



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:14 AM UTC

PDB ID : 4H0L / pdb_00004h0l
Title : Cytochrome b6f Complex Crystal Structure from Mastigocladus laminosus with n-Side Inhibitor NQNO
Authors : Hasan, S.S.; Yamashita, E.; Baniulis, D.; Cramer, W.A.
Deposited on : 2012-09-08
Resolution : 3.25 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

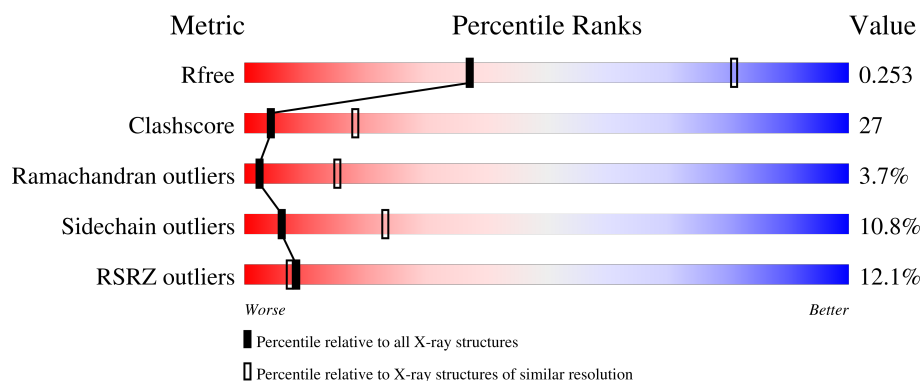
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	215	3% 65% 30% ..
2	B	160	6% 55% 38% 6% .
3	C	289	15% 49% 39% 10% ..
4	D	179	22% 49% 33% 7% 10%
5	E	32	12% 25% 50% 16% 9%

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Mol	Chain	Length	Quality of chain
6	F	35	
7	G	37	
8	H	29	

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	UMQ	A	306	X	-	-	-
12	UMQ	A	307	X	-	-	-
12	UMQ	A	309	X	-	-	-
12	UMQ	C	301	X	-	-	-
13	QNO	A	308	X	-	-	-
14	CLA	B	202	X	-	-	-
16	SQD	D	201	X	-	-	-
17	BCR	G	101	-	X	-	-

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 16219 atoms, of which 8226 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 b6.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	213	Total	C	H	N	O	S	0	0	0
			3420	1132	1722	270	286	10			

- Molecule 2 is a protein called Cytochrome b6-f complex subunit 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	160	Total	C	H	N	O	S	0	0	0
			2558	841	1309	193	209	6			

- Molecule 3 is a protein called Apocytochrome f.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	286	Total	C	H	N	O	S	0	0	0
			4419	1406	2219	366	421	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	11	PRO	GLU	SEE REMARK 999	UNP P83793

- Molecule 4 is a protein called Cytochrome b6-f complex iron-sulfur subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	161	Total	C	H	N	O	S	0	0	0
			2460	791	1224	213	225	7			

- Molecule 5 is a protein called Cytochrome b6-f complex subunit 6.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	E	32	Total	C	H	N	O	S	0	0	0
			532	179	284	34	34	1			

- Molecule 6 is a protein called Cytochrome b6-f complex subunit 7.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
6	F	32	Total	C	H	N	O	S	0	0	0
			502	165	260	35	40	2			

- Molecule 7 is a protein called Cytochrome b6-f complex subunit 5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	G	37	Total	C	H	N	O	S	0	0	0
			572	188	289	44	50	1			

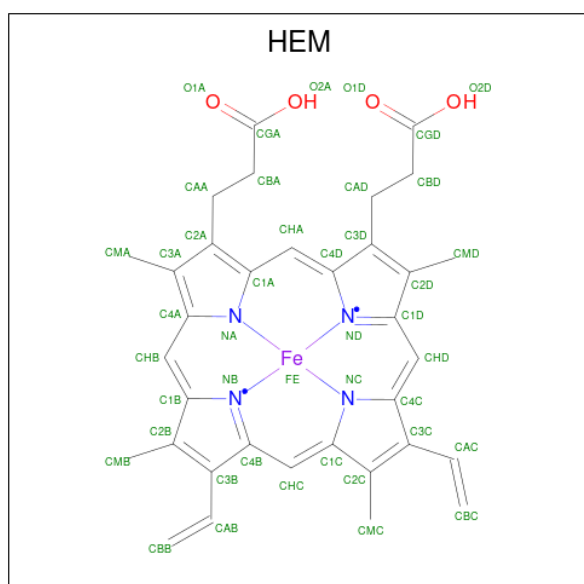
- Molecule 8 is a protein called Cytochrome b6-f complex subunit 8.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
8	H	29	Total	C	H	N	O	S	0	0	0
			469	156	239	36	36	2			

- Molecule 9 is CADMIUM ION (CCD ID: CD) (formula: Cd).

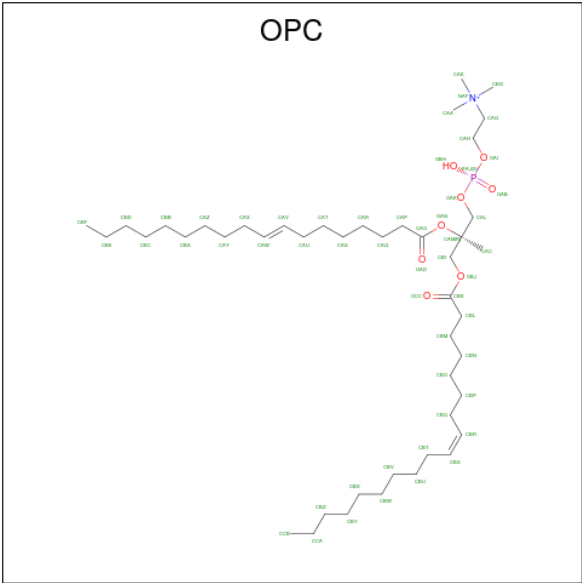
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Cd	0	0
			1	1		
9	B	1	Total	Cd	0	0
			1	1		

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



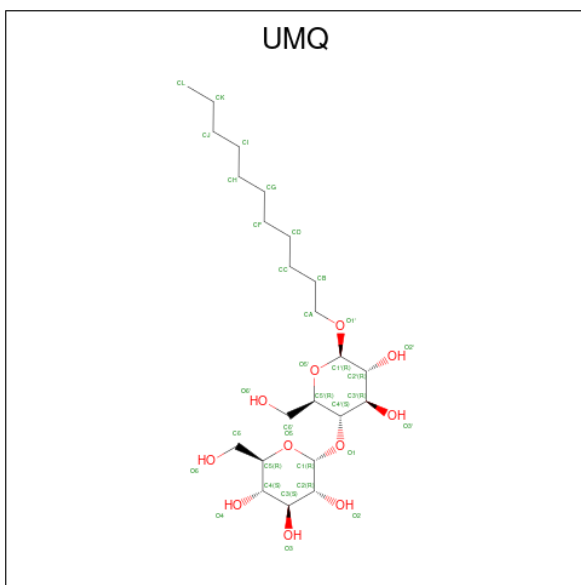
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
10	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
10	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
10	C	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- Molecule 11 is (7R,17E)-4-HYDROXY-N,N,N,7-TETRAMETHYL-7-[(8E)-OCTADEC-8-ENOYLOXY]-10-OXO-3,5,9-TRIOXA-4-PHOSPHAHEPTACOS-17-EN-1-AMINIUM 4-OXIDE (CCD ID: OPC) (formula: C₄₅H₈₇NO₈P).



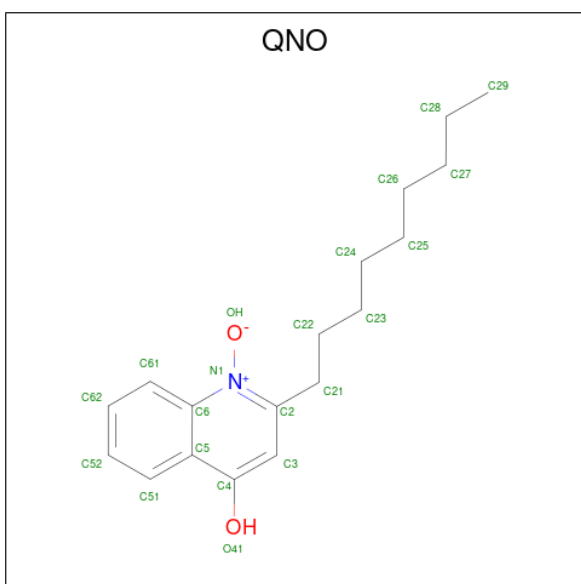
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
11	A	1	Total	C	H	N	O	P	0	0
			137	44	83	1	8	1		
11	B	1	Total	C	H	N	O	P	0	0
			137	44	83	1	8	1		

- Molecule 12 is UNDECYL-MALTOSIDE (CCD ID: UMQ) (formula: C₂₃H₄₄O₁₁).



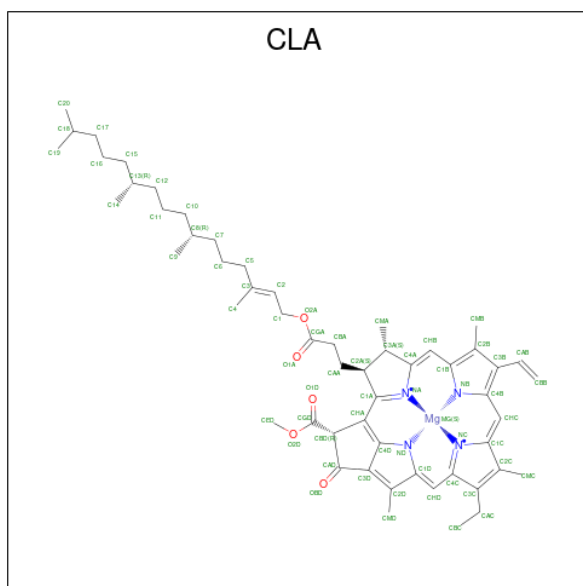
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	A	1	Total	C	H	O	0	0
			77	23	43	11		
12	A	1	Total	C	H	O	0	0
			77	23	43	11		
12	A	1	Total	C	H	O	0	0
			77	23	43	11		
12	C	1	Total	C	H	O	0	0
			78	23	44	11		

- Molecule 13 is 2-NONYL-4-HYDROXYQUINOLINE N-OXIDE (CCD ID: QNO) (formula: $C_{18}H_{25}NO_2$).



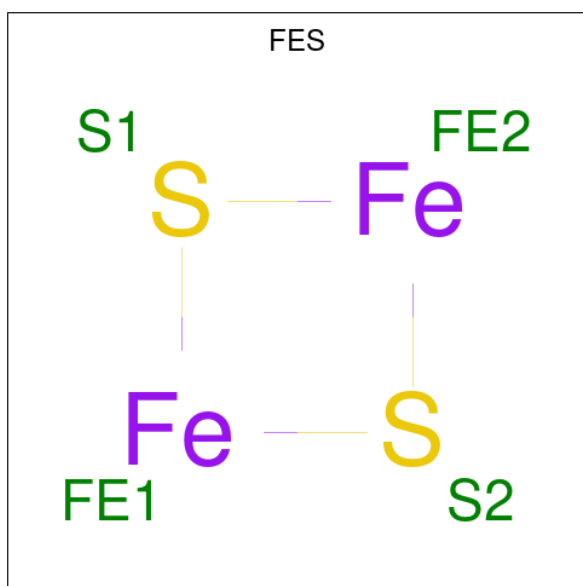
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	A	1	Total	C	H	N	O	0	0
			46	18	25	1	2		

- Molecule 14 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



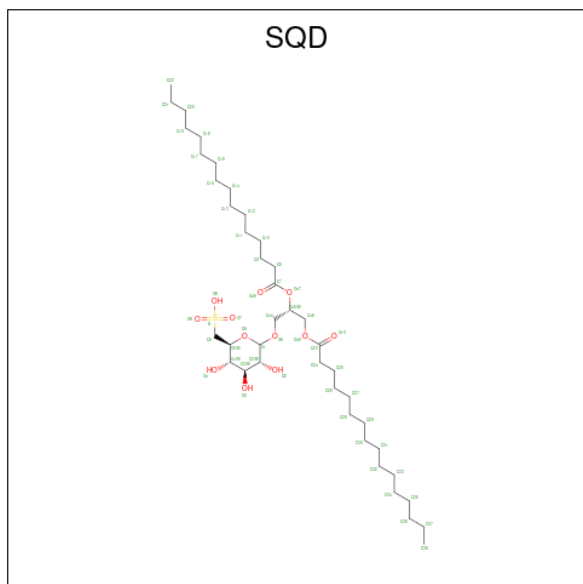
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
14	B	1	Total	C	H	Mg	N	O	0	0
			127	55	62	1	4	5		

- Molecule 15 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	D	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 16 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
17	G	1	Total	C	H	0	0
			96	40	56		

