEM	CBD-CAD-C3D	-2.44	105.78	112.53
5	A	800	HEM	CAB-C3B-C2B	2.41	136.26	128.43
5	A	800	HEM	CHB-C1B-C2B	-2.34	120.30	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	801	HAS	CBD-CAD-C3D	-2.33	106.09	112.53
6	A	801	HAS	O1A-CGA-CBA	-2.31	115.75	123.09
6	A	801	HAS	CMB-C2B-C1B	2.28	128.59	125.03
8	A	572	OLC	O20-C21-C22	2.22	116.31	105.85
8	A	574	OLC	C3-C2-C1	-2.17	105.73	113.69
8	A	566	OLC	C3-C2-C1	-2.11	105.95	113.69
6	A	801	HAS	C1C-CHC-C4B	-2.10	121.30	126.25
6	A	801	HAS	C2B-C1B-NB	2.10	112.33	109.90
6	A	801	HAS	CHA-C4D-C3D	2.09	127.82	124.77
8	A	574	OLC	C21-C22-C24	-2.08	104.76	111.77
5	A	800	HEM	C3A-C4A-NA	2.06	113.44	110.14
6	A	801	HAS	CAD-CBD-CGD	-2.03	108.29	113.67
6	A	801	HAS	C24-C23-C22	-2.03	116.62	121.17
5	A	800	HEM	CMB-C2B-C3B	-2.02	123.53	128.43
8	A	571	OLC	O20-C21-C22	2.02	115.33	105.85
5	A	800	HEM	O2A-CGA-CBA	2.01	120.36	114.00
8	A	566	OLC	C21-O20-C1	2.00	124.44	117.12
8	A	573	OLC	O20-C1-O19	2.00	128.64	123.63

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	801	HAS	NA

All (153) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	565	OLC	O20-C21-C22-C24
8	A	565	OLC	O20-C21-C22-O23
8	A	566	OLC	C21-C22-C24-O25
8	A	566	OLC	O23-C22-C24-O25
8	A	569	OLC	O19-C1-O20-C21
8	A	570	OLC	O20-C21-C22-C24
8	A	572	OLC	C21-C22-C24-O25
8	A	572	OLC	O20-C21-C22-C24
8	A	574	OLC	O20-C21-C22-C24
8	A	574	OLC	O20-C21-C22-O23
8	B	169	OLC	C21-C22-C24-O25
8	B	171	OLC	C21-C22-C24-O25
8	A	568	OLC	O19-C1-O20-C21
8	A	568	OLC	C2-C1-O20-C21
8	A	567	OLC	O20-C21-C22-O23

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Mol	Chain	Res	Type	Atoms
8	A	569	OLC	O20-C21-C22-O23
8	A	572	OLC	O20-C21-C22-O23
8	A	564	OLC	C2-C1-O20-C21
8	A	565	OLC	C2-C1-O20-C21
8	A	572	OLC	C2-C3-C4-C5
8	A	566	OLC	O20-C21-C22-C24
8	A	567	OLC	O20-C21-C22-C24
8	A	568	OLC	O20-C21-C22-C24
8	C	35	OLC	O20-C21-C22-C24
8	A	564	OLC	O19-C1-O20-C21
8	A	568	OLC	O20-C21-C22-O23
8	B	170	OLC	O20-C21-C22-O23
8	A	565	OLC	O19-C1-O20-C21
8	B	172	OLC	C13-C14-C15-C16
8	A	572	OLC	O23-C22-C24-O25
8	B	171	OLC	C1-C2-C3-C4
8	A	574	OLC	C10-C11-C12-C13
8	A	566	OLC	O20-C21-C22-O23
8	C	35	OLC	O20-C21-C22-O23
8	A	574	OLC	C4-C5-C6-C7
8	A	572	OLC	C2-C1-O20-C21
8	B	170	OLC	O20-C21-C22-C24
8	A	570	OLC	O20-C21-C22-O23
8	A	573	OLC	C21-C22-C24-O25
8	A	564	OLC	C5-C6-C7-C8
8	A	571	OLC	C2-C1-O20-C21
8	A	566	OLC	C12-C13-C14-C15
8	A	573	OLC	O23-C22-C24-O25
8	B	169	OLC	O23-C22-C24-O25
8	B	171	OLC	O23-C22-C24-O25
8	A	564	OLC	C14-C15-C16-C17
8	B	169	OLC	C11-C12-C13-C14
8	A	572	OLC	C13-C14-C15-C16
8	B	169	OLC	C14-C15-C16-C17
8	A	573	OLC	C1-C2-C3-C4
8	A	572	OLC	O19-C1-O20-C21
8	A	572	OLC	C12-C13-C14-C15
8	B	172	OLC	C2-C1-O20-C21
8	A	571	OLC	O19-C1-O20-C21
8	B	169	OLC	C3-C4-C5-C6
8	A	573	OLC	C3-C4-C5-C6
8	A	565	OLC	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
8	B	170	OLC	C2-C3-C4-C5
8	A	566	OLC	C11-C12-C13-C14
8	C	35	OLC	C3-C4-C5-C6
8	A	569	OLC	O20-C21-C22-C24
8	A	567	OLC	C6-C7-C8-C9
8	B	170	OLC	C6-C7-C8-C9
8	B	169	OLC	C13-C14-C15-C16
8	C	35	OLC	C11-C12-C13-C14
8	A	565	OLC	C10-C11-C12-C13
8	B	169	OLC	C6-C7-C8-C9
8	A	570	OLC	C4-C5-C6-C7
8	A	570	OLC	C3-C4-C5-C6
8	B	171	OLC	C13-C14-C15-C16
8	A	571	OLC	C2-C3-C4-C5
8	A	572	OLC	C4-C5-C6-C7
8	A	572	OLC	C14-C15-C16-C17
8	A	571	OLC	C6-C7-C8-C9
8	A	567	OLC	C1-C2-C3-C4
8	A	564	OLC	C10-C11-C12-C13
8	A	574	OLC	C6-C7-C8-C9
8	A	573	OLC	C2-C1-O20-C21
8	A	564	OLC	C4-C5-C6-C7
8	A	565	OLC	C3-C4-C5-C6
8	A	574	OLC	C12-C13-C14-C15
8	B	171	OLC	C10-C11-C12-C13
8	A	564	OLC	C11-C12-C13-C14
8	A	564	OLC	C15-C16-C17-C18
8	B	172	OLC	C15-C16-C17-C18
8	B	171	OLC	C15-C16-C17-C18
8	B	170	OLC	C3-C4-C5-C6
8	A	566	OLC	C6-C7-C8-C9
6	A	801	HAS	C23-C24-C28-C29
8	A	571	OLC	C3-C4-C5-C6
8	B	169	OLC	C2-C1-O20-C21
8	B	170	OLC	C2-C1-O20-C21
8	A	573	OLC	O19-C1-O20-C21
8	A	565	OLC	C15-C16-C17-C18
8	A	572	OLC	C11-C12-C13-C14
8	C	35	OLC	C4-C5-C6-C7
8	C	35	OLC	C12-C13-C14-C15
8	C	35	OLC	C1-C2-C3-C4
8	A	573	OLC	O20-C21-C22-C24

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Mol	Chain	Res	Type	Atoms
8	B	172	OLC	C10-C11-C12-C13
8	B	172	OLC	C11-C12-C13-C14
8	A	572	OLC	C15-C16-C17-C18
8	B	169	OLC	O19-C1-O20-C21
8	B	171	OLC	C5-C6-C7-C8
8	B	172	OLC	O19-C1-O20-C21
8	B	170	OLC	O19-C1-O20-C21
8	B	172	OLC	C4-C5-C6-C7
8	B	170	OLC	C1-C2-C3-C4
8	C	35	OLC	C2-C3-C4-C5
8	A	567	OLC	C4-C5-C6-C7
8	A	564	OLC	C2-C3-C4-C5
8	B	172	OLC	C5-C6-C7-C8
8	A	564	OLC	C9-C10-C11-C12
8	A	566	OLC	C7-C8-C9-C10
8	C	35	OLC	C5-C6-C7-C8
8	B	171	OLC	C3-C4-C5-C6
8	B	169	OLC	C7-C8-C9-C10
8	A	567	OLC	C3-C4-C5-C6
8	A	564	OLC	C6-C7-C8-C9
8	B	169	OLC	C10-C11-C12-C13
8	A	574	OLC	C15-C16-C17-C18
8	B	170	OLC	C9-C10-C11-C12
8	A	574	OLC	C14-C15-C16-C17
8	A	565	OLC	C9-C10-C11-C12
8	C	35	OLC	C9-C10-C11-C12
8	A	571	OLC	C4-C5-C6-C7
8	A	564	OLC	C12-C13-C14-C15
8	A	565	OLC	C6-C7-C8-C9
8	A	566	OLC	C10-C11-C12-C13
8	A	572	OLC	C9-C10-C11-C12
6	A	801	HAS	CAD-CBD-CGD-O2D
8	A	566	OLC	C3-C4-C5-C6
8	B	170	OLC	O23-C22-C24-O25
8	A	571	OLC	C9-C10-C11-C12
8	A	572	OLC	C10-C11-C12-C13
6	A	801	HAS	C11-C12-C13-C14
6	A	801	HAS	CAA-CBA-CGA-O2A
8	A	564	OLC	C1-C2-C3-C4
8	B	171	OLC	C7-C8-C9-C10
8	B	172	OLC	C7-C8-C9-C10
8	A	573	OLC	O20-C21-C22-O23