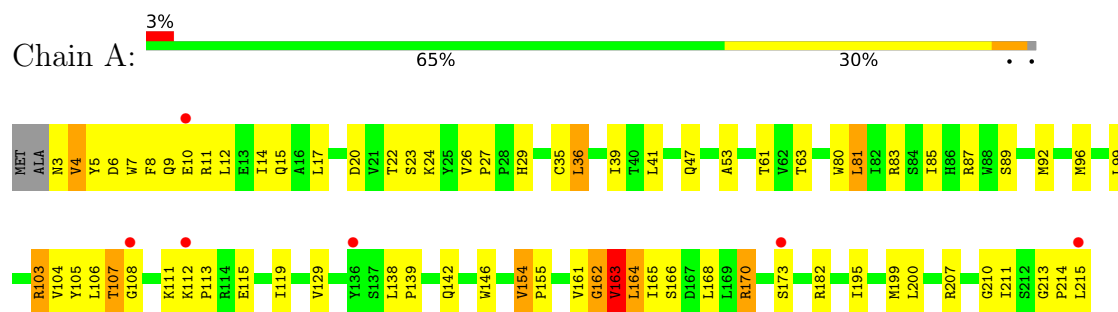
- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	2	Total	O	0	0
			2	2		
18	B	3	Total	O	0	0
			3	3		
18	C	1	Total	O	0	0
			1	1		

3 Residue-property plots [i](#)

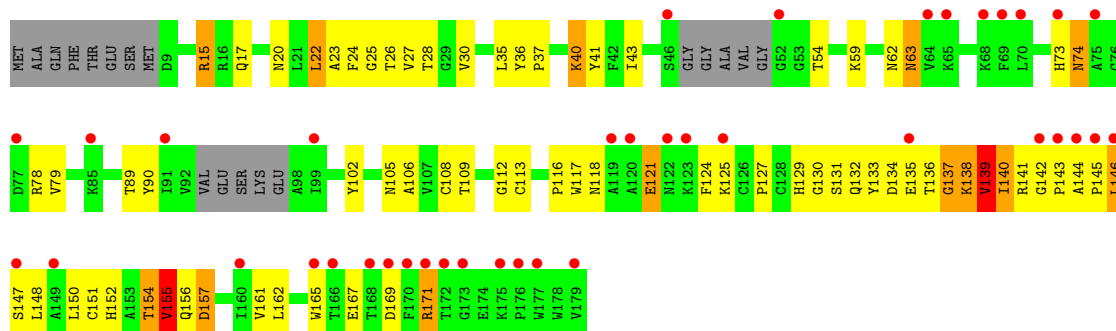
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Cytochrome b6





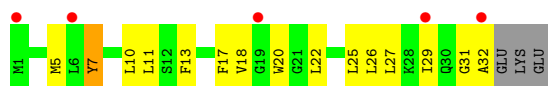
• Molecule 4: Cytochrome b6-f complex iron-sulfur subunit



• Molecule 5: Cytochrome b6-f complex subunit 6



• Molecule 6: Cytochrome b6-f complex subunit 7



• Molecule 7: Cytochrome b6-f complex subunit 5



• Molecule 8: Cytochrome b6-f complex subunit 8



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	159.13Å 159.13Å 362.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.45 – 3.25 48.45 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.45-3.25) 99.6 (48.45-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.7.0029, PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.218 , 0.247 0.227 , 0.253	Depositor DCC
R_{free} test set	2186 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	96.8	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 69.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	16219	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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: FES, OPC, CLA, CD, SQD, QNO, UMQ, BCR, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.54	0/1750	0.89	7/2388 (0.3%)
2	B	0.47	0/1288	0.94	5/1765 (0.3%)
3	C	0.51	0/2248	0.96	8/3061 (0.3%)
4	D	0.41	0/1267	0.84	1/1725 (0.1%)
5	E	0.65	0/253	1.32	5/340 (1.5%)
6	F	0.61	0/246	0.92	0/331
7	G	0.55	0/289	1.02	0/391
8	H	0.61	0/236	0.90	2/323 (0.6%)
All	All	0.51	0/7577	0.93	28/10324 (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
2	B	0	2
5	E	0	1
7	G	0	1
8	H	0	2
All	All	0	6

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	200	GLN	N-CA-C	8.64	120.16	108.23
3	C	211	ILE	CA-C-N	6.98	127.02	119.90
3	C	211	ILE	C-N-CA	6.98	127.02	119.90
5	E	12	ILE	N-CA-C	-6.54	101.12	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	178	GLY	N-CA-C	6.51	120.11	110.60
3	C	104	GLN	CA-C-N	6.24	126.20	119.78
3	C	104	GLN	C-N-CA	6.24	126.20	119.78
5	E	12	ILE	N-CA-CB	6.05	117.75	110.31
2	B	32	TRP	CA-C-N	5.78	127.06	119.84
2	B	32	TRP	C-N-CA	5.78	127.06	119.84
1	A	26	VAL	CA-C-N	5.75	123.80	119.66
1	A	26	VAL	C-N-CA	5.75	123.80	119.66
8	H	28	GLY	N-CA-C	5.68	121.45	111.57
5	E	9	ILE	N-CA-C	-5.62	101.47	109.51
1	A	27	PRO	CA-C-N	5.56	126.78	119.84
1	A	27	PRO	C-N-CA	5.56	126.78	119.84
2	B	32	TRP	C-N-CD	-5.40	102.87	125.00
4	D	137	GLY	N-CA-C	-5.39	104.88	111.35
3	C	207	VAL	N-CA-C	5.39	118.29	109.78
3	C	10	PRO	N-CA-C	5.29	117.16	110.70
5	E	23	ILE	N-CA-CB	5.26	119.90	111.23
5	E	23	ILE	N-CA-C	-5.23	98.46	109.34
8	H	3	ILE	N-CA-C	-5.20	104.59	111.09
1	A	154	VAL	CB-CA-C	-5.16	108.80	113.70
2	B	126	ARG	CA-C-N	5.10	124.71	119.05
2	B	126	ARG	C-N-CA	5.10	124.71	119.05
1	A	213	GLY	CA-C-N	5.02	125.49	120.52
1	A	213	GLY	C-N-CA	5.02	125.49	120.52

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	2	ALA	Peptide
2	B	32	TRP	Peptide
5	E	28	SER	Peptide
7	G	33	ASN	Peptide
8	H	2	GLU	Peptide
8	H	27	ASN	Peptide

5.2 Too-close contacts [i](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1698	1722	1720	75	2
2	B	1249	1309	1308	64	0
3	C	2200	2219	2218	129	2
4	D	1236	1224	1219	94	0
5	E	248	284	284	50	0
6	F	242	260	260	16	0
7	G	283	289	289	27	0
8	H	230	239	239	12	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	129	90	90	13	0
10	C	43	30	30	11	0
11	A	54	83	83	10	0
11	B	54	83	83	4	0
12	A	102	129	128	8	0
12	C	34	44	42	4	0
13	A	21	25	25	2	0
14	B	65	62	71	5	0
15	D	4	0	0	1	0
16	D	53	78	74	17	0
17	G	40	56	56	9	0
18	A	2	0	0	0	0
18	B	3	0	0	0	0
18	C	1	0	0	0	0
All	All	7993	8226	8219	434	2

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 27.

All (434) 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)
4:D:15:ARG:NH1	5:E:30:LYS:O	1.87	1.07
3:C:22:CYS:SG	10:C:302:HEM:C3B	2.51	1.04
3:C:25:CYS:SG	10:C:302:HEM:CAC	2.51	0.99
4:D:25:GLY:HA3	16:D:201:SQD:H341	1.42	0.99
4:D:25:GLY:HA2	16:D:201:SQD:H311	1.52	0.92
4:D:25:GLY:O	16:D:201:SQD:H332	1.72	0.89
5:E:6:VAL:O	5:E:9:ILE:O	1.92	0.88
5:E:20:VAL:HG22	6:F:29:ILE:HD11	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:25:GLY:HA3	16:D:201:SQD:C34	2.06	0.85
5:E:20:VAL:HG22	6:F:29:ILE:CD1	2.04	0.85
1:A:92:MET:HE3	11:A:305:OPC:HB2	1.57	0.85
14:B:202:CLA:HHC	14:B:202:CLA:HBB1	1.58	0.85
1:A:163:VAL:HG12	1:A:164:LEU:N	1.92	0.84
3:C:22:CYS:SG	10:C:302:HEM:CAB	2.68	0.81
4:D:134:ASP:OD2	4:D:171:ARG:NH2	2.15	0.79
1:A:35:CYS:SG	10:A:304:HEM:CAB	2.71	0.79
4:D:138:LYS:HD3	4:D:171:ARG:CZ	2.11	0.79
3:C:35:GLU:OE1	3:C:51:LYS:NZ	2.13	0.79
2:B:109:ILE:O	2:B:112:PRO:HD2	1.84	0.77
1:A:92:MET:HE3	11:A:305:OPC:HCB2	1.66	0.77
3:C:117:GLY:HA2	3:C:119:LEU:HG	1.66	0.76
3:C:25:CYS:SG	10:C:302:HEM:CBC	2.73	0.76
1:A:35:CYS:SG	10:A:304:HEM:CBB	2.74	0.76
3:C:41:LEU:HD22	3:C:252:PRO:HG3	1.67	0.75
6:F:22:LEU:O	6:F:26:LEU:HD23	1.86	0.75
7:G:4:PRO:O	7:G:7:ASP:N	2.20	0.74
3:C:271:MET:HE1	4:D:22:LEU:HD23	1.69	0.74
2:B:32:TRP:CD1	2:B:33:PRO:HD3	2.23	0.74
5:E:26:ILE:HG23	5:E:31:LEU:HB3	1.71	0.73
4:D:25:GLY:C	16:D:201:SQD:H332	2.13	0.72
4:D:15:ARG:NH2	5:E:29:ILE:O	2.22	0.72
4:D:25:GLY:HA2	16:D:201:SQD:C31	2.19	0.72
2:B:104:VAL:HB	2:B:105:PRO:HD3	1.72	0.71
4:D:136:THR:OG1	4:D:171:ARG:NE	2.18	0.71
10:A:302:HEM:HBB2	10:A:302:HEM:HMB2	1.73	0.70
1:A:8:PHE:HB3	1:A:14:ILE:HG13	1.73	0.70
4:D:25:GLY:CA	16:D:201:SQD:H341	2.21	0.70
4:D:118:ASN:OD1	4:D:121:GLU:HB2	1.91	0.70
8:H:17:TRP:O	8:H:21:MET:HG2	1.91	0.70
4:D:25:GLY:CA	16:D:201:SQD:H311	2.22	0.70
3:C:65:GLY:O	3:C:66:SER:O	2.10	0.69
1:A:111:LYS:NZ	2:B:120:PHE:O	2.25	0.69
4:D:15:ARG:CZ	5:E:30:LYS:O	2.39	0.69
1:A:41:LEU:HD23	10:A:304:HEM:HBC2	1.74	0.69
3:C:251:ASP:HB3	3:C:254:ARG:HD3	1.75	0.69
3:C:283:GLN:O	3:C:286:GLU:HG2	1.92	0.69
4:D:102:TYR:OH	4:D:136:THR:HA	1.93	0.68
4:D:15:ARG:HH12	5:E:31:LEU:HA	1.58	0.68
5:E:8:TYR:CZ	5:E:12:ILE:HD11	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:303:HEM:HBC2	10:A:303:HEM:HMC2	1.75	0.68
3:C:232:THR:O	3:C:233:ASN:OD1	2.11	0.67
5:E:22:ILE:O	5:E:23:ILE:O	2.12	0.67
1:A:113:PRO:HG3	2:B:22:MET:CE	2.24	0.67
3:C:225:VAL:CG1	3:C:229:GLU:HG2	2.24	0.67
3:C:21:VAL:O	3:C:24:ASN:HB2	1.95	0.67
4:D:62:ASN:O	4:D:63:ASN:ND2	2.28	0.67
1:A:83:ARG:NH2	2:B:61:MET:O	2.28	0.67
1:A:24:LYS:NZ	12:A:306:UMQ:O3	2.27	0.67
4:D:131:SER:HA	4:D:142:GLY:HA3	1.76	0.67
1:A:142:GLN:HG3	2:B:72:PRO:HG3	1.76	0.66
3:C:268:ALA:HB2	4:D:26:THR:HG22	1.78	0.66
2:B:82:TYR:HB2	2:B:83:PRO:HD3	1.77	0.66
3:C:276:LYS:HE2	8:H:25:GLY:O	1.95	0.66
4:D:73:HIS:CE1	4:D:79:VAL:HG13	2.31	0.66
3:C:271:MET:HE2	4:D:22:LEU:HB3	1.78	0.66
3:C:270:LEU:HA	8:H:21:MET:HE2	1.78	0.66
4:D:138:LYS:HD3	4:D:171:ARG:NH1	2.11	0.65
1:A:3:ASN:ND2	1:A:6:ASP:OD2	2.30	0.65
17:G:101:BCR:C21	17:G:101:BCR:H382	2.26	0.65
4:D:109:THR:HG22	4:D:144:ALA:HB1	1.77	0.65
3:C:219:VAL:HG21	3:C:231:LEU:HB2	1.79	0.65
7:G:33:ASN:O	7:G:34:GLU:O	2.14	0.65
1:A:113:PRO:HG3	2:B:22:MET:HE2	1.79	0.65
3:C:271:MET:CE	4:D:22:LEU:HD23	2.26	0.65
1:A:161:VAL:HG12	1:A:165:ILE:HG13	1.79	0.65
3:C:22:CYS:SG	10:C:302:HEM:C4B	2.89	0.65
3:C:211:ILE:O	3:C:211:ILE:HG13	1.96	0.64
4:D:136:THR:HG1	4:D:171:ARG:HE	1.43	0.64
4:D:25:GLY:CA	16:D:201:SQD:C34	2.75	0.64
4:D:129:HIS:HB2	15:D:200:FES:S1	2.38	0.64
3:C:64:ASP:OD1	3:C:65:GLY:N	2.31	0.64
4:D:139:VAL:O	4:D:140:ILE:HB	1.97	0.64
3:C:174:ALA:HB2	3:C:231:LEU:HD23	1.80	0.63
3:C:175:SER:HB2	3:C:209:ASP:OD1	1.98	0.63
6:F:31:GLY:O	6:F:32:ALA:CB	2.47	0.63
6:F:27:LEU:HD11	8:H:27:ASN:HA	1.81	0.63
2:B:128:VAL:O	2:B:132:ILE:HD12	1.99	0.63
4:D:137:GLY:O	4:D:138:LYS:O	2.17	0.63
4:D:145:PRO:O	4:D:146:LEU:HD13	1.99	0.63
2:B:154:THR:HG23	2:B:155:LEU:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:25:GLY:CA	16:D:201:SQD:C33	2.78	0.62
5:E:9:ILE:O	5:E:10:VAL:HG23	1.98	0.62
3:C:25:CYS:SG	10:C:302:HEM:HAC	2.40	0.62
5:E:14:LEU:O	5:E:18:ILE:HG13	1.98	0.62
11:A:305:OPC:HBZ2	17:G:101:BCR:H333	1.80	0.62
4:D:25:GLY:HA2	16:D:201:SQD:C32	2.30	0.62
4:D:165:TRP:CD1	4:D:167:GLU:O	2.52	0.62
3:C:193:VAL:HB	3:C:213:ALA:HB2	1.82	0.61
1:A:39:ILE:HD11	17:G:101:BCR:H313	1.83	0.61
2:B:142:TRP:CZ2	2:B:155:LEU:O	2.54	0.61
5:E:16:PHE:HZ	6:F:25:LEU:HD22	1.65	0.61
3:C:279:VAL:O	3:C:283:GLN:HG3	1.99	0.61
2:B:151:LEU:O	2:B:154:THR:HG22	2.01	0.61
2:B:37:LEU:HD23	2:B:38:TYR:CE2	2.36	0.61
3:C:144:PHE:CZ	3:C:251:ASP:HB2	2.36	0.61
1:A:92:MET:HE3	11:A:305:OPC:CBY	2.28	0.60
1:A:113:PRO:CG	2:B:22:MET:HE2	2.31	0.60
2:B:74:GLU:OE2	2:B:75:ILE:N	2.34	0.60
1:A:161:VAL:CG1	1:A:165:ILE:HG13	2.30	0.60
3:C:262:ILE:HG23	8:H:14:VAL:HG13	1.83	0.60
1:A:35:CYS:HG	10:A:304:HEM:CAB	2.10	0.60
2:B:45:MET:HE1	4:D:27:VAL:HA	1.83	0.60
3:C:3:PHE:HB2	3:C:6:GLN:NE2	2.16	0.60
3:C:144:PHE:CE1	3:C:251:ASP:HB2	2.37	0.60
3:C:34:VAL:HG22	3:C:151:LEU:HD22	1.84	0.60
1:A:103:ARG:O	1:A:107:THR:HB	2.02	0.59
4:D:73:HIS:O	4:D:74:ASN:HB2	2.01	0.59
2:B:32:TRP:CD1	2:B:33:PRO:CD	2.86	0.59
4:D:152:HIS:CE1	4:D:165:TRP:CE3	2.90	0.59
3:C:5:ALA:HB2	10:C:302:HEM:HBB2	1.83	0.59
2:B:123:PRO:HD2	7:G:25:ALA:HB1	1.84	0.59
5:E:5:ALA:O	5:E:9:ILE:HG12	2.03	0.58
5:E:12:ILE:O	5:E:13:ALA:CB	2.52	0.58
1:A:111:LYS:O	1:A:112:LYS:C	2.45	0.58
3:C:58:LEU:HD12	3:C:59:GLN:N	2.18	0.58
5:E:12:ILE:O	5:E:13:ALA:HB2	2.04	0.58
5:E:24:PHE:O	5:E:25:ALA:C	2.46	0.58
3:C:251:ASP:HB3	3:C:254:ARG:CD	2.33	0.58
4:D:165:TRP:NE1	4:D:167:GLU:O	2.37	0.58
3:C:173:THR:OG1	3:C:174:ALA:N	2.37	0.57
10:A:304:HEM:O2D	13:A:308:QNO:H3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:VAL:HG13	2:B:101:MET:CG	2.34	0.57
3:C:172:PHE:HB2	3:C:232:THR:HG21	1.86	0.57
3:C:273:ILE:HD12	8:H:25:GLY:HA3	1.85	0.57
7:G:4:PRO:O	7:G:5:LEU:C	2.46	0.57
3:C:171:VAL:HG12	3:C:234:ASN:HA	1.87	0.57
2:B:79:TRP:CD1	7:G:6:LEU:CD1	2.87	0.57
4:D:118:ASN:OD1	4:D:121:GLU:CB	2.53	0.56
6:F:13:PHE:CE2	6:F:17:PHE:HE1	2.23	0.56
3:C:173:THR:O	3:C:231:LEU:HG	2.05	0.56
4:D:124:PHE:HB2	4:D:133:TYR:HB2	1.87	0.56
3:C:194:LYS:O	3:C:195:TYR:C	2.48	0.56
4:D:15:ARG:NH1	5:E:31:LEU:HA	2.21	0.56
5:E:27:LYS:O	5:E:30:LYS:N	2.39	0.56
1:A:142:GLN:OE1	1:A:142:GLN:HA	2.05	0.56
3:C:84:ILE:HD12	3:C:103:PHE:CD1	2.41	0.56
3:C:197:VAL:O	3:C:209:ASP:N	2.38	0.56
7:G:28:GLN:C	7:G:30:LYS:H	2.14	0.56
2:B:95:LEU:O	2:B:95:LEU:HD23	2.06	0.55
6:F:31:GLY:O	6:F:32:ALA:HB2	2.06	0.55
4:D:143:PRO:O	4:D:145:PRO:HD3	2.07	0.55
4:D:36:TYR:HB3	4:D:37:PRO:HD3	1.88	0.55
6:F:7:TYR:O	6:F:11:LEU:HD12	2.07	0.55
3:C:71:ASN:HB2	10:C:302:HEM:O2A	2.06	0.55
3:C:194:LYS:O	3:C:196:GLN:N	2.40	0.55
12:C:301:UMQ:H6'2	12:C:301:UMQ:O5	2.06	0.55
3:C:187:GLU:HG3	3:C:187:GLU:O	2.07	0.55
3:C:225:VAL:HG11	3:C:229:GLU:HG2	1.89	0.55
12:A:309:UMQ:HJ1	16:D:201:SQD:H121	1.88	0.54
3:C:52:ILE:HG12	3:C:153:ALA:HB1	1.88	0.54
3:C:199:ILE:C	3:C:200:GLN:HG3	2.32	0.54
4:D:15:ARG:NH2	5:E:30:LYS:O	2.39	0.54
5:E:9:ILE:O	5:E:10:VAL:CB	2.54	0.54
1:A:8:PHE:HB3	1:A:14:ILE:CG1	2.36	0.54
7:G:20:GLY:N	17:G:101:BCR:H363	2.23	0.54
3:C:225:VAL:HG12	3:C:229:GLU:HG2	1.89	0.54
3:C:154:ASN:CG	3:C:155:ARG:N	2.65	0.54
3:C:273:ILE:HG13	8:H:21:MET:HE3	1.90	0.54
11:A:305:OPC:CBP	7:G:5:LEU:HD11	2.37	0.54
1:A:106:LEU:HD12	7:G:21:LEU:HD23	1.89	0.54
10:A:304:HEM:HMB1	10:A:304:HEM:HBB2	1.90	0.54
4:D:138:LYS:HA	4:D:147:SER:OG	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:LEU:O	1:A:182:ARG:NH1	2.41	0.53
5:E:23:ILE:O	5:E:26:ILE:N	2.42	0.53
1:A:92:MET:CE	11:A:305:OPC:HBY2	2.34	0.53
1:A:103:ARG:NH1	1:A:104:VAL:HA	2.24	0.53
3:C:90:ILE:HG23	3:C:94:LEU:HD13	1.90	0.53
3:C:160:ILE:O	10:C:302:HEM:HMD1	2.08	0.53
1:A:7:TRP:NE1	1:A:11:ARG:HH21	2.06	0.53
4:D:25:GLY:CA	16:D:201:SQD:H332	2.39	0.53
2:B:122:ASN:OD1	2:B:123:PRO:HD2	2.09	0.53
4:D:78:ARG:HG3	4:D:117:TRP:CD1	2.44	0.53
11:A:305:OPC:CBW	7:G:9:LEU:HD21	2.39	0.52
3:C:30:LYS:HB3	3:C:31:PRO:HD2	1.90	0.52
1:A:35:CYS:SG	10:A:304:HEM:C3B	3.02	0.52
11:A:305:OPC:HAX1	11:A:305:OPC:HBC1	1.90	0.52
1:A:163:VAL:O	1:A:166:SER:N	2.42	0.52
3:C:281:LYS:O	3:C:282:VAL:C	2.52	0.52
1:A:35:CYS:O	1:A:39:ILE:HD12	2.10	0.52
2:B:154:THR:CG2	2:B:155:LEU:N	2.73	0.52
2:B:37:LEU:CD2	2:B:38:TYR:CE2	2.93	0.52
4:D:116:PRO:HD2	4:D:125:LYS:O	2.09	0.52
4:D:138:LYS:HA	4:D:147:SER:CB	2.40	0.52
7:G:29:TYR:O	7:G:29:TYR:CD2	2.63	0.52
2:B:158:GLY:O	2:B:159:LEU:HD23	2.10	0.52
3:C:30:LYS:HB2	3:C:155:ARG:NH1	2.25	0.51
4:D:154:THR:C	4:D:155:VAL:HG22	2.35	0.51
7:G:26:TYR:O	7:G:30:LYS:HG3	2.11	0.51
1:A:146:TRP:CD1	2:B:72:PRO:HD3	2.44	0.51
3:C:84:ILE:HD12	3:C:103:PHE:CG	2.46	0.51
4:D:15:ARG:HH12	5:E:30:LYS:C	2.12	0.51
3:C:139:ASP:CG	3:C:142:ILE:HG12	2.36	0.51
3:C:231:LEU:HD12	3:C:232:THR:HG23	1.93	0.51
7:G:29:TYR:HD2	7:G:30:LYS:HG2	1.76	0.51
2:B:86:GLN:O	2:B:90:SER:OG	2.27	0.51
5:E:26:ILE:O	5:E:31:LEU:HB2	2.11	0.51
1:A:138:LEU:N	1:A:139:PRO:CD	2.74	0.51
3:C:34:VAL:HG22	3:C:151:LEU:CD2	2.41	0.50
10:C:302:HEM:HBC2	10:C:302:HEM:HMC2	1.93	0.50
4:D:138:LYS:HD2	4:D:171:ARG:HG3	1.92	0.50
1:A:39:ILE:HG22	1:A:96:MET:HG3	1.93	0.50
4:D:130:GLY:C	4:D:141:ARG:HH21	2.19	0.50
1:A:195:ILE:O	1:A:199:MET:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LEU:HB2	7:G:28:GLN:OE1	2.12	0.50
1:A:103:ARG:HH11	1:A:104:VAL:HA	1.76	0.50