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Mol	Chain	Res	Type	Atoms
8	A	569	OLC	C22-C21-O20-C1
6	A	801	HAS	CAA-CBA-CGA-O1A
8	C	35	OLC	C7-C8-C9-C10
8	A	565	OLC	C2-C3-C4-C5
8	A	573	OLC	C6-C7-C8-C9
8	B	171	OLC	C11-C12-C13-C14
8	C	35	OLC	C13-C14-C15-C16
6	A	801	HAS	CAD-CBD-CGD-O1D
8	A	568	OLC	O20-C1-C2-C3
8	A	573	OLC	C4-C5-C6-C7
8	A	568	OLC	O19-C1-C2-C3
8	A	570	OLC	C1-C2-C3-C4

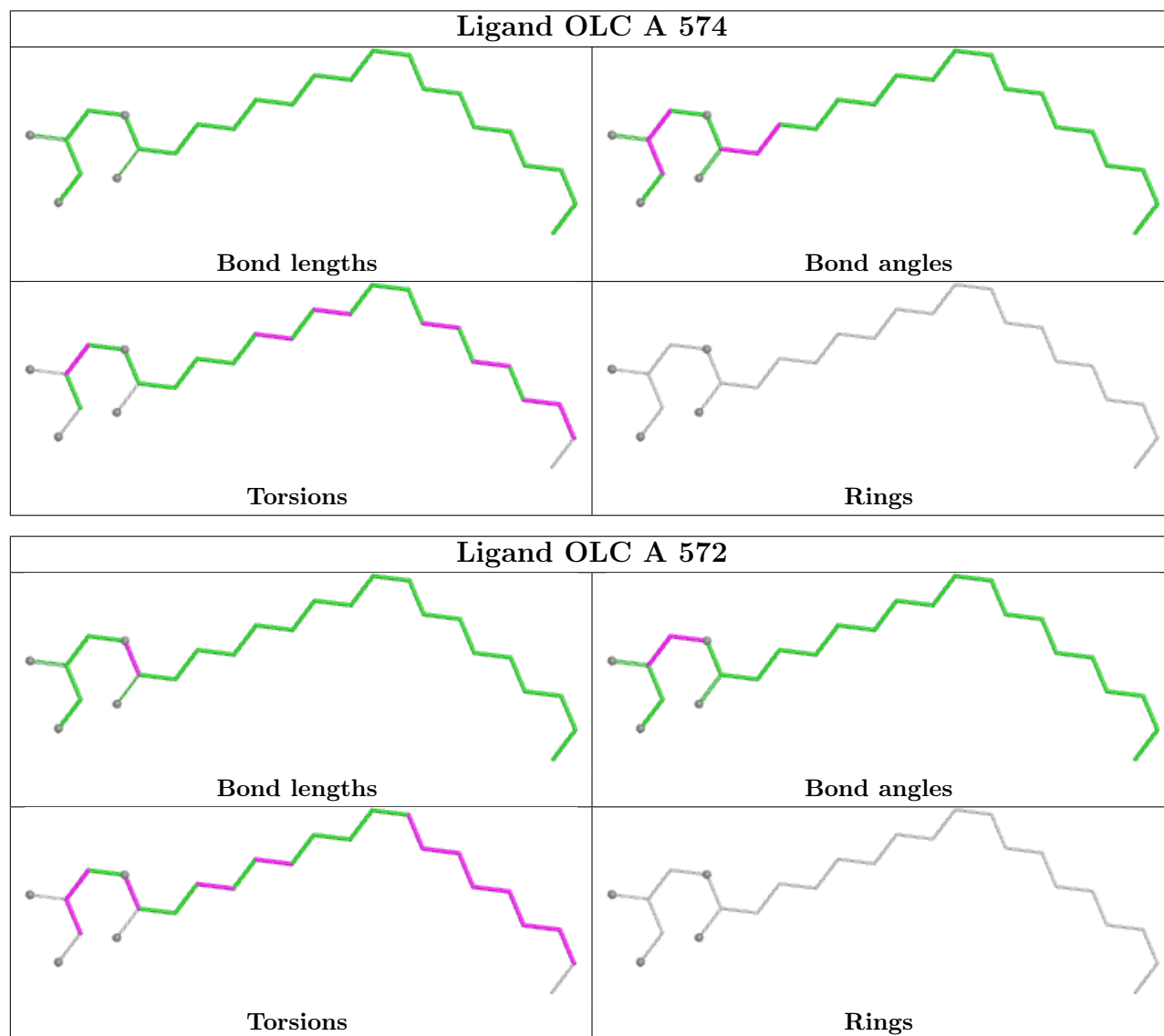
There are no ring outliers.

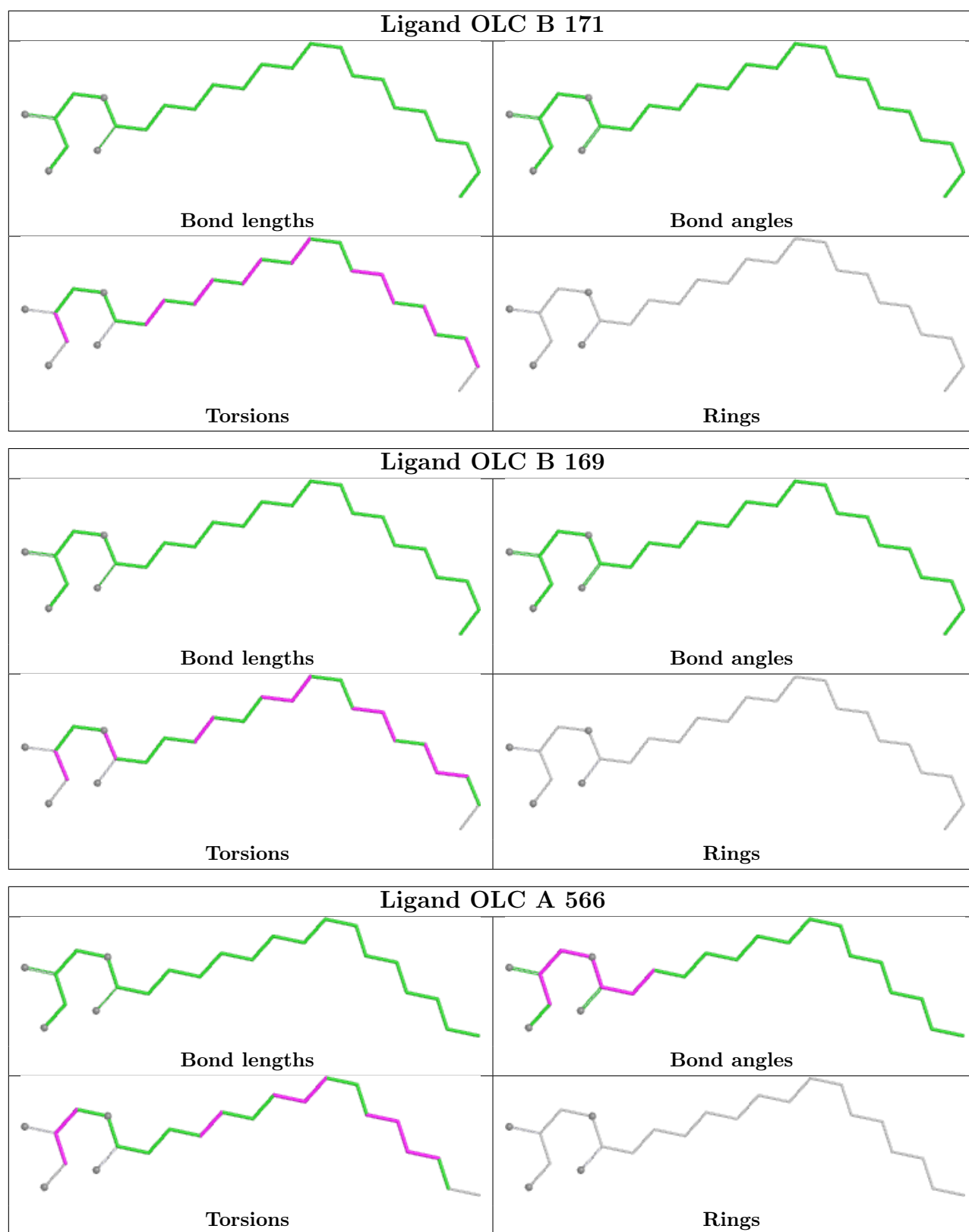
16 monomers are involved in 44 short contacts:

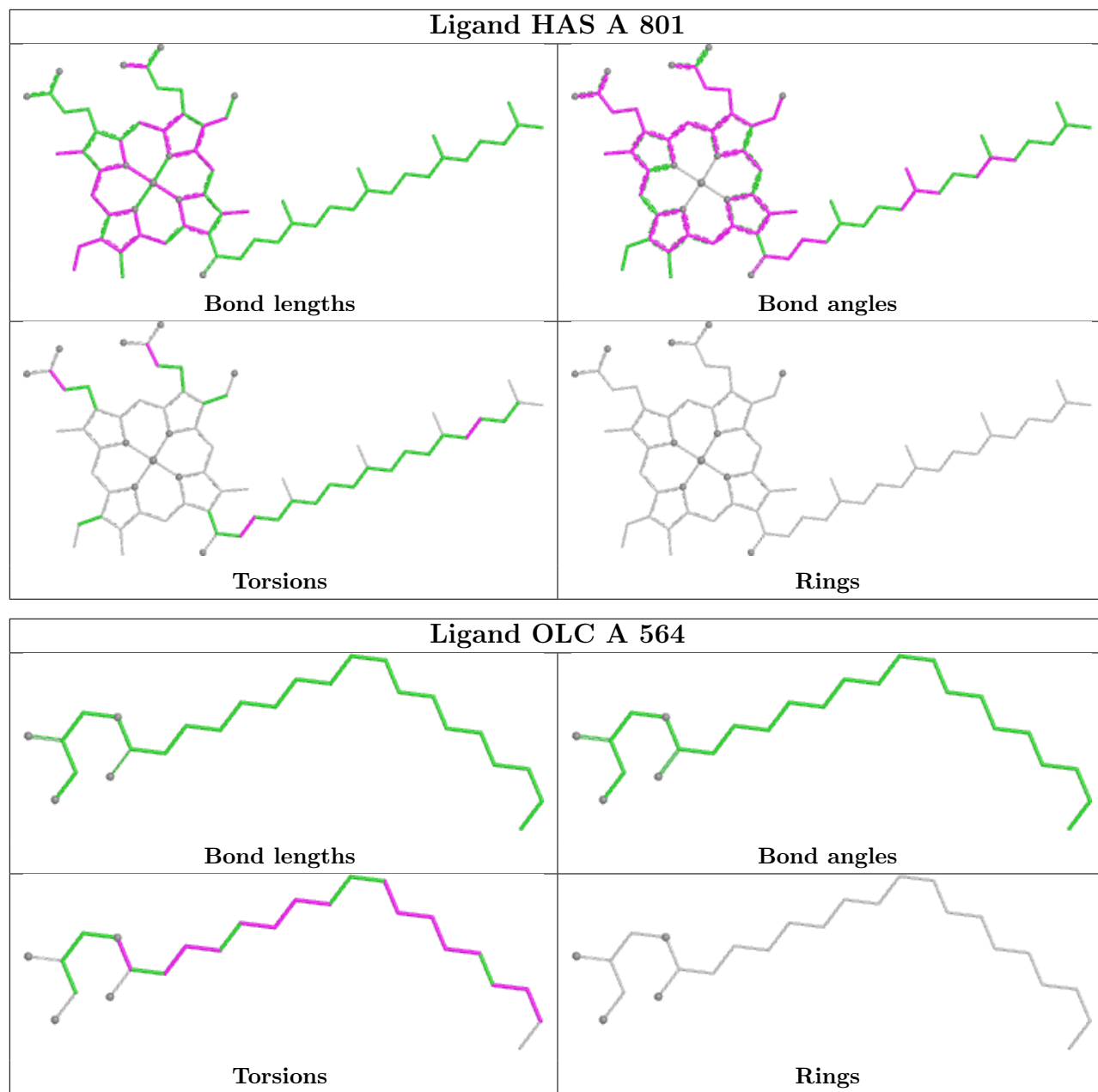
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	574	OLC	1	0
8	A	572	OLC	6	0
8	B	171	OLC	1	0
8	B	169	OLC	4	0
8	A	566	OLC	2	0
6	A	801	HAS	3	0
8	A	564	OLC	1	0
8	B	170	OLC	10	0
8	A	565	OLC	4	0
7	A	563	PER	1	0
8	A	570	OLC	7	0
5	A	800	HEM	3	0
8	A	571	OLC	2	0
8	B	172	OLC	1	0
8	C	35	OLC	1	0
8	A	569	OLC	4	0

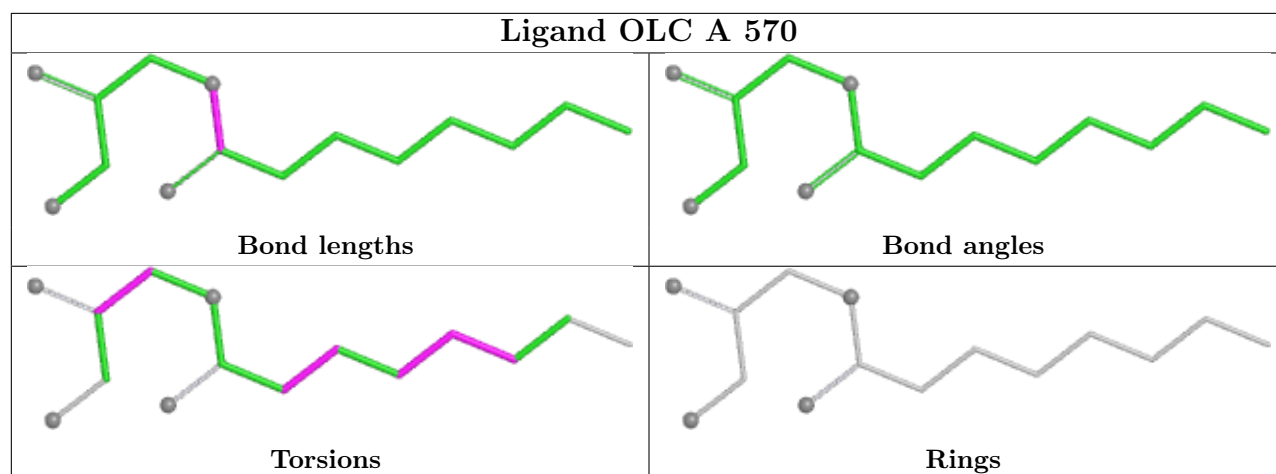
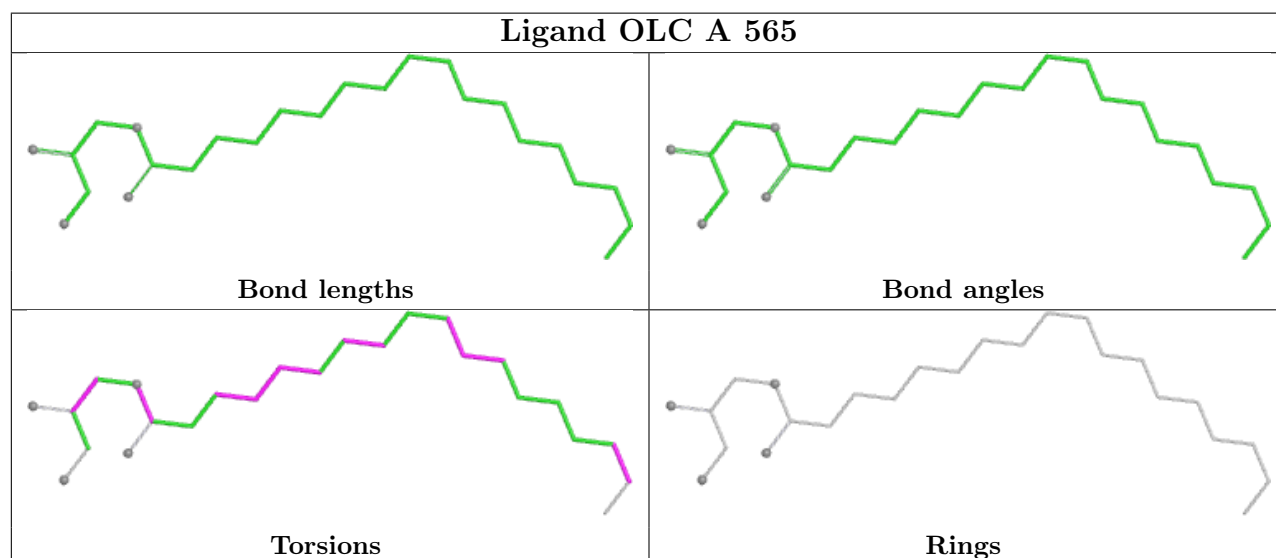
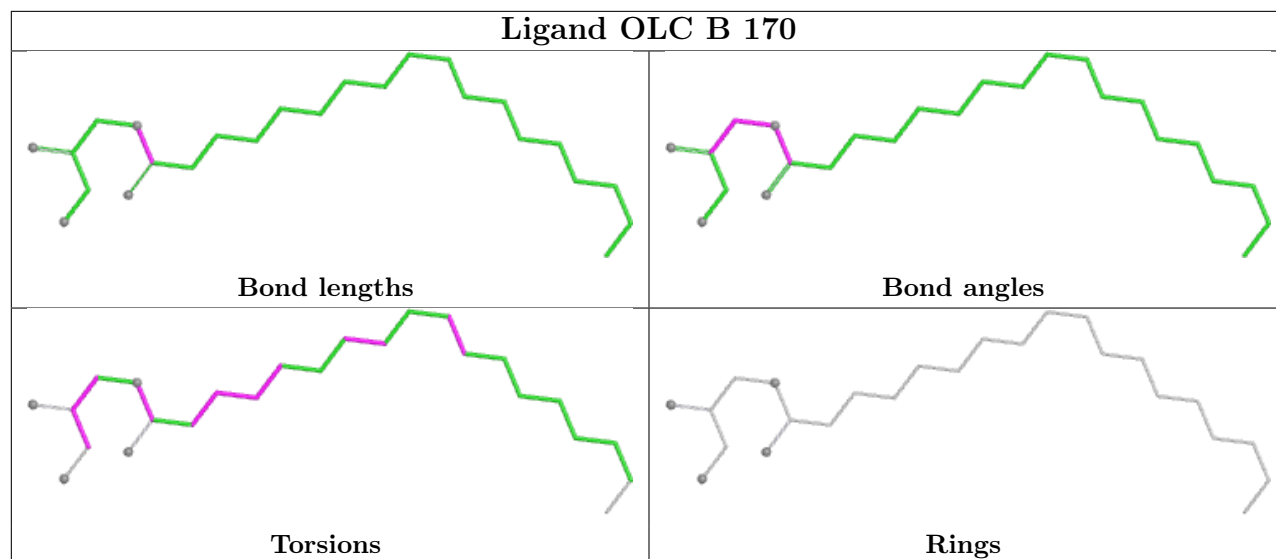
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