2:B:11:ASP:O	2:B:15:ARG:HG3	2.12	0.50
3:C:200:GLN:HA	3:C:205:LYS:HG2	1.94	0.50
5:E:16:PHE:CE2	6:F:26:LEU:HD22	2.47	0.50
3:C:266:MET:HE1	5:E:11:PHE:CE2	2.47	0.49
4:D:28:THR:HB	16:D:201:SQD:H322	1.93	0.49
3:C:84:ILE:HD11	3:C:114:LEU:HD13	1.94	0.49
1:A:47:GLN:NE2	1:A:89:SER:HB3	2.28	0.49
10:A:304:HEM:HBC2	10:A:304:HEM:HHD	1.95	0.49
5:E:22:ILE:O	5:E:22:ILE:HG22	2.11	0.49
6:F:25:LEU:O	6:F:29:ILE:HG23	2.13	0.49
1:A:210:GLY:HA2	10:A:304:HEM:O1A	2.13	0.49
4:D:36:TYR:HB3	4:D:37:PRO:CD	2.42	0.49
1:A:4:VAL:O	1:A:5:TYR:C	2.55	0.49
1:A:22:THR:HG21	12:A:309:UMQ:H2'1	1.95	0.49
1:A:113:PRO:HG3	2:B:22:MET:HE3	1.95	0.49
1:A:115:GLU:O	1:A:119:ILE:HG13	2.13	0.49
2:B:102:ALA:O	2:B:105:PRO:HD2	2.12	0.49
2:B:113:PHE:O	2:B:116:ASN:HB2	2.13	0.49
3:C:71:ASN:OD1	3:C:120:PRO:HA	2.11	0.49
3:C:151:LEU:HD12	3:C:152:GLY:H	1.77	0.49
4:D:154:THR:C	4:D:155:VAL:CG2	2.85	0.49
6:F:13:PHE:CE2	6:F:17:PHE:CE1	3.00	0.49
1:A:103:ARG:HA	7:G:21:LEU:HD21	1.94	0.48
1:A:166:SER:HB3	1:A:170:ARG:NH2	2.28	0.48
3:C:180:ILE:HG13	3:C:198:SER:O	2.13	0.48
10:C:302:HEM:HBB2	10:C:302:HEM:HHC	1.95	0.48
4:D:130:GLY:C	4:D:141:ARG:NH2	2.71	0.48
1:A:20:ASP:OD1	12:A:306:UMQ:O3	2.15	0.48
3:C:226:LYS:HG2	3:C:227:ALA:H	1.79	0.48
1:A:35:CYS:C	1:A:39:ILE:HD12	2.38	0.48
3:C:180:ILE:HD11	3:C:197:VAL:HG13	1.94	0.48
2:B:84:VAL:HG13	2:B:101:MET:HG2	1.94	0.48
3:C:275:LYS:HE2	4:D:20:ASN:OD1	2.13	0.48
4:D:156:GLN:HB2	4:D:161:VAL:CG2	2.44	0.48
2:B:142:TRP:HZ2	2:B:155:LEU:O	1.96	0.48
3:C:180:ILE:CD1	3:C:197:VAL:CG1	2.92	0.48
2:B:37:LEU:HD23	2:B:38:TYR:CD2	2.49	0.48
2:B:100:LEU:CD2	11:B:203:OPC:HBX2	2.43	0.48
14:B:202:CLA:C3C	11:B:203:OPC:HBT1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:5:LEU:O	7:G:9:LEU:HB2	2.14	0.48
7:G:10:VAL:O	7:G:14:VAL:HG23	2.13	0.48
2:B:142:TRP:CH2	2:B:155:LEU:HD23	2.48	0.47
5:E:22:ILE:O	5:E:22:ILE:CG2	2.62	0.47
2:B:99:LEU:O	2:B:103:SER:OG	2.30	0.47
5:E:9:ILE:O	5:E:10:VAL:HB	2.14	0.47
7:G:31:ARG:HH11	7:G:31:ARG:HG2	1.79	0.47
3:C:94:LEU:O	3:C:98:VAL:HG23	2.14	0.47
4:D:25:GLY:HA2	16:D:201:SQD:C33	2.42	0.47
4:D:156:GLN:O	4:D:157:ASP:C	2.57	0.47
3:C:58:LEU:HD12	3:C:58:LEU:C	2.38	0.47
3:C:281:LYS:HG2	3:C:282:VAL:N	2.29	0.47
4:D:73:HIS:CE1	4:D:79:VAL:CG1	2.98	0.47
3:C:36:VAL:HG21	3:C:247:ILE:HB	1.97	0.47
3:C:199:ILE:C	3:C:200:GLN:CG	2.88	0.47
2:B:104:VAL:O	2:B:108:LEU:HB2	2.15	0.47
4:D:156:GLN:HB2	4:D:161:VAL:HG23	1.95	0.47
16:D:201:SQD:H131	16:D:201:SQD:H161	1.55	0.47
3:C:36:VAL:HG11	3:C:149:ILE:HD13	1.96	0.47
12:C:301:UMQ:HL3	4:D:37:PRO:CG	2.45	0.47
5:E:9:ILE:O	5:E:10:VAL:CG2	2.61	0.46
5:E:16:PHE:CZ	6:F:25:LEU:HD22	2.48	0.46
5:E:22:ILE:O	5:E:23:ILE:C	2.53	0.46
5:E:26:ILE:CG2	5:E:31:LEU:HB3	2.44	0.46
4:D:15:ARG:NH1	5:E:31:LEU:HG	2.30	0.46
5:E:24:PHE:O	5:E:27:LYS:N	2.48	0.46
3:C:271:MET:HB3	4:D:23:ALA:HA	1.97	0.46
4:D:125:LYS:O	4:D:127:PRO:HD3	2.14	0.46
17:G:101:BCR:H382	17:G:101:BCR:H21C	1.97	0.46
2:B:118:ASN:ND2	11:B:203:OPC:HAH1	2.30	0.46
3:C:60:GLN:OE1	3:C:157:ARG:HG3	2.16	0.46
4:D:141:ARG:HG2	4:D:142:GLY:H	1.80	0.46
3:C:3:PHE:O	3:C:6:GLN:HG2	2.16	0.46
4:D:169:ASP:OD2	4:D:171:ARG:HB3	2.15	0.46
5:E:2:ILE:O	5:E:6:VAL:HG23	2.14	0.46
2:B:10:SER:O	2:B:12:PRO:HD3	2.15	0.46
3:C:59:GLN:HB3	3:C:68:VAL:O	2.16	0.46
2:B:79:TRP:CD1	7:G:6:LEU:HD11	2.51	0.46
1:A:154:VAL:HB	1:A:155:PRO:HD3	1.98	0.46
3:C:88:GLU:O	3:C:88:GLU:HG2	2.16	0.46
4:D:108:CYS:HB2	4:D:113:CYS:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:124:PHE:O	4:D:132:GLN:HA	2.15	0.46
11:B:203:OPC:HAE2	11:B:203:OPC:OAI	2.15	0.46
3:C:229:GLU:OE2	3:C:230:ALA:N	2.48	0.46
4:D:152:HIS:ND1	4:D:165:TRP:CE3	2.84	0.46
5:E:9:ILE:HG12	5:E:9:ILE:H	1.59	0.45
12:C:301:UMQ:H6'2	12:C:301:UMQ:C5	2.46	0.45
4:D:102:TYR:HA	4:D:151:CYS:O	2.17	0.45
5:E:16:PHE:CE2	6:F:26:LEU:CD2	3.00	0.45
1:A:29:HIS:CG	1:A:214:PRO:HA	2.51	0.45
2:B:145:ILE:O	2:B:148:THR:HB	2.17	0.45
4:D:73:HIS:CE1	4:D:79:VAL:HG22	2.52	0.45
11:A:305:OPC:HBW2	7:G:9:LEU:HD21	1.97	0.45
2:B:45:MET:HE2	4:D:30:VAL:HB	1.98	0.45
14:B:202:CLA:O2A	14:B:202:CLA:C4	2.65	0.45
4:D:152:HIS:O	4:D:162:LEU:HD23	2.16	0.45
2:B:111:VAL:N	2:B:112:PRO:HD2	2.32	0.45
3:C:54:TYR:OH	3:C:121:GLY:HA3	2.16	0.45
1:A:111:LYS:HE2	2:B:115:GLU:O	2.16	0.45
3:C:12:THR:OG1	3:C:13:PRO:HD2	2.17	0.45
2:B:37:LEU:CD2	2:B:38:TYR:CZ	3.00	0.45
5:E:22:ILE:O	5:E:26:ILE:HB	2.17	0.45
1:A:39:ILE:CD1	17:G:101:BCR:C31	2.95	0.45
3:C:180:ILE:HD12	3:C:197:VAL:CG1	2.47	0.45
1:A:161:VAL:O	1:A:162:GLY:C	2.60	0.44
2:B:33:PRO:HA	2:B:37:LEU:HB3	1.99	0.44
4:D:73:HIS:ND1	4:D:79:VAL:CG2	2.80	0.44
7:G:29:TYR:O	7:G:29:TYR:CG	2.69	0.44
1:A:207:ARG:NH1	13:A:308:QNO:H3	2.32	0.44
4:D:40:LYS:HA	4:D:40:LYS:HD2	1.83	0.44
2:B:77:PRO:HB2	2:B:81:LEU:HD12	1.99	0.44
3:C:1:TYR:O	3:C:2:PRO:C	2.59	0.44
3:C:266:MET:SD	8:H:13:VAL:HG12	2.58	0.44
3:C:1:TYR:HD2	3:C:118:PRO:HG3	1.83	0.44
4:D:73:HIS:ND1	4:D:79:VAL:HG22	2.32	0.44
3:C:151:LEU:HD12	3:C:152:GLY:N	2.33	0.44
3:C:255:VAL:O	3:C:259:ILE:HG13	2.17	0.44
7:G:34:GLU:O	7:G:35:LEU:HD12	2.17	0.44
5:E:13:ALA:O	5:E:14:LEU:C	2.59	0.44
11:A:305:OPC:OAI	11:A:305:OPC:HBG3	2.17	0.44
3:C:262:ILE:HG23	8:H:14:VAL:CG1	2.47	0.43
5:E:23:ILE:O	5:E:24:PHE:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:47:LYS:HG3	3:C:128:VAL:HG13	2.00	0.43
8:H:23:VAL:O	8:H:27:ASN:N	2.51	0.43
2:B:4:LEU:HG	2:B:5:LYS:N	2.33	0.43
2:B:32:TRP:NE1	16:D:201:SQD:O3	2.50	0.43
2:B:33:PRO:O	2:B:34:ASN:C	2.60	0.43
3:C:271:MET:CE	4:D:22:LEU:HB3	2.47	0.43
4:D:133:TYR:CD2	4:D:148:LEU:HG	2.53	0.43
4:D:145:PRO:O	4:D:146:LEU:CD1	2.65	0.43
1:A:166:SER:O	1:A:170:ARG:HG2	2.18	0.43
3:C:9:TYR:O	3:C:106:TYR:OH	2.32	0.43
1:A:4:VAL:C	1:A:6:ASP:N	2.74	0.43
2:B:53:ALA:O	2:B:57:LEU:HG	2.18	0.43
3:C:20:ILE:HD13	3:C:152:GLY:HA3	2.01	0.43
3:C:211:ILE:O	3:C:211:ILE:CG1	2.65	0.43
2:B:3:THR:O	2:B:29:GLU:HA	2.19	0.43
3:C:219:VAL:HG12	3:C:220:SER:N	2.34	0.43
7:G:21:LEU:HD12	7:G:21:LEU:HA	1.89	0.43
2:B:134:LEU:HD12	2:B:134:LEU:HA	1.79	0.43
3:C:10:PRO:N	3:C:11:PRO:HD3	2.33	0.43
3:C:109:GLY:O	3:C:111:ASP:N	2.50	0.43
3:C:206:THR:O	3:C:206:THR:CG2	2.65	0.43
4:D:78:ARG:HG3	4:D:117:TRP:NE1	2.34	0.43
4:D:90:TYR:CD1	4:D:106:ALA:HB2	2.53	0.43
7:G:30:LYS:C	7:G:32:PRO:HD3	2.44	0.43
5:E:26:ILE:HG21	5:E:32:ILE:CD1	2.49	0.43
3:C:161:TYR:O	3:C:163:THR:N	2.52	0.42
3:C:262:ILE:HG22	3:C:263:CYS:N	2.34	0.42
14:B:202:CLA:O2A	14:B:202:CLA:H42	2.19	0.42
3:C:178:GLY:HA3	3:C:202:ASP:OD2	2.19	0.42
3:C:251:ASP:OD2	3:C:252:PRO:HD2	2.19	0.42
3:C:281:LYS:O	3:C:284:ALA:N	2.47	0.42
4:D:89:THR:HG22	4:D:105:ASN:HA	2.01	0.42
1:A:3:ASN:CG	1:A:4:VAL:H	2.27	0.42
12:A:306:UMQ:O2'	12:A:306:UMQ:HB2	2.18	0.42
3:C:68:VAL:HG22	3:C:69:GLY:N	2.33	0.42
3:C:245:THR:OG1	3:C:246:GLU:N	2.51	0.42
4:D:138:LYS:HA	4:D:147:SER:HB3	2.01	0.42
5:E:23:ILE:HD13	5:E:23:ILE:HG21	1.85	0.42
5:E:26:ILE:HG23	5:E:31:LEU:CB	2.47	0.42
1:A:6:ASP:O	1:A:10:GLU:HG3	2.20	0.42
5:E:16:PHE:HE1	5:E:20:VAL:HG21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ARG:HD2	10:A:302:HEM:O1D	2.20	0.42
1:A:108:GLY:HA3	2:B:121:GLN:HA	2.01	0.42
1:A:154:VAL:HG22	2:B:88:LEU:HD21	2.02	0.42
1:A:161:VAL:HG13	1:A:164:LEU:HD12	2.02	0.42
12:A:306:UMQ:O2'	12:A:306:UMQ:CA	2.68	0.42
12:A:306:UMQ:O5	12:A:306:UMQ:C3'	2.67	0.42
3:C:36:VAL:HG23	3:C:37:PRO:O	2.18	0.42
3:C:43:ASP:HA	3:C:133:SER:O	2.19	0.42
4:D:15:ARG:HH12	5:E:31:LEU:CA	2.31	0.42
1:A:103:ARG:HD2	1:A:103:ARG:C	2.44	0.42
2:B:37:LEU:HD21	4:D:24:PHE:HZ	1.84	0.42
3:C:233:ASN:OD1	3:C:233:ASN:C	2.62	0.41
3:C:10:PRO:N	3:C:11:PRO:CD	2.83	0.41
3:C:35:GLU:HB2	3:C:49:VAL:HB	2.01	0.41
17:G:101:BCR:H15C	17:G:101:BCR:H351	1.89	0.41
1:A:9:GLN:OE1	1:A:15:GLN:HB2	2.20	0.41
1:A:39:ILE:HD11	17:G:101:BCR:C31	2.49	0.41
3:C:161:TYR:C	3:C:163:THR:N	2.77	0.41
3:C:264:LEU:HD13	4:D:30:VAL:CG2	2.49	0.41
7:G:29:TYR:C	7:G:30:LYS:CG	2.93	0.41
3:C:3:PHE:C	3:C:6:GLN:HG2	2.46	0.41
2:B:40:PHE:HB2	2:B:41:PRO:HD3	2.02	0.41
12:C:301:UMQ:HL3	4:D:37:PRO:HG3	2.02	0.41
5:E:10:VAL:O	5:E:14:LEU:HD12	2.19	0.41
3:C:270:LEU:HA	8:H:21:MET:CE	2.48	0.41
3:C:273:ILE:HD12	8:H:25:GLY:CA	2.50	0.41
5:E:18:ILE:O	5:E:22:ILE:HG13	2.21	0.41
1:A:53:ALA:HB1	4:D:41:TYR:CE2	2.56	0.41
1:A:80:TRP:CH2	3:C:254:ARG:HG2	2.55	0.41
3:C:187:GLU:O	3:C:188:ASP:C	2.62	0.41
5:E:29:ILE:O	5:E:29:ILE:HG22	2.21	0.41
5:E:23:ILE:O	5:E:26:ILE:HB	2.20	0.41
7:G:29:TYR:HD2	7:G:30:LYS:CG	2.33	0.41
1:A:14:ILE:HG22	12:A:307:UMQ:HD1	2.03	0.41
1:A:103:ARG:O	1:A:103:ARG:HD2	2.21	0.41
1:A:211:ILE:N	10:A:304:HEM:O1A	2.54	0.41
2:B:32:TRP:CG	2:B:33:PRO:N	2.89	0.41
2:B:45:MET:HE2	4:D:30:VAL:CB	2.51	0.41
3:C:72:VAL:HG21	3:C:124:TYR:O	2.20	0.41
3:C:223:GLN:HB3	3:C:225:VAL:CG2	2.51	0.41
3:C:281:LYS:O	3:C:283:GLN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:117:GLY:HA2	3:C:118:PRO:C	2.46	0.41
2:B:126:ARG:N	2:B:127:PRO:HD3	2.35	0.40
3:C:161:TYR:C	3:C:163:THR:H	2.30	0.40
3:C:171:VAL:HG12	3:C:233:ASN:O	2.21	0.40
1:A:36:LEU:HD23	1:A:99:LEU:C	2.47	0.40
1:A:105:TYR:C	1:A:107:THR:H	2.29	0.40
1:A:129:VAL:HG21	14:B:202:CLA:H43	2.02	0.40
2:B:75:ILE:HG12	2:B:75:ILE:O	2.20	0.40
6:F:18:VAL:O	6:F:22:LEU:HG	2.21	0.40
1:A:81:LEU:HD22	1:A:85:ILE:HG13	2.04	0.40
3:C:70:LEU:HD23	3:C:70:LEU:H	1.86	0.40
4:D:140:ILE:O	4:D:140:ILE:HG13	2.21	0.40
6:F:20:TRP:C	6:F:20:TRP:CD1	2.98	0.40
1:A:105:TYR:OH	2:B:115:GLU:OE2	2.37	0.40
3:C:134:PRO:HB2	3:C:142:ILE:HG21	2.04	0.40
7:G:23:TYR:CD1	17:G:101:BCR:H21C	2.56	0.40