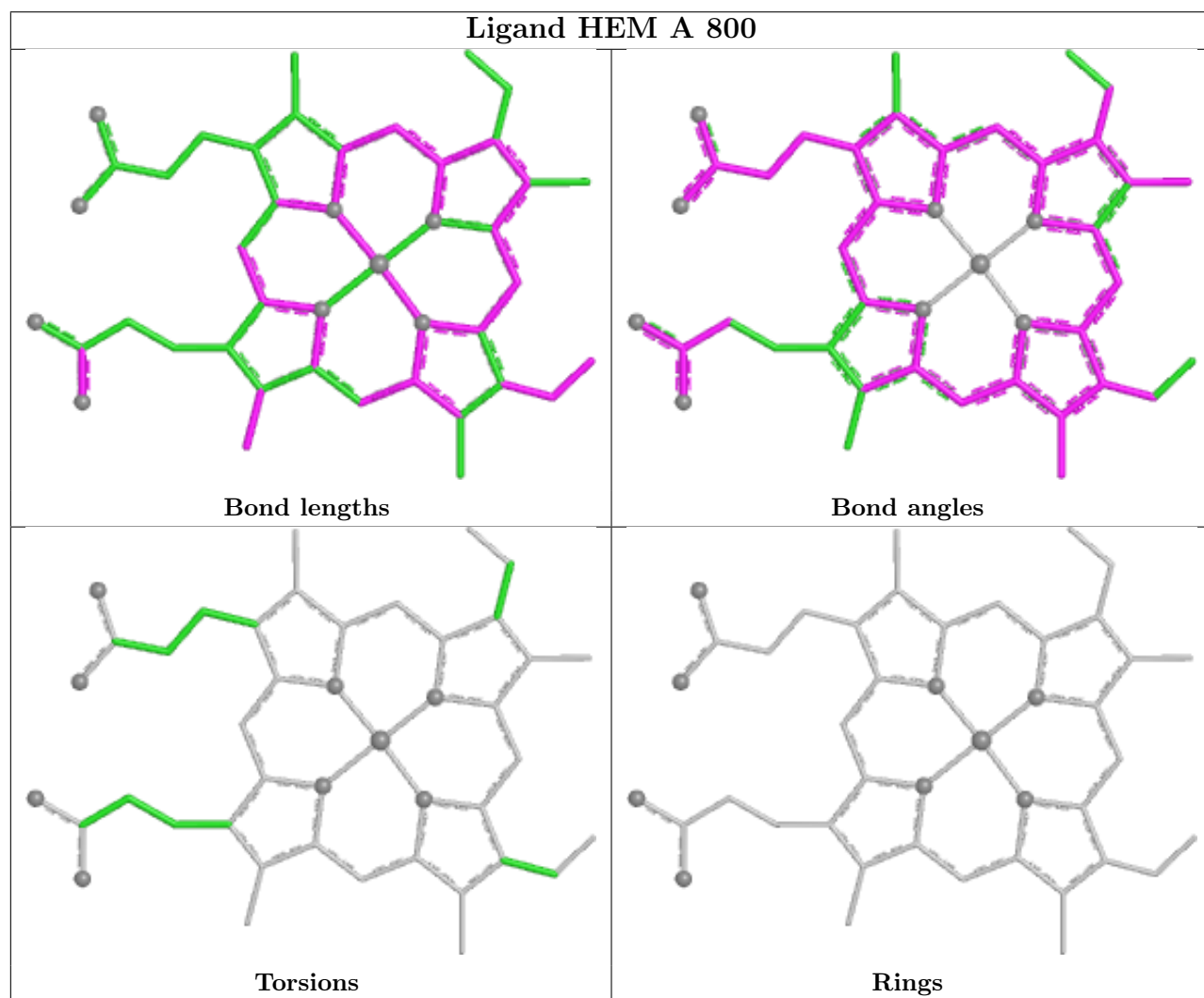
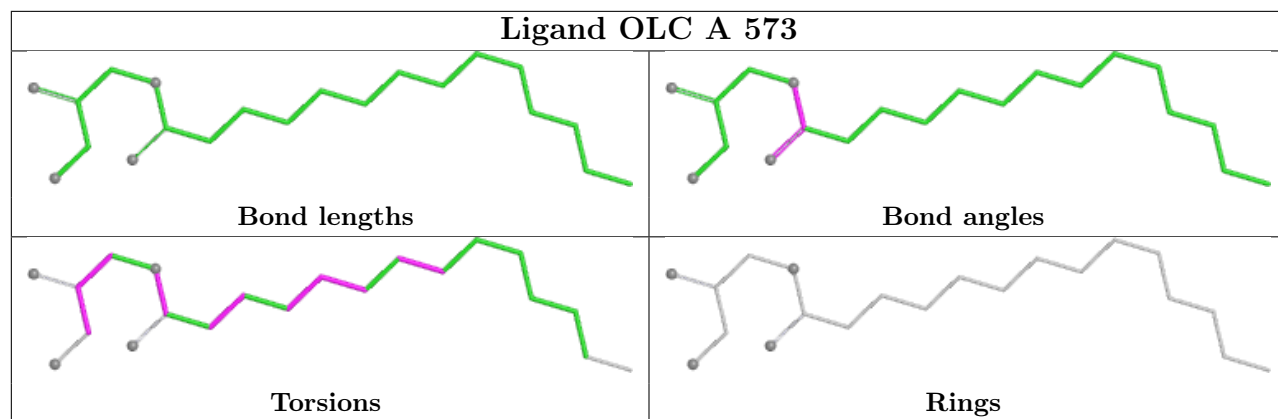
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

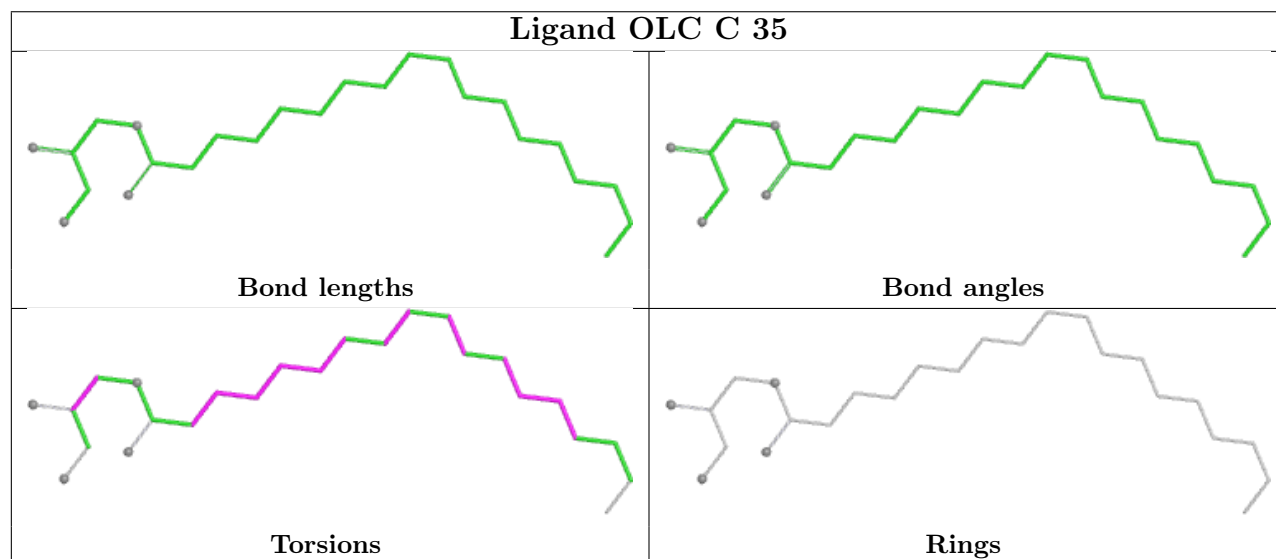
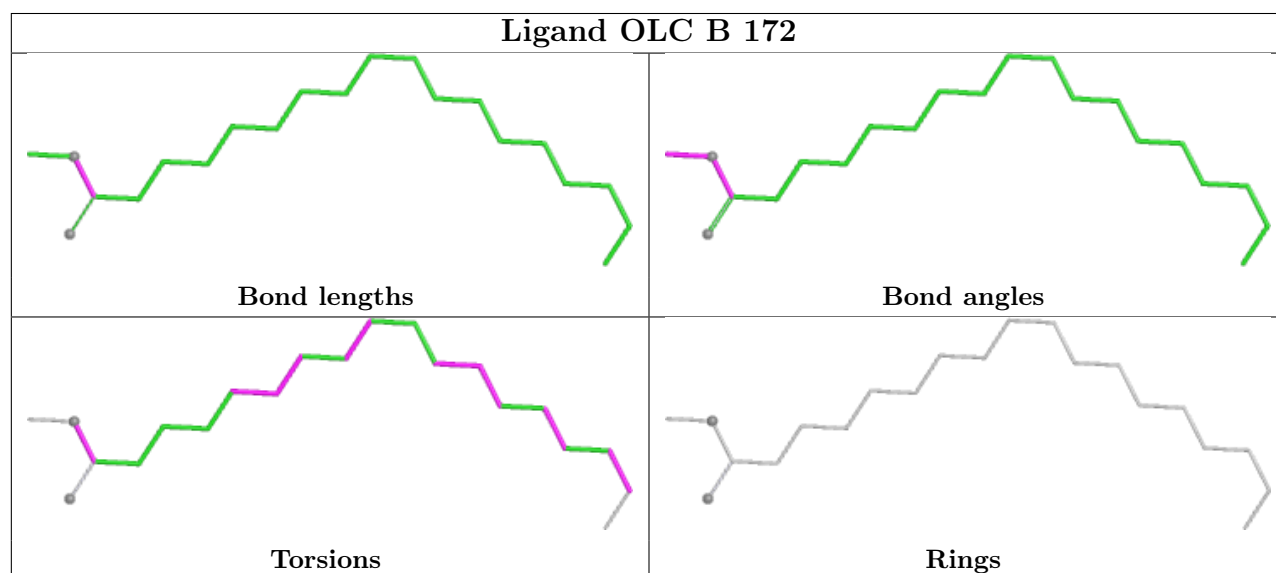
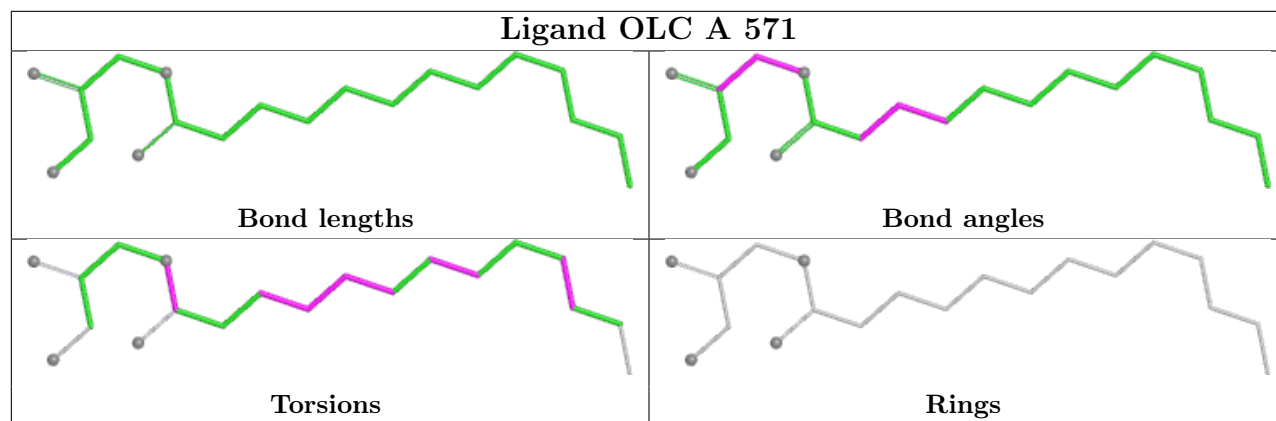


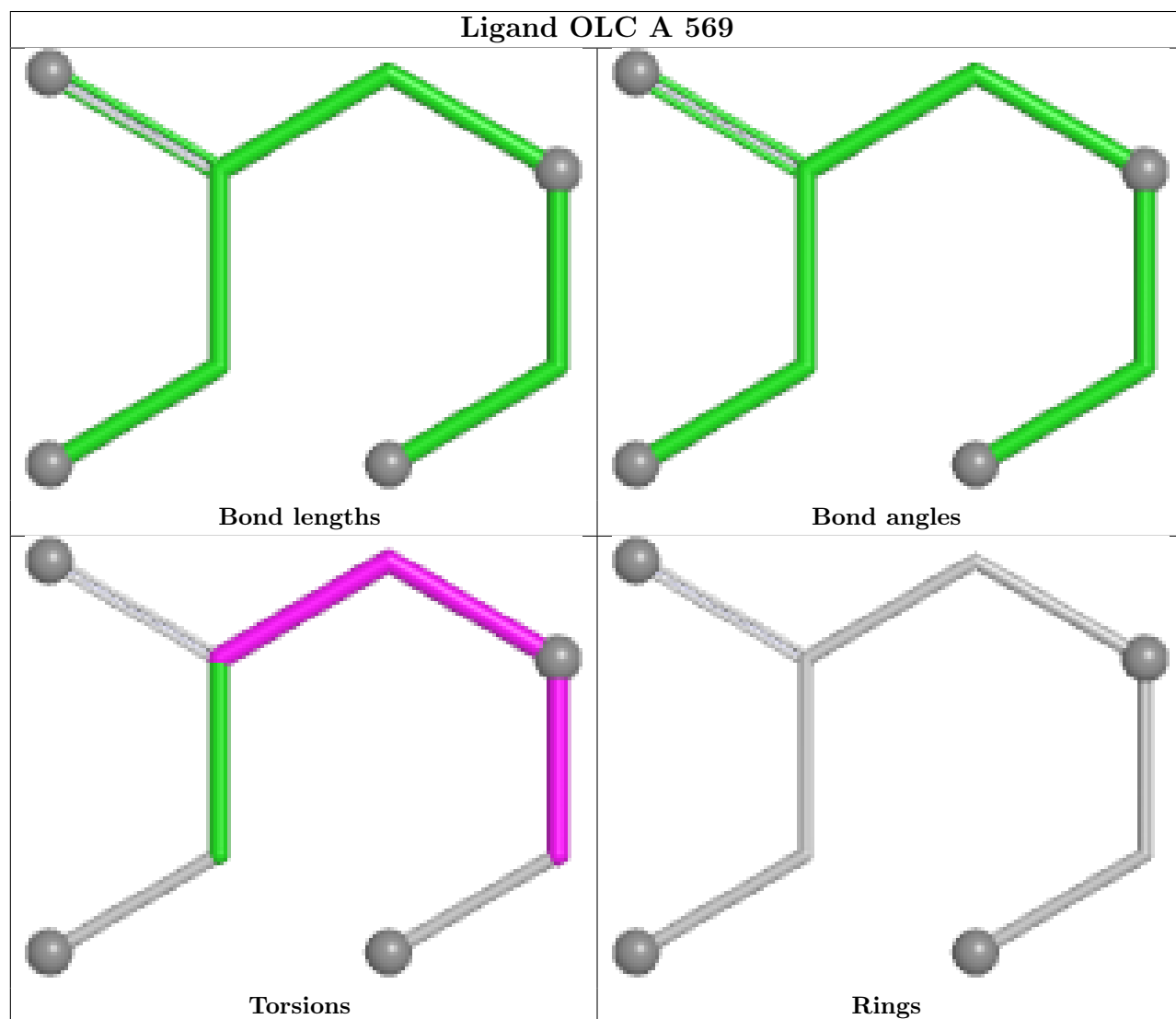
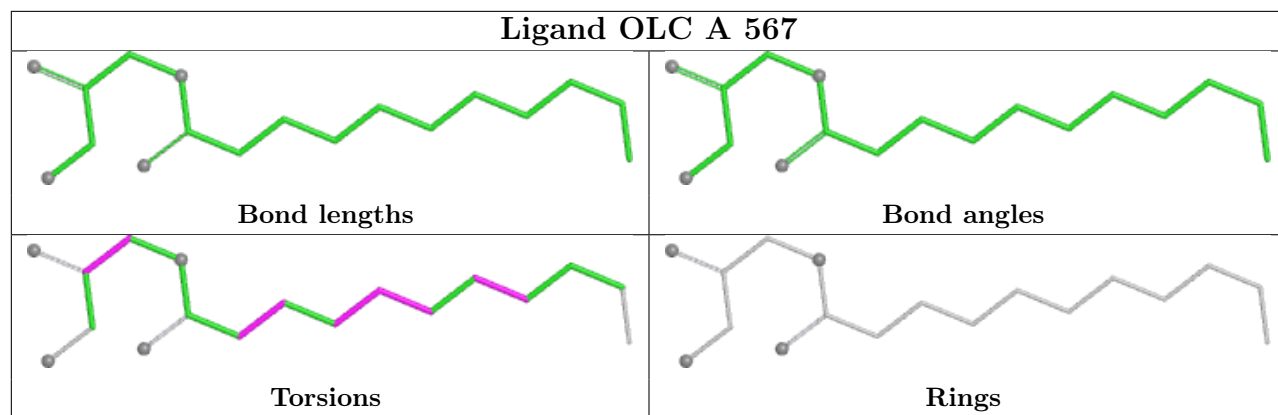