All (2) 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)
1:A:112:LYS:NZ	3:C:87:GLU:OE1[8_665]	1.82	0.38
1:A:112:LYS:HZ2	3:C:87:GLU:OE1[8_665]	1.41	0.19

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	211/215 (98%)	187 (89%)	19 (9%)	5 (2%)	4	23
2	B	158/160 (99%)	143 (90%)	11 (7%)	4 (2%)	4	22
3	C	284/289 (98%)	235 (83%)	41 (14%)	8 (3%)	4	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	155/179 (87%)	123 (79%)	22 (14%)	10 (6%)	1	7
5	E	30/32 (94%)	16 (53%)	11 (37%)	3 (10%)	0	3
6	F	30/35 (86%)	29 (97%)	1 (3%)	0	100	100
7	G	35/37 (95%)	26 (74%)	6 (17%)	3 (9%)	0	4
8	H	27/29 (93%)	26 (96%)	0	1 (4%)	2	15
All	All	930/976 (95%)	785 (84%)	111 (12%)	34 (4%)	2	15

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	GLY
2	B	33	PRO
2	B	34	ASN
2	B	75	ILE
3	C	66	SER
3	C	186	GLU
3	C	192	ASN
3	C	195	TYR
4	D	138	LYS
4	D	139	VAL
4	D	140	ILE
5	E	10	VAL
5	E	13	ALA
5	E	23	ILE
7	G	34	GLU
1	A	23	SER
2	B	22	MET
3	C	233	ASN
4	D	63	ASN
4	D	121	GLU
4	D	171	ARG
1	A	4	VAL
3	C	187	GLU
3	C	282	VAL
4	D	74	ASN
4	D	112	GLY
4	D	155	VAL
1	A	170	ARG
3	C	206	THR
4	D	157	ASP

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Mol	Chain	Res	Type
7	G	5	LEU
7	G	33	ASN
8	H	2	GLU
1	A	163	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	183/184 (100%)	170 (93%)	13 (7%)	13	39
2	B	137/137 (100%)	126 (92%)	11 (8%)	11	35
3	C	240/243 (99%)	204 (85%)	36 (15%)	3	13
4	D	133/146 (91%)	119 (90%)	14 (10%)	6	24
5	E	25/25 (100%)	20 (80%)	5 (20%)	1	5
6	F	24/27 (89%)	21 (88%)	3 (12%)	4	19
7	G	28/28 (100%)	25 (89%)	3 (11%)	6	24
8	H	24/24 (100%)	23 (96%)	1 (4%)	26	53
All	All	794/814 (98%)	708 (89%)	86 (11%)	6	23

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	17	LEU
1	A	36	LEU
1	A	61	THR
1	A	63	THR
1	A	81	LEU
1	A	87	ARG
1	A	103	ARG
1	A	107	THR
1	A	163	VAL
1	A	164	LEU

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Mol	Chain	Res	Type
1	A	173	SER
1	A	200	LEU
2	B	35	ASP
2	B	39	VAL
2	B	64	GLU
2	B	74	GLU
2	B	76	LEU
2	B	95	LEU
2	B	96	LEU
2	B	100	LEU
2	B	134	LEU
2	B	138	LEU
2	B	159	LEU
3	C	22	CYS
3	C	24	ASN
3	C	34	VAL
3	C	58	LEU
3	C	60	GLN
3	C	67	LYS
3	C	84	ILE
3	C	88	GLU
3	C	94	LEU
3	C	107	LYS
3	C	123	GLN
3	C	131	VAL
3	C	137	THR
3	C	160	ILE
3	C	171	VAL
3	C	180	ILE
3	C	181	THR
3	C	186	GLU
3	C	193	VAL
3	C	205	LYS
3	C	206	THR
3	C	208	VAL
3	C	211	ILE
3	C	223	GLN
3	C	225	VAL
3	C	229	GLU
3	C	245	THR
3	C	249	LEU
3	C	254	ARG

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Mol	Chain	Res	Type
3	C	256	LYS
3	C	262	ILE
3	C	264	LEU
3	C	267	LEU
3	C	270	LEU
3	C	281	LYS
3	C	282	VAL
4	D	15	ARG
4	D	17	GLN
4	D	22	LEU
4	D	35	LEU
4	D	40	LYS
4	D	43	ILE
4	D	54	THR
4	D	59	LYS
4	D	135	GLU
4	D	139	VAL
4	D	146	LEU
4	D	150	LEU
4	D	154	THR
4	D	155	VAL
5	E	9	ILE
5	E	12	ILE
5	E	14	LEU
5	E	31	LEU
5	E	32	ILE
6	F	5	MET
6	F	7	TYR
6	F	10	LEU
7	G	6	LEU
7	G	9	LEU
7	G	21	LEU
8	H	2	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	209	GLN
3	C	154	ASN
3	C	233	ASN
4	D	63	ASN

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Mol	Chain	Res	Type
4	D	82	GLN
4	D	156	GLN
4	D	159	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 2 are monoatomic - leaving 15 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	$\# Z > 2$
13	QNO	A	308	10	21,22,22	2.76	5 (23%)	22,28,28	2.65	2 (9%)
10	HEM	A	303	1	50,50,50	1.79	6 (12%)	67,82,82	1.31	6 (8%)
12	UMQ	C	301	-	35,35,35	1.29	5 (14%)	46,46,46	2.00	10 (21%)
12	UMQ	A	306	-	35,35,35	1.16	5 (14%)	46,46,46	1.80	8 (17%)
17	BCR	G	101	-	41,41,41	2.20	20 (48%)	56,56,56	2.44	26 (46%)
10	HEM	C	302	3	50,50,50	1.82	8 (16%)	67,82,82	1.50	11 (16%)
15	FES	D	200	4	0,4,4	-	-	-	-	-
10	HEM	A	302	1	50,50,50	1.80	9 (18%)	67,82,82	1.25	6 (8%)
11	OPC	A	305	-	53,53,54	1.02	4 (7%)	59,61,64	1.14	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	SQD	D	201	-	51,53,54	3.21	17 (33%)	60,63,65	2.46	18 (30%)
11	OPC	B	203	-	53,53,54	1.06	3 (5%)	59,61,64	0.95	3 (5%)
12	UMQ	A	309	-	35,35,35	1.23	5 (14%)	46,46,46	2.63	18 (39%)
14	CLA	B	202	18	69,73,73	1.22	7 (10%)	82,113,113	1.45	10 (12%)
10	HEM	A	304	13,18	50,50,50	2.09	7 (14%)	67,82,82	1.42	6 (8%)
12	UMQ	A	307	-	35,35,35	1.26	5 (14%)	46,46,46	2.04	13 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	QNO	A	308	10	1/1/0/0	4/9/9/9	0/2/2/2
10	HEM	A	303	1	-	2/14/54/54	-
12	UMQ	A	306	-	1/1/10/10	10/20/60/60	0/2/2/2
17	BCR	G	101	-	-	24/29/63/63	0/2/2/2
10	HEM	C	302	3	-	3/14/54/54	-
15	FES	D	200	4	-	-	0/1/1/1
10	HEM	A	302	1	-	4/14/54/54	-
11	OPC	A	305	-	-	24/57/57/60	-
16	SQD	D	201	-	3/3/9/9	27/49/65/69	0/1/1/1
11	OPC	B	203	-	-	23/57/57/60	-
12	UMQ	A	307	-	2/2/10/10	8/20/60/60	0/2/2/2
12	UMQ	A	309	-	4/4/10/10	16/20/60/60	0/2/2/2
14	CLA	B	202	18	2/2/17/20	16/39/115/115	-
10	HEM	A	304	13,18	-	7/14/54/54	-
12	UMQ	C	301	-	1/1/10/10	7/20/60/60	0/2/2/2

All (106) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	D	201	SQD	C2-C3	-10.49	1.32	1.52
16	D	201	SQD	O6-C44	9.55	1.60	1.43
10	A	304	HEM	C3D-C2D	8.23	1.54	1.36
16	D	201	SQD	C8-C7	7.78	1.73	1.50
10	C	302	HEM	C3D-C2D	7.68	1.53	1.36
10	A	302	HEM	C3D-C2D	7.67	1.53	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	303	HEM	C3D-C2D	7.53	1.53	1.36
13	A	308	QNO	OH-N1	-7.10	1.30	1.38
16	D	201	SQD	C4-C5	-6.23	1.39	1.53
13	A	308	QNO	C5-C6	-5.99	1.33	1.42
16	D	201	SQD	O47-C7	5.96	1.51	1.34
16	D	201	SQD	O5-C1	5.71	1.57	1.42
10	A	304	HEM	FE-ND	5.62	2.12	1.94
13	A	308	QNO	C3-C2	5.35	1.47	1.38
13	A	308	QNO	C4-C5	-5.25	1.31	1.42
10	A	304	HEM	FE-NB	5.10	2.10	1.94
10	C	302	HEM	FE-NB	5.09	2.10	1.94
10	A	302	HEM	FE-ND	5.02	2.10	1.94
16	D	201	SQD	O47-C45	4.89	1.58	1.46
10	A	304	HEM	FE-NC	4.72	2.10	1.95
16	D	201	SQD	C46-C45	-4.41	1.37	1.50
16	D	201	SQD	C3-C4	4.38	1.59	1.52
10	A	303	HEM	FE-NB	4.09	2.07	1.94
14	B	202	CLA	C1D-ND	3.82	1.42	1.37
11	A	305	OPC	OAN-CAO	3.69	1.44	1.34
16	D	201	SQD	C2-C1	-3.63	1.41	1.50
10	A	303	HEM	FE-ND	3.57	2.05	1.94
11	B	203	OPC	OAN-CAO	3.51	1.44	1.34
17	G	101	BCR	C23-C22	3.49	1.53	1.46
17	G	101	BCR	C20-C21	3.47	1.53	1.43
17	G	101	BCR	C15-C14	3.43	1.53	1.43
14	B	202	CLA	C4B-NB	3.43	1.42	1.37
13	A	308	QNO	C2-N1	3.42	1.43	1.36
17	G	101	BCR	C26-C25	3.37	1.40	1.34
17	G	101	BCR	C11-C10	3.36	1.53	1.43
10	A	302	HEM	FE-NC	3.29	2.06	1.95
17	G	101	BCR	C16-C17	3.26	1.53	1.43
10	A	304	HEM	CAB-C3B	3.26	1.56	1.47
17	G	101	BCR	C12-C13	3.25	1.52	1.46
17	G	101	BCR	C19-C18	3.21	1.52	1.46
16	D	201	SQD	O5-C5	3.18	1.52	1.44
10	C	302	HEM	CAB-C3B	3.09	1.55	1.47
10	A	303	HEM	CAB-C3B	3.05	1.55	1.47
12	A	307	UMQ	C4-C5	-2.96	1.46	1.53
10	A	304	HEM	CAC-C3C	2.94	1.55	1.47
17	G	101	BCR	C31-C1	-2.92	1.48	1.53
10	A	302	HEM	FE-NB	2.91	2.03	1.94
12	A	306	UMQ	C4-C5	-2.88	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	C	302	HEM	CAC-C3C	2.86	1.55	1.47
17	G	101	BCR	C8-C9	2.83	1.52	1.46
11	B	203	OPC	OBJ-CBK	2.81	1.41	1.33
12	C	301	UMQ	C4-C5	-2.79	1.47	1.53
10	A	302	HEM	CAC-C3C	2.76	1.54	1.47
12	C	301	UMQ	O5'-C5'	-2.75	1.37	1.44
16	D	201	SQD	O48-C46	-2.75	1.39	1.45
17	G	101	BCR	C32-C1	-2.71	1.48	1.53
10	A	302	HEM	CAB-C3B	2.70	1.54	1.47
12	A	309	UMQ	C4-C5	-2.69	1.47	1.53
14	B	202	CLA	C3B-C4B	2.68	1.50	1.42
12	C	301	UMQ	O2'-C2'	-2.68	1.36	1.43
14	B	202	CLA	C1B-C2B	2.66	1.49	1.43
10	A	303	HEM	CAC-C3C	2.63	1.54	1.47
16	D	201	SQD	C10-C9	2.62	1.64	1.51
10	C	302	HEM	FE-ND	2.59	2.02	1.94
16	D	201	SQD	C9-C8	2.59	1.61	1.52
10	A	303	HEM	FE-NC	2.53	2.03	1.95
10	A	302	HEM	CMB-C2B	2.53	1.55	1.50
12	A	309	UMQ	O5'-C5'	-2.53	1.38	1.44
17	G	101	BCR	C24-C23	2.49	1.40	1.33
11	A	305	OPC	OBJ-CBI	-2.47	1.39	1.45
12	A	307	UMQ	O5'-C5'	-2.46	1.38	1.44
17	G	101	BCR	C40-C30	-2.45	1.49	1.53
12	A	309	UMQ	C3-C4	-2.42	1.46	1.52
17	G	101	BCR	C24-C25	2.39	1.53	1.45
11	A	305	OPC	OBJ-CBK	2.39	1.40	1.33
14	B	202	CLA	CHC-C1C	2.39	1.43	1.38
12	A	306	UMQ	O2'-C2'	-2.39	1.37	1.43
12	A	309	UMQ	O2'-C2'	-2.38	1.37	1.43
12	A	307	UMQ	O3'-C3'	-2.35	1.37	1.43
10	A	302	HEM	CMC-C2C	2.34	1.55	1.50
12	A	306	UMQ	O5'-C5'	-2.34	1.38	1.44
10	C	302	HEM	CMB-C2B	2.32	1.55	1.50
16	D	201	SQD	C18-C17	2.32	1.63	1.51
17	G	101	BCR	C1-C6	-2.31	1.50	1.53
12	A	307	UMQ	C3-C4	-2.30	1.46	1.52
12	A	307	UMQ	O2'-C2'	-2.30	1.37	1.43
17	G	101	BCR	C20-C19	2.28	1.40	1.34
12	C	301	UMQ	C3-C4	-2.27	1.46	1.52
10	A	304	HEM	FE-NA	2.22	2.02	1.95
11	A	305	OPC	CAV-CAW	2.22	1.44	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	203	OPC	CAV-CAW	2.21	1.44	1.31
17	G	101	BCR	C11-C12	2.20	1.40	1.34
10	A	302	HEM	C2A-C3A	-2.19	1.33	1.38
16	D	201	SQD	C11-C10	2.18	1.62	1.51
12	A	306	UMQ	O3'-C3'	-2.18	1.37	1.43
17	G	101	BCR	C39-C30	-2.16	1.49	1.53
10	C	302	HEM	FE-NA	2.16	2.02	1.95
12	C	301	UMQ	O3'-C3'	-2.14	1.37	1.43
17	G	101	BCR	C29-C28	-2.13	1.47	1.52
17	G	101	BCR	C7-C6	2.12	1.52	1.45
14	B	202	CLA	CMB-C2B	-2.10	1.46	1.50
16	D	201	SQD	O6-C1	2.06	1.46	1.40
14	B	202	CLA	CMC-C2C	-2.06	1.46	1.50
10	C	302	HEM	CMA-C3A	2.05	1.55	1.50
12	A	309	UMQ	O3'-C3'	-2.05	1.37	1.43
12	A	306	UMQ	O5-C5	-2.02	1.39	1.44