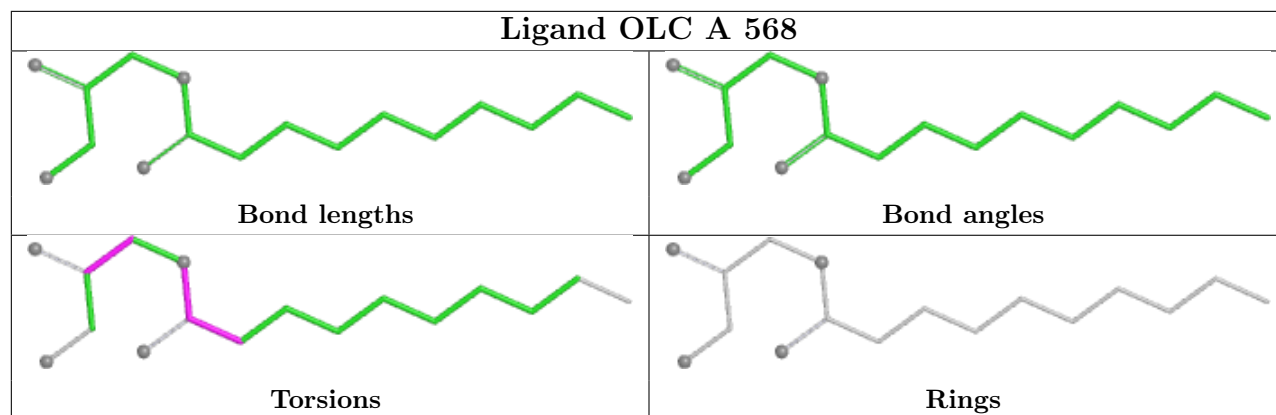












5.7 Other polymers [i](#)

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	554/569 (97%)	0.34	36 (6%) 25 23	15, 29, 53, 84	4 (0%)
2	B	166/168 (98%)	0.28	6 (3%) 46 46	16, 30, 48, 65	1 (0%)
3	C	31/34 (91%)	0.35	0 100 100	24, 30, 40, 55	0
All	All	751/771 (97%)	0.33	42 (5%) 30 29	15, 29, 51, 84	5 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	12	TYR	6.0
1	A	513	SER	5.2
1	A	515	PRO	4.7
1	A	10	ARG	4.2
1	A	492	LEU	4.1
1	A	519	ARG	4.0
1	A	9	SER	3.9
1	A	520	LEU	3.8
1	A	491	VAL	3.8
2	B	50	LEU	3.4
1	A	499	PRO	3.2
1	A	11	VAL	3.1
1	A	514	GLY	3.0
1	A	493	LEU	3.0
1	A	400	SER	2.7
2	B	5	HIS	2.6
1	A	517	ASP	2.6
2	B	38	ALA	2.6
1	A	332	LEU	2.5
1	A	552	HIS	2.5
1	A	512	ILE	2.5
1	A	536	ILE	2.5
1	A	516[A]	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	548	GLN	2.4
1	A	164	LEU	2.3
1	A	172	ALA	2.3
1	A	195	LEU	2.3
1	A	333	PHE	2.3
1	A	530	TRP	2.2
1	A	521	VAL	2.2
2	B	23	LEU	2.2
1	A	535	ALA	2.2
1	A	214	GLY	2.2
2	B	12	LEU	2.2
2	B	7	ALA	2.1
1	A	322	PHE	2.1
1	A	490	SER	2.1
1	A	500	GLU	2.1
1	A	326	LEU	2.1
1	A	518	ARG	2.1
1	A	553	LEU	2.0
1	A	331	GLY	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
8	OLC	A	568	17/25	0.68	0.26	59,63,79,80	0
8	OLC	B	172	21/25	0.74	0.20	60,63,76,79	0
8	OLC	C	35	25/25	0.74	0.17	67,81,92,93	0
8	OLC	B	170	25/25	0.76	0.21	56,63,72,76	0

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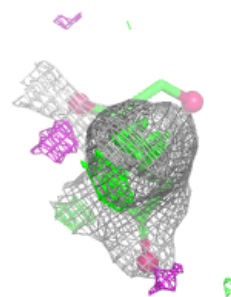
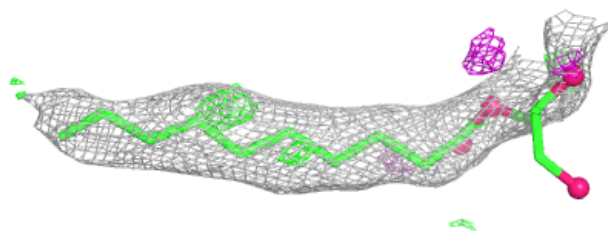
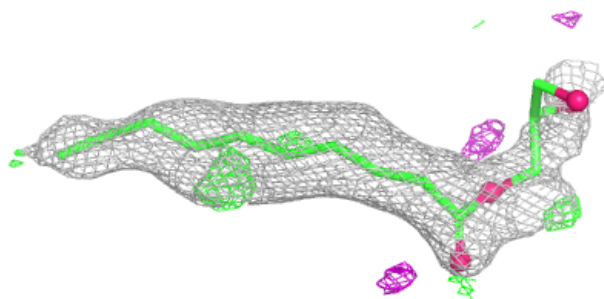
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	OLC	A	569	8/25	0.80	0.14	68,68,70,71	0
8	OLC	B	171	25/25	0.80	0.17	65,68,73,74	0
8	OLC	A	567	18/25	0.82	0.17	47,60,73,74	0
8	OLC	B	169	25/25	0.82	0.15	54,65,72,73	0
8	OLC	A	564	25/25	0.82	0.17	45,55,73,76	0
8	OLC	A	572	25/25	0.83	0.18	48,59,64,68	0
8	OLC	A	571	20/25	0.84	0.16	54,66,71,71	0
8	OLC	A	565	25/25	0.84	0.16	44,65,90,92	0
8	OLC	A	573	21/25	0.84	0.15	56,66,81,82	0
8	OLC	A	570	15/25	0.84	0.18	47,64,76,77	0
8	OLC	A	574	25/25	0.85	0.14	51,58,68,70	0
8	OLC	A	566	23/25	0.87	0.13	30,45,65,66	0
7	PER	A	563	2/2	0.96	0.05	19,19,19,21	0
6	HAS	A	801	65/65	0.98	0.06	11,20,34,39	0
4	CU	A	803	1/1	0.99	0.02	22,22,22,22	0
5	HEM	A	800	43/43	0.99	0.05	10,15,19,21	0
9	CUA	B	802	2/2	0.99	0.03	20,20,20,21	0

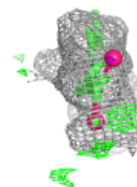
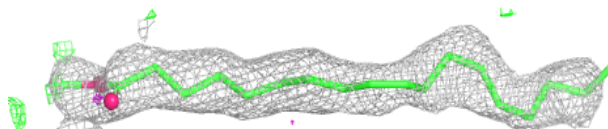
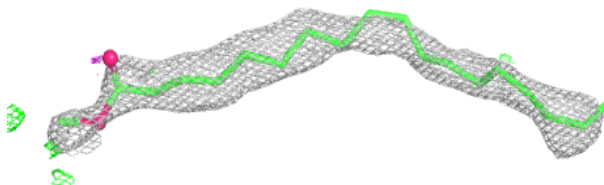
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC A 568:

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

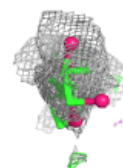
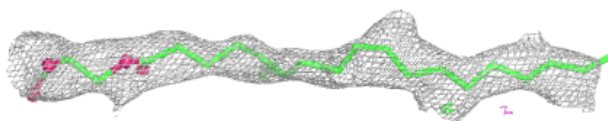
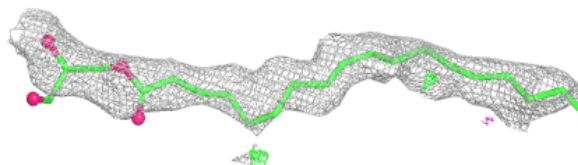
**Electron density around OLC B 172:**

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

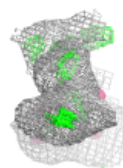
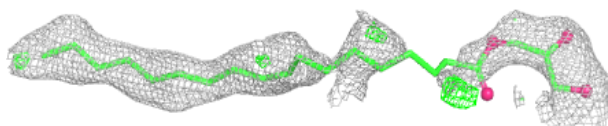
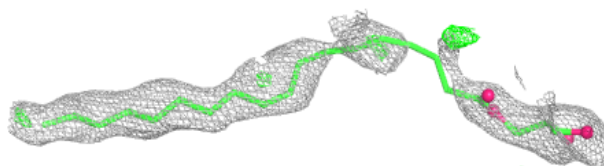