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	D	201	SQD	C3-C4-C5	9.62	119.63	109.99
13	A	308	QNO	C3-C2-N1	-9.08	108.97	118.94
13	A	308	QNO	C4-C3-C2	-7.35	112.89	118.45
14	B	202	CLA	C4A-NA-C1A	6.94	109.85	106.68
12	A	309	UMQ	O5'-C1'-C2'	6.56	123.84	110.37
12	A	309	UMQ	O1'-C1'-C2'	6.50	118.15	108.27
12	C	301	UMQ	O1'-C1'-C2'	6.47	118.10	108.27
16	D	201	SQD	C2-C3-C4	6.13	119.50	110.67
17	G	101	BCR	C7-C8-C9	-6.13	117.17	126.23
10	A	304	HEM	C4D-ND-C1D	5.58	111.81	105.21
16	D	201	SQD	C1-O5-C5	5.44	121.42	113.05
12	A	306	UMQ	CA-O1'-C1'	5.43	122.96	113.68
10	C	302	HEM	C4D-ND-C1D	5.30	111.49	105.21
12	C	301	UMQ	O1-C1-O5	5.16	124.27	110.69
11	A	305	OPC	OAN-CAO-CAP	5.15	122.62	111.48
17	G	101	BCR	C16-C17-C18	-5.00	120.27	127.28
12	A	307	UMQ	O2'-C2'-C1'	4.94	121.85	110.08
16	D	201	SQD	O4-C4-C5	4.92	121.45	109.32
17	G	101	BCR	C20-C21-C22	-4.88	120.43	127.28
17	G	101	BCR	C15-C14-C13	-4.82	120.51	127.28
10	A	303	HEM	C4D-ND-C1D	4.80	110.90	105.21
12	A	309	UMQ	CA-O1'-C1'	4.73	121.75	113.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	306	UMQ	O1-C4'-C5'	4.70	121.81	109.48
12	A	307	UMQ	O2'-C2'-C3'	4.69	121.42	110.38
12	A	309	UMQ	C2'-C3'-C4'	4.64	120.22	109.68
12	A	307	UMQ	CA-O1'-C1'	4.62	121.57	113.68
16	D	201	SQD	O3-C3-C4	4.55	119.57	110.15
17	G	101	BCR	C1-C6-C5	-4.52	116.46	122.64
17	G	101	BCR	C24-C23-C22	-4.51	119.57	126.23
10	A	302	HEM	C4D-ND-C1D	4.49	110.53	105.21
12	A	309	UMQ	O3-C3-C4	4.48	120.94	110.38
12	C	301	UMQ	C1'-C2'-C3'	-4.47	100.61	110.01
16	D	201	SQD	O3-C3-C2	4.42	120.86	109.86
17	G	101	BCR	C33-C5-C6	-4.41	119.68	124.48
12	A	307	UMQ	O2-C2-C1	4.39	120.54	110.08
12	C	301	UMQ	O1-C1-C2	4.33	118.75	108.09
12	A	309	UMQ	O2-C2-C1	4.26	120.22	110.08
12	A	309	UMQ	O3-C3-C2	4.25	120.39	110.38
12	A	309	UMQ	C4-C3-C2	4.25	118.28	110.83
12	A	309	UMQ	O2-C2-C3	4.21	120.30	110.38
12	A	306	UMQ	C3'-C4'-C5'	4.19	120.22	110.93
12	A	307	UMQ	C1-C2-C3	4.12	118.67	110.01
12	A	307	UMQ	O2-C2-C3	4.06	119.96	110.38
16	D	201	SQD	O4-C4-C3	4.03	118.29	110.05
12	A	309	UMQ	O3'-C3'-C4'	3.99	120.18	109.94
16	D	201	SQD	O9-S-C6	3.93	112.63	106.76
16	D	201	SQD	O9-S-O7	-3.92	101.09	113.82
12	A	309	UMQ	C1-C2-C3	3.88	118.17	110.01
12	A	306	UMQ	O1-C4'-C3'	3.77	116.81	107.23
16	D	201	SQD	O47-C7-C8	3.73	119.55	111.48
17	G	101	BCR	C23-C24-C25	-3.67	117.18	127.00
14	B	202	CLA	O2D-CGD-O1D	-3.64	116.76	123.85
12	A	309	UMQ	O3'-C3'-C2'	3.63	118.92	110.38
10	A	304	HEM	CHC-C1C-NC	3.61	128.39	124.45
16	D	201	SQD	O7-S-C6	3.58	112.11	106.76
11	B	203	OPC	OAN-CAO-CAP	3.41	118.85	111.48
10	C	302	HEM	C3B-C4B-NB	-3.38	107.04	109.47
17	G	101	BCR	C38-C26-C25	-3.31	120.88	124.48
12	A	306	UMQ	C1-O1-C4'	-3.28	110.19	117.98
12	C	301	UMQ	C1'-O5'-C5'	-3.27	107.34	113.72
17	G	101	BCR	C20-C19-C18	-3.21	117.56	126.36
17	G	101	BCR	C33-C5-C4	3.21	120.44	113.60
12	C	301	UMQ	C1-C2-C3	-3.18	103.32	110.01
16	D	201	SQD	C44-O6-C1	3.16	120.53	113.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	303	HEM	CAD-C3D-C4D	3.14	130.17	124.70
12	C	301	UMQ	C1-O5-C5	-3.11	107.64	113.72
12	A	307	UMQ	C1'-O5'-C5'	-3.09	107.69	113.72
12	A	307	UMQ	O5'-C1'-C2'	-3.07	104.06	110.37
17	G	101	BCR	C29-C30-C25	3.06	114.89	110.44
14	B	202	CLA	CAA-CBA-CGA	-3.06	104.52	113.21
17	G	101	BCR	C31-C1-C6	-3.05	105.45	110.24
12	A	309	UMQ	O5'-C1'-O1'	3.04	117.22	110.04
10	A	302	HEM	CBA-CAA-C2A	-2.95	104.39	112.53
12	A	307	UMQ	C1'-C2'-C3'	2.92	116.15	110.01
10	C	302	HEM	CHC-C4B-C3B	2.89	130.84	125.07
10	A	304	HEM	CAC-C3C-C4C	2.87	131.68	124.82
10	C	302	HEM	CHD-C4C-NC	2.87	127.58	124.45
10	A	304	HEM	CHD-C4C-C3C	2.87	130.04	125.21
11	B	203	OPC	OBJ-CBK-CBL	2.85	120.52	111.83
12	A	306	UMQ	O1-C1-C2	2.84	115.08	108.09
14	B	202	CLA	C3B-C4B-NB	-2.84	108.00	110.53
12	A	307	UMQ	O1'-C1'-C2'	2.77	112.47	108.27
12	A	306	UMQ	C1-C2-C3	2.66	115.61	110.01
14	B	202	CLA	C9-C8-C10	2.66	120.74	111.27
10	A	302	HEM	CHD-C4C-NC	2.65	127.34	124.45
17	G	101	BCR	C37-C22-C21	-2.64	118.54	122.82
17	G	101	BCR	C8-C9-C10	2.64	123.16	119.01
14	B	202	CLA	CHB-C4A-NA	2.61	128.17	124.40
17	G	101	BCR	C38-C26-C27	2.58	119.10	113.60
10	C	302	HEM	CHB-C1B-NB	2.52	127.48	124.37
12	A	309	UMQ	O5-C5-C4	2.51	114.23	109.70
10	A	304	HEM	CBA-CAA-C2A	-2.48	105.67	112.53
10	A	303	HEM	CHC-C4B-NB	2.47	127.08	124.42
12	C	301	UMQ	C4-C3-C2	-2.47	106.50	110.83
10	A	304	HEM	CAC-C3C-C2C	-2.47	120.41	128.43
10	C	302	HEM	CAB-C3B-C2B	-2.45	120.47	128.43
17	G	101	BCR	C1-C6-C7	2.43	122.25	115.65
11	A	305	OPC	CBI-CAM-CAL	-2.42	106.14	111.78
16	D	201	SQD	O6-C1-C2	-2.42	106.38	109.02
12	C	301	UMQ	O5-C1-C2	2.42	115.33	110.37
12	A	309	UMQ	C1-O5-C5	2.39	118.39	113.72
17	G	101	BCR	C3-C4-C5	2.38	118.29	114.06
11	A	305	OPC	OAN-CAO-OAD	-2.38	118.15	123.70
11	A	305	OPC	OBJ-CBK-CBL	2.38	119.08	111.83
10	C	302	HEM	CMD-C2D-C1D	2.37	128.74	125.03
17	G	101	BCR	C11-C10-C9	-2.37	123.96	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	G	101	BCR	C34-C9-C10	-2.35	119.00	122.82
14	B	202	CLA	CAA-C2A-C1A	-2.35	104.27	111.97
11	B	203	OPC	OAN-CAO-OAD	-2.35	118.21	123.70
12	A	307	UMQ	O5'-C5'-C4'	2.35	114.57	109.72
12	C	301	UMQ	O5'-C1'-C2'	-2.33	105.58	110.37
16	D	201	SQD	C45-O47-C7	2.32	123.36	117.80
12	A	306	UMQ	O1'-C1'-C2'	2.31	111.78	108.27
16	D	201	SQD	C13-C12-C11	2.31	126.04	114.37
16	D	201	SQD	O5-C1-C2	2.30	114.41	110.84
12	A	309	UMQ	O5'-C5'-C4'	2.29	114.47	109.72
16	D	201	SQD	O48-C23-C24	2.27	118.76	111.83
12	A	307	UMQ	C1-O5-C5	-2.27	109.30	113.72
10	A	302	HEM	CHA-C1A-NA	2.24	127.93	123.86
10	A	302	HEM	C2A-C1A-NA	-2.24	107.67	110.15
10	A	303	HEM	C2A-C1A-NA	-2.23	107.68	110.15
10	C	302	HEM	C3B-C2B-C1B	2.17	108.04	106.41
10	C	302	HEM	C1B-NB-C4B	2.17	107.77	105.21
10	A	303	HEM	O2A-CGA-CBA	2.17	120.84	114.00
12	A	309	UMQ	O5-C5-C6	2.16	111.81	106.44
10	C	302	HEM	CHC-C4B-NB	-2.14	122.12	124.42
14	B	202	CLA	CAA-C2A-C3A	-2.11	107.29	113.00
17	G	101	BCR	C8-C7-C6	-2.11	121.37	127.00
10	A	302	HEM	CHC-C4B-NB	2.10	126.68	124.42
17	G	101	BCR	C4-C5-C6	-2.09	119.89	122.70
17	G	101	BCR	C30-C25-C26	-2.08	119.80	122.64
17	G	101	BCR	C40-C30-C25	-2.06	107.01	110.24
14	B	202	CLA	O1D-CGD-CBD	2.06	128.58	124.52
17	G	101	BCR	C10-C11-C12	-2.05	117.26	123.20
12	A	309	UMQ	C6'-C5'-C4'	-2.04	107.63	113.38
12	A	307	UMQ	C6-C5-C4	-2.03	108.03	113.02
16	D	201	SQD	O48-C23-O10	-2.02	118.58	123.63
10	C	302	HEM	C1D-C2D-C3D	-2.02	104.86	106.98
14	B	202	CLA	C3A-C2A-C1A	2.01	104.35	101.34
17	G	101	BCR	C30-C25-C24	2.01	121.10	115.65
10	A	303	HEM	CHD-C1D-ND	2.00	126.58	124.42

All (14) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	A	306	UMQ	C4'
12	A	307	UMQ	C2
12	A	307	UMQ	C2'

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Mol	Chain	Res	Type	Atom
12	A	309	UMQ	C2
12	A	309	UMQ	C3
12	A	309	UMQ	C1'
12	A	309	UMQ	C3'
12	C	301	UMQ	C1
13	A	308	QNO	C2
14	B	202	CLA	ND
14	B	202	CLA	C8
16	D	201	SQD	C5
16	D	201	SQD	C3
16	D	201	SQD	C4

All (175) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	305	OPC	CAH-OAI-PAJ-OAB
11	A	305	OPC	NAF-CAG-CAH-OAI
11	B	203	OPC	CAH-OAI-PAJ-OAK
11	B	203	OPC	CAH-OAI-PAJ-OAB
11	B	203	OPC	NAF-CAG-CAH-OAI
12	A	306	UMQ	C2'-C1'-O1'-CA
14	B	202	CLA	C1A-C2A-CAA-CBA
14	B	202	CLA	C3A-C2A-CAA-CBA
14	B	202	CLA	CBD-CGD-O2D-CED
14	B	202	CLA	O2A-C1-C2-C3
16	D	201	SQD	C2-C1-O6-C44
16	D	201	SQD	O5-C1-O6-C44
16	D	201	SQD	O47-C45-C46-O48
16	D	201	SQD	C5-C6-S-O7
16	D	201	SQD	C5-C6-S-O8
16	D	201	SQD	C5-C6-S-O9
17	G	101	BCR	C1-C6-C7-C8
17	G	101	BCR	C5-C6-C7-C8
17	G	101	BCR	C6-C7-C8-C9
17	G	101	BCR	C7-C8-C9-C10
17	G	101	BCR	C7-C8-C9-C34
17	G	101	BCR	C11-C12-C13-C14
17	G	101	BCR	C11-C12-C13-C35
17	G	101	BCR	C20-C21-C22-C37
17	G	101	BCR	C21-C22-C23-C24
17	G	101	BCR	C37-C22-C23-C24
17	G	101	BCR	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
12	A	306	UMQ	C3'-C4'-O1-C1
14	B	202	CLA	O1D-CGD-O2D-CED
12	C	301	UMQ	O5-C1-O1-C4'
16	D	201	SQD	O49-C7-O47-C45
12	A	307	UMQ	O5-C5-C6-O6
16	D	201	SQD	C13-C14-C15-C16
12	A	309	UMQ	O5-C5-C6-O6
11	B	203	OPC	OAD-CAO-OAN-CAM
12	A	306	UMQ	O5'-C5'-C6'-O6'
12	A	307	UMQ	C4-C5-C6-O6
11	B	203	OPC	CAP-CAO-OAN-CAM
16	D	201	SQD	C8-C7-O47-C45
12	C	301	UMQ	O5'-C5'-C6'-O6'
12	C	301	UMQ	C4'-C5'-C6'-O6'
12	A	306	UMQ	O5'-C1'-O1'-CA
12	A	309	UMQ	O5'-C5'-C6'-O6'
16	D	201	SQD	C33-C34-C35-C36
16	D	201	SQD	C31-C32-C33-C34
12	A	309	UMQ	C4'-C5'-C6'-O6'
12	A	306	UMQ	C4'-C5'-C6'-O6'
12	A	309	UMQ	C4-C5-C6-O6
12	A	309	UMQ	C2'-C1'-O1'-CA
17	G	101	BCR	C36-C18-C19-C20
14	B	202	CLA	C13-C15-C16-C17
11	B	203	OPC	CBK-CBL-CBM-CBN
11	A	305	OPC	CAO-CAP-CAQ-CAR
11	B	203	OPC	CAO-CAP-CAQ-CAR
13	A	308	QNO	C2-C21-C22-C23
11	B	203	OPC	CBQ-CBR-CBS-CBT
16	D	201	SQD	C23-C24-C25-C26
12	A	309	UMQ	O5-C1-O1-C4'
12	A	309	UMQ	O1'-CA-CB-CC
14	B	202	CLA	C10-C11-C12-C13
17	G	101	BCR	C12-C13-C14-C15
17	G	101	BCR	C16-C17-C18-C19
12	A	309	UMQ	O5'-C1'-O1'-CA
14	B	202	CLA	C16-C17-C18-C20
11	A	305	OPC	CAP-CAQ-CAR-CAS
12	A	309	UMQ	CC-CD-CF-CG
16	D	201	SQD	C29-C30-C31-C32
12	C	301	UMQ	CH-CI-CJ-CK
11	B	203	OPC	CAR-CAS-CAT-CAU