Electron density around OLC C 35:

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

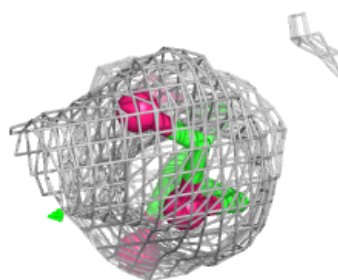
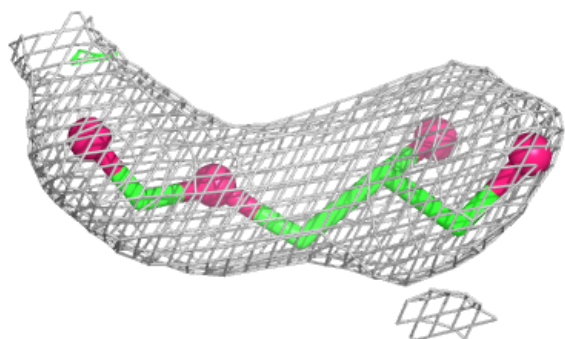
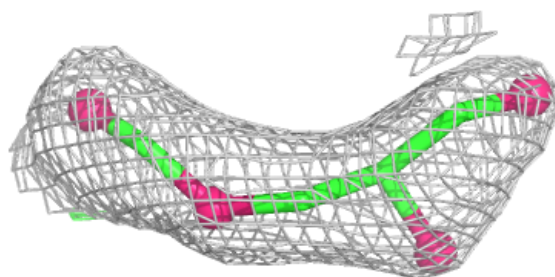
**Electron density around OLC B 170:**

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

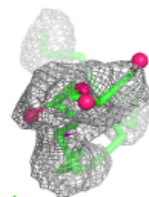
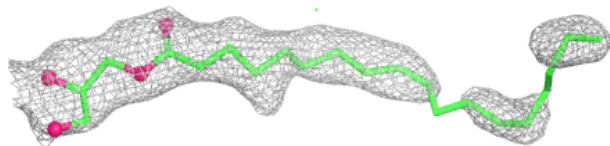
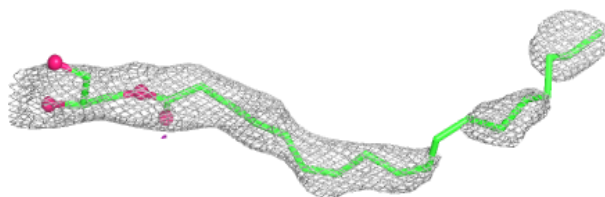


Electron density around OLC A 569:

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

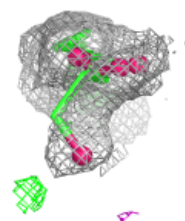
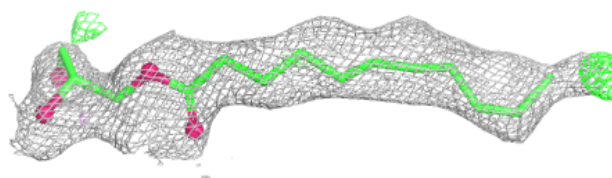
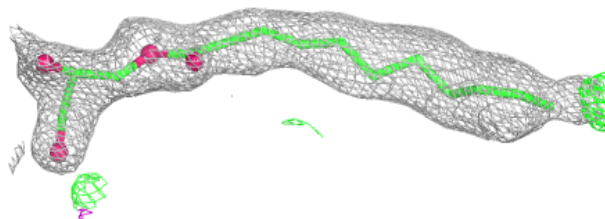
**Electron density around OLC B 171:**

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

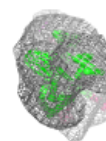
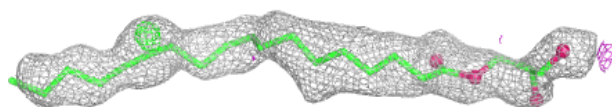
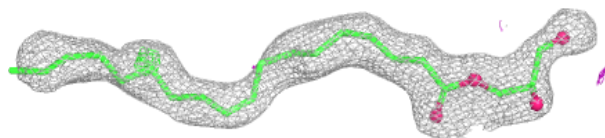


Electron density around OLC A 567:

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

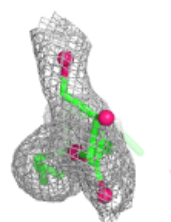
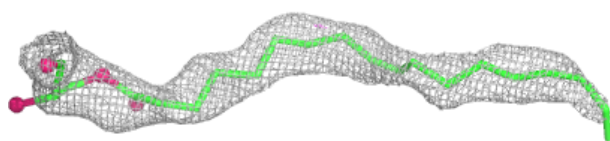
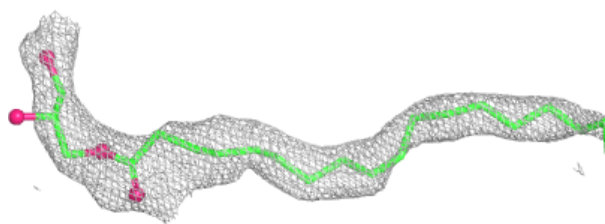
**Electron density around OLC B 169:**

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

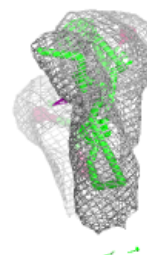
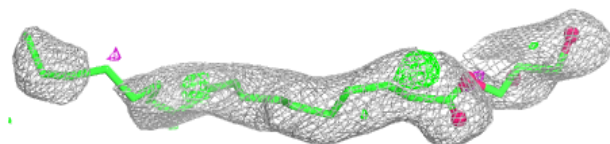
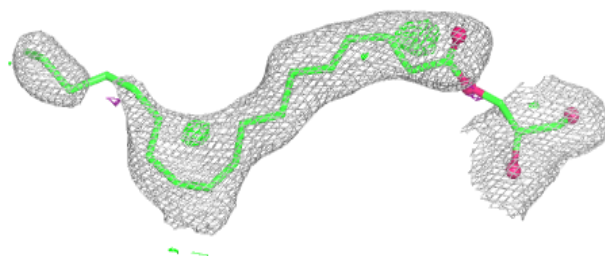


Electron density around OLC A 564:

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

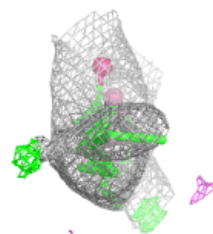
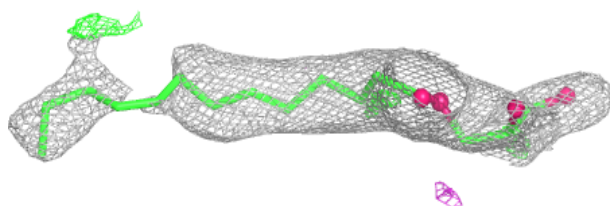
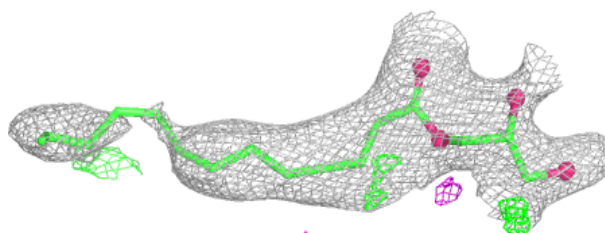
**Electron density around OLC A 572:**

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

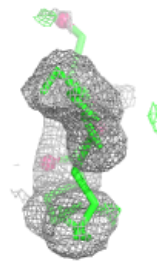
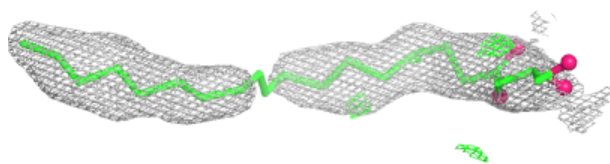
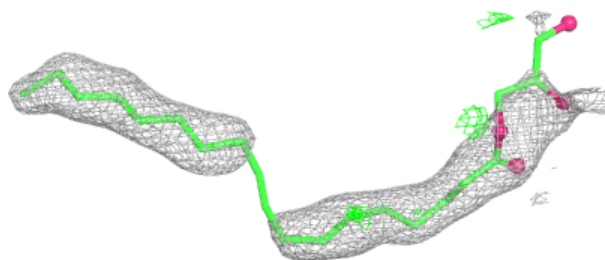


Electron density around OLC A 571:

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

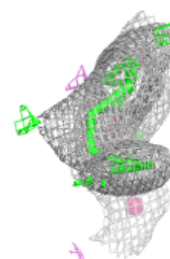
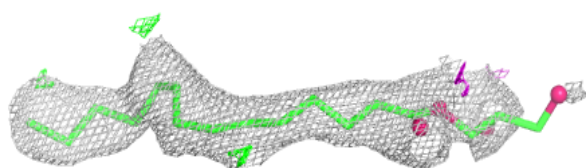
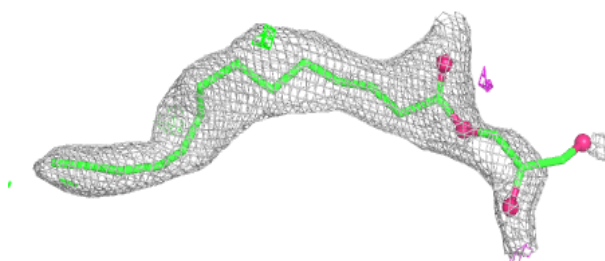
**Electron density around OLC A 565:**

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

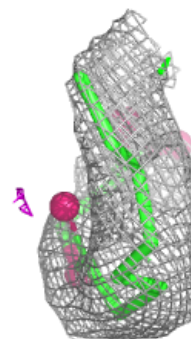
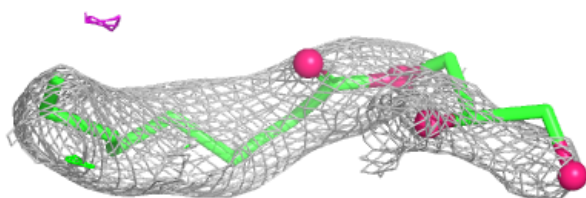
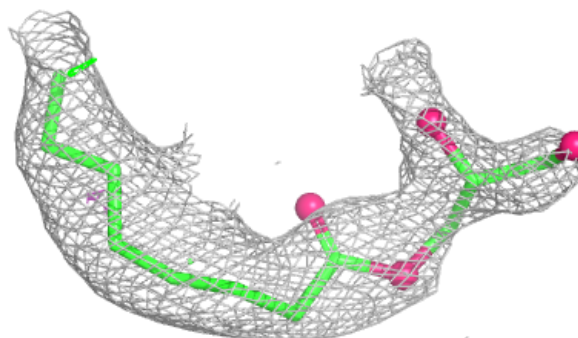


Electron density around OLC A 573:

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

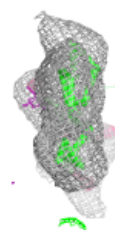
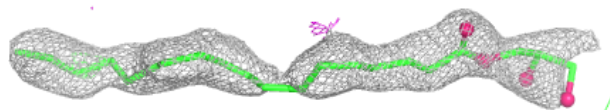
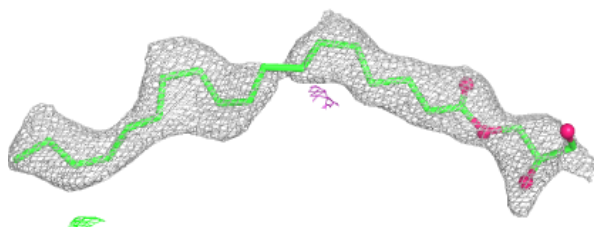
**Electron density around OLC A 570:**

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

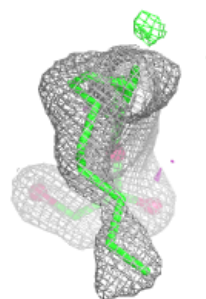
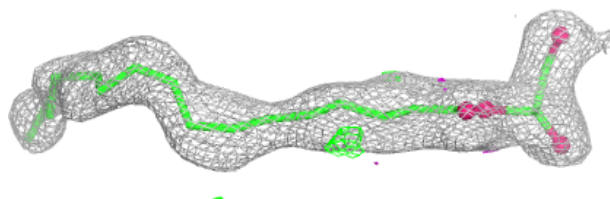
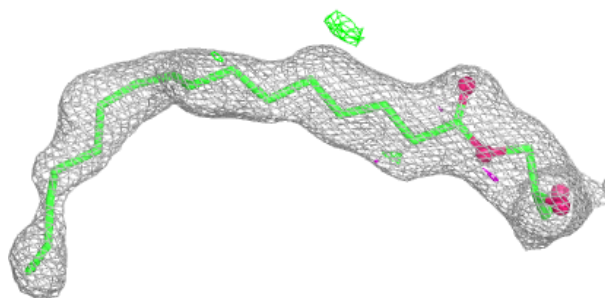


Electron density around OLC A 574:

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

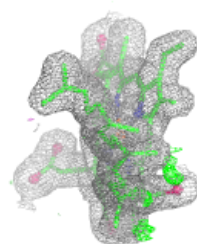
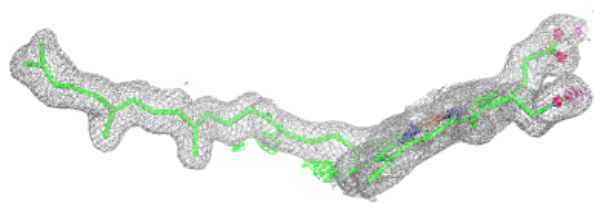
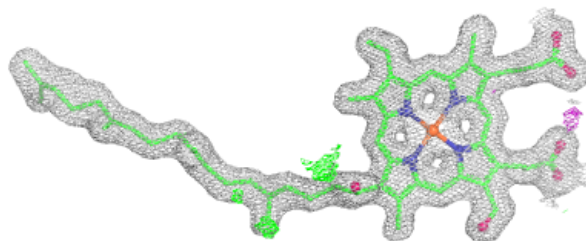
**Electron density around OLC A 566:**

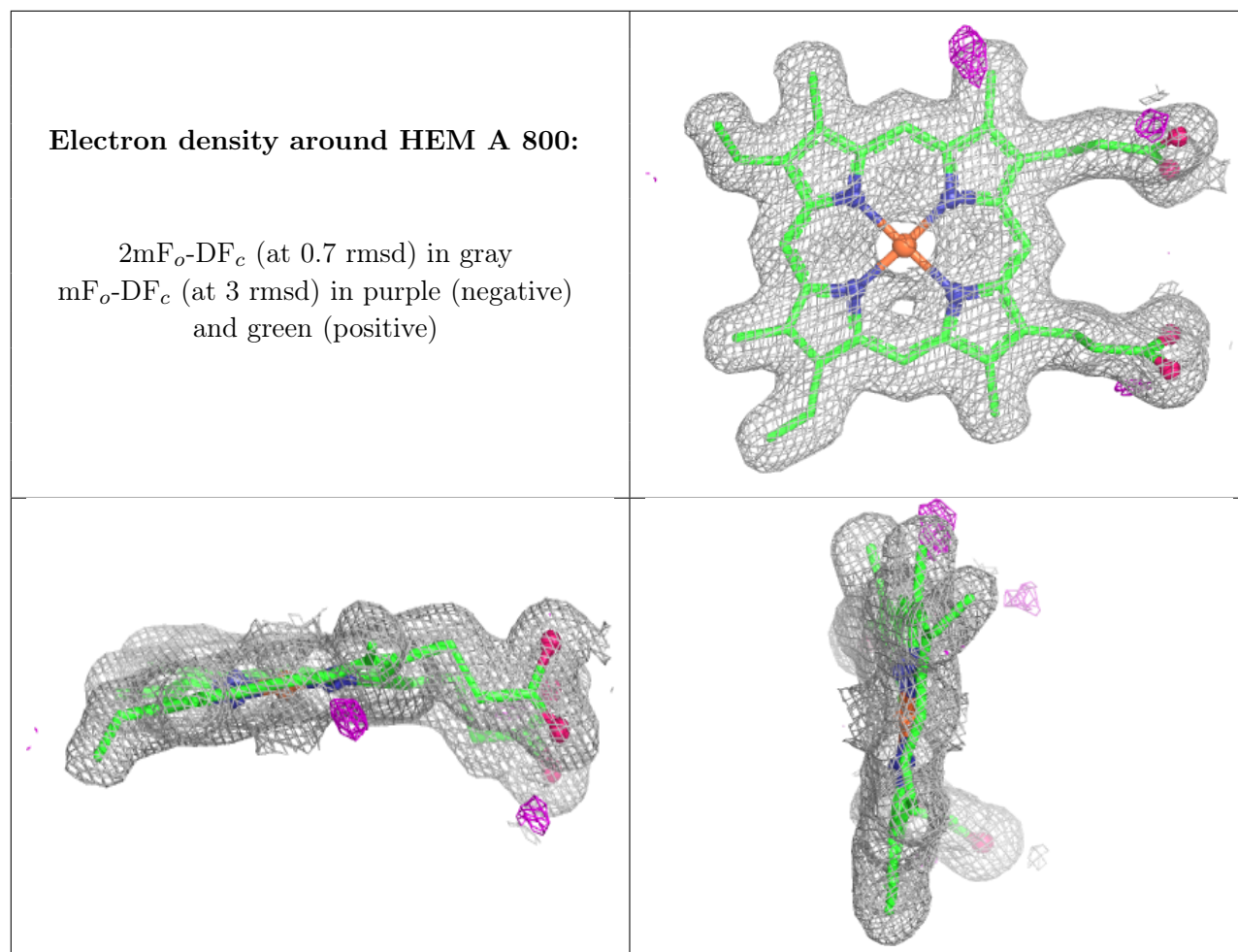
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HAS A 801:

$2mF_o-DF_c$ (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.