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Mol	Chain	Res	Type	Atoms
12	A	307	UMQ	C4'-C5'-C6'-O6'
12	A	307	UMQ	CH-CI-CJ-CK
12	A	306	UMQ	CB-CC-CD-CF
16	D	201	SQD	C9-C10-C11-C12
12	C	301	UMQ	CD-CF-CG-CH
16	D	201	SQD	C18-C19-C20-C21
14	B	202	CLA	C3-C5-C6-C7
11	A	305	OPC	OCC-CBK-OBJ-CBI
11	A	305	OPC	CBV-CBW-CBX-CBY
17	G	101	BCR	C10-C11-C12-C13
17	G	101	BCR	C18-C19-C20-C21
11	A	305	OPC	CBN-CBO-CBP-CBQ
12	A	307	UMQ	CF-CG-CH-CI
11	A	305	OPC	CAX-CAY-CAZ-CBA
16	D	201	SQD	C14-C15-C16-C17
11	A	305	OPC	CAY-CAZ-CBA-CBB
12	A	309	UMQ	CF-CG-CH-CI
11	A	305	OPC	CBK-CBL-CBM-CBN
11	A	305	OPC	CAW-CAX-CAY-CAZ
16	D	201	SQD	C44-C45-C46-O48
11	A	305	OPC	CBS-CBT-CBU-CBV
11	B	203	OPC	CBM-CBN-CBO-CBP
16	D	201	SQD	C28-C29-C30-C31
12	A	306	UMQ	O5-C5-C6-O6
16	D	201	SQD	C24-C25-C26-C27
11	A	305	OPC	CBL-CBK-OBJ-CBI
12	A	309	UMQ	CB-CC-CD-CF
11	A	305	OPC	OAN-CAM-CBI-OBJ
13	A	308	QNO	C22-C23-C24-C25
11	B	203	OPC	CBL-CBM-CBN-CBO
12	C	301	UMQ	CI-CJ-CK-CL
10	A	302	HEM	C3D-CAD-CBD-CGD
11	A	305	OPC	CAQ-CAR-CAS-CAT
17	G	101	BCR	C17-C18-C19-C20
13	A	308	QNO	C21-C22-C23-C24
11	A	305	OPC	CAL-CAM-CBI-OBJ
16	D	201	SQD	C11-C10-C9-C8
17	G	101	BCR	C23-C24-C25-C30
11	B	203	OPC	CBS-CBT-CBU-CBV
16	D	201	SQD	O10-C23-O48-C46
14	B	202	CLA	C11-C10-C8-C9
14	B	202	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
11	B	203	OPC	CBO-CBP-CBQ-CBR
17	G	101	BCR	C16-C17-C18-C36
14	B	202	CLA	C11-C10-C8-C7
11	A	305	OPC	CBO-CBP-CBQ-CBR
11	B	203	OPC	CAS-CAT-CAU-CAV
17	G	101	BCR	C14-C15-C16-C17
12	A	306	UMQ	CI-CJ-CK-CL
10	A	304	HEM	C4C-C3C-CAC-CBC
10	C	302	HEM	C4B-C3B-CAB-CBB
11	A	305	OPC	CBY-CBZ-CCA-CCB
16	D	201	SQD	C27-C28-C29-C30
14	B	202	CLA	C6-C7-C8-C10
12	A	309	UMQ	CG-CH-CI-CJ
11	A	305	OPC	CAH-OAI-PAJ-OAK
11	A	305	OPC	CAH-OAI-PAJ-OBH
17	G	101	BCR	C9-C10-C11-C12
16	D	201	SQD	C44-C45-O47-C7
12	A	307	UMQ	O5'-C5'-C6'-O6'
12	A	309	UMQ	CH-CI-CJ-CK
11	B	203	OPC	CBU-CBV-CBW-CBX
12	A	306	UMQ	CB-CA-O1'-C1'
12	A	307	UMQ	CB-CA-O1'-C1'
12	A	307	UMQ	CA-CB-CC-CD
11	A	305	OPC	CAT-CAU-CAV-CAW
16	D	201	SQD	C12-C13-C14-C15
17	G	101	BCR	C11-C10-C9-C34
11	B	203	OPC	CBN-CBO-CBP-CBQ
10	C	302	HEM	CAD-CBD-CGD-O1D
17	G	101	BCR	C11-C10-C9-C8
10	A	304	HEM	CAA-CBA-CGA-O1A
11	A	305	OPC	CAZ-CBA-CBB-CBC
17	G	101	BCR	C23-C24-C25-C26
11	B	203	OPC	CBP-CBQ-CBR-CBS
16	D	201	SQD	O6-C44-C45-O47
10	A	302	HEM	CAA-CBA-CGA-O1A
10	A	302	HEM	CAA-CBA-CGA-O2A
10	A	304	HEM	CAA-CBA-CGA-O2A
12	C	301	UMQ	O1'-CA-CB-CC
10	A	304	HEM	C4D-C3D-CAD-CBD
10	A	304	HEM	C2D-C3D-CAD-CBD
13	A	308	QNO	C26-C27-C28-C29
10	C	302	HEM	CAD-CBD-CGD-O2D

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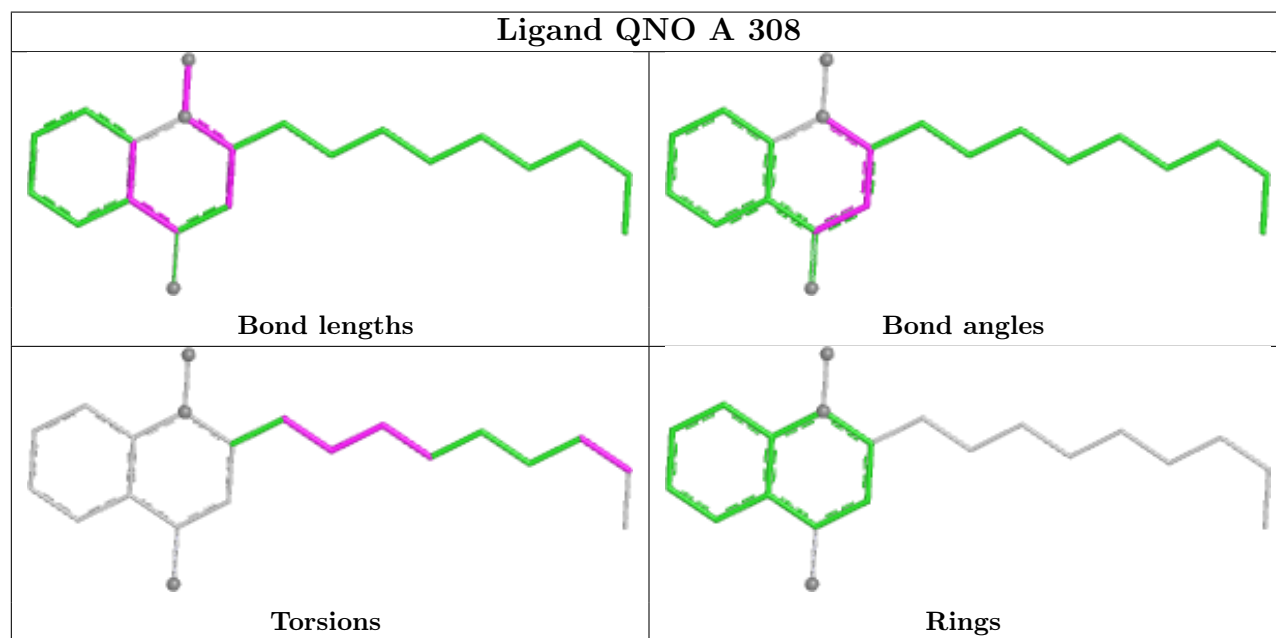
Mol	Chain	Res	Type	Atoms
11	B	203	OPC	CAV-CAW-CAX-CAY
12	A	309	UMQ	CD-CF-CG-CH
11	B	203	OPC	CBC-CBD-CBE-CBF
11	A	305	OPC	CBM-CBN-CBO-CBP
14	B	202	CLA	C8-C10-C11-C12
10	A	304	HEM	CAD-CBD-CGD-O2D
12	A	306	UMQ	CA-CB-CC-CD
11	B	203	OPC	CBT-CBU-CBV-CBW
10	A	304	HEM	CAD-CBD-CGD-O1D
12	A	309	UMQ	CB-CA-O1'-C1'
14	B	202	CLA	C4B-C3B-CAB-CBB
11	B	203	OPC	CAQ-CAR-CAS-CAT
11	B	203	OPC	CAH-CAG-NAF-CAE
11	A	305	OPC	OAN-CAO-CAP-CAQ
16	D	201	SQD	C7-C8-C9-C10
14	B	202	CLA	C6-C7-C8-C9
11	B	203	OPC	CAH-CAG-NAF-CAA
10	A	303	HEM	CAA-CBA-CGA-O1A
16	D	201	SQD	O49-C7-C8-C9
10	A	303	HEM	C1A-C2A-CAA-CBA
10	A	302	HEM	CAD-CBD-CGD-O2D
12	A	309	UMQ	C2-C1-O1-C4'

There are no ring outliers.

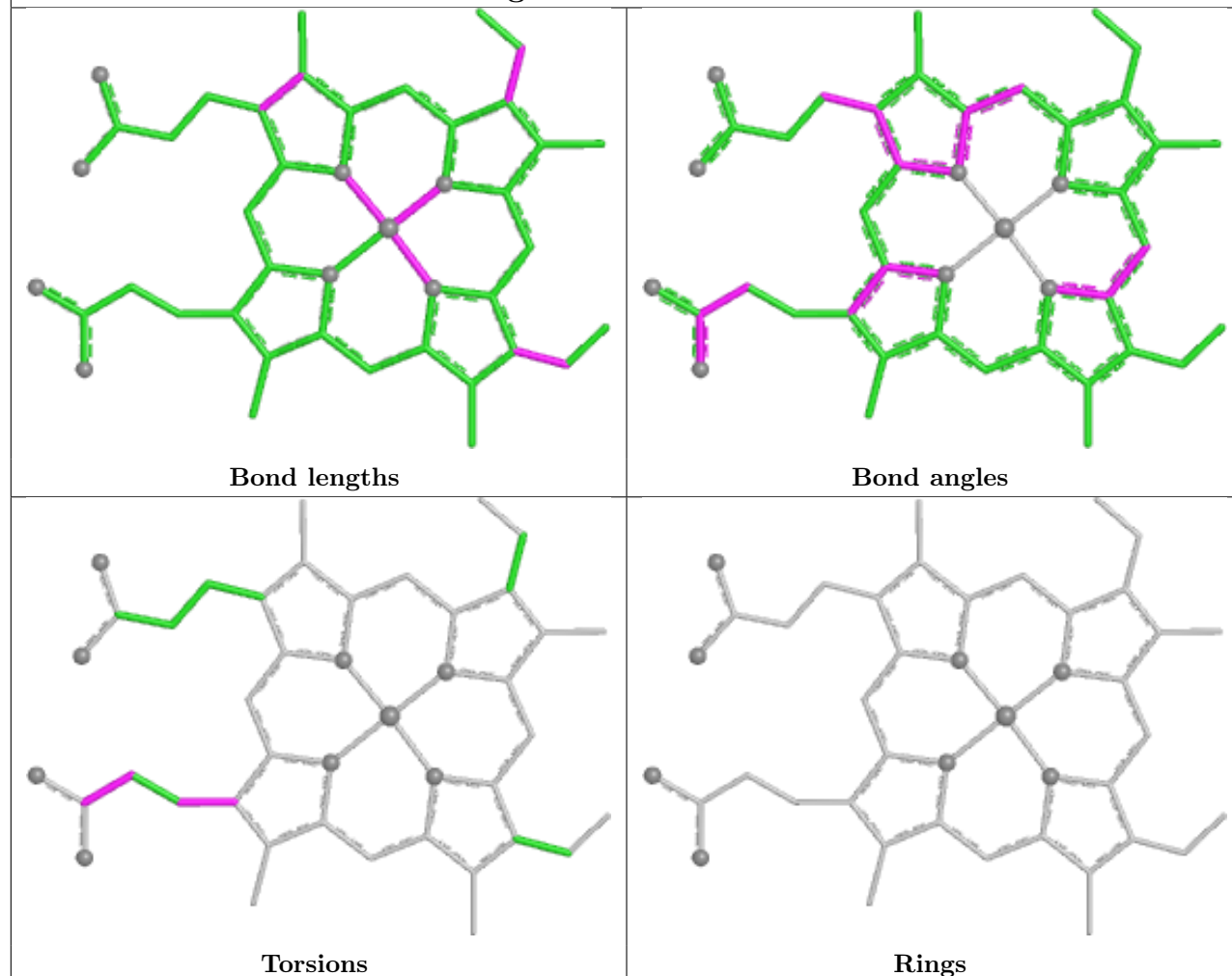
15 monomers are involved in 80 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	308	QNO	2	0
10	A	303	HEM	1	0
12	C	301	UMQ	4	0
12	A	306	UMQ	5	0
17	G	101	BCR	9	0
10	C	302	HEM	11	0
15	D	200	FES	1	0
10	A	302	HEM	2	0
11	A	305	OPC	10	0
16	D	201	SQD	17	0
11	B	203	OPC	4	0
12	A	309	UMQ	2	0
14	B	202	CLA	5	0
10	A	304	HEM	10	0
12	A	307	UMQ	1	0

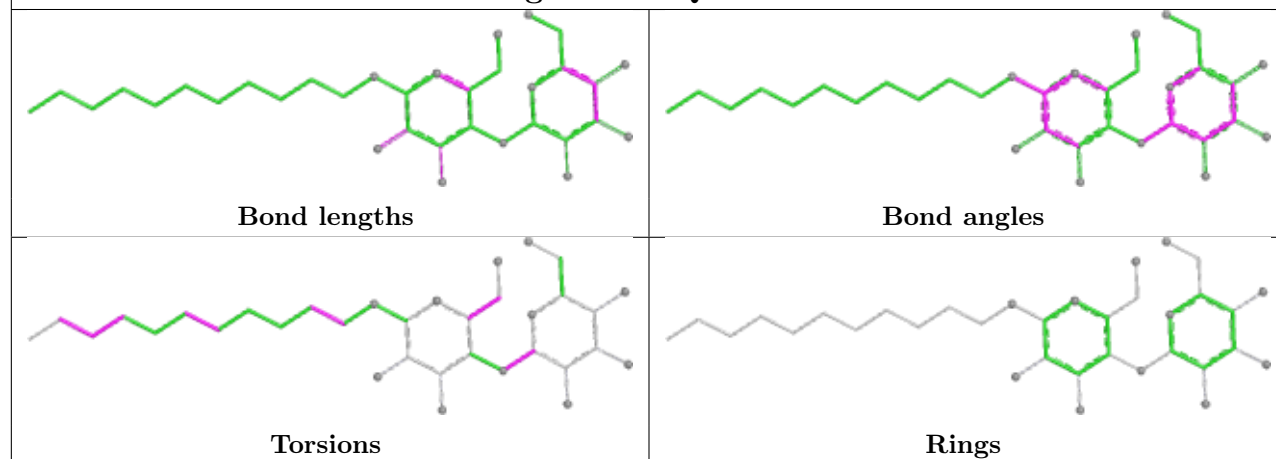
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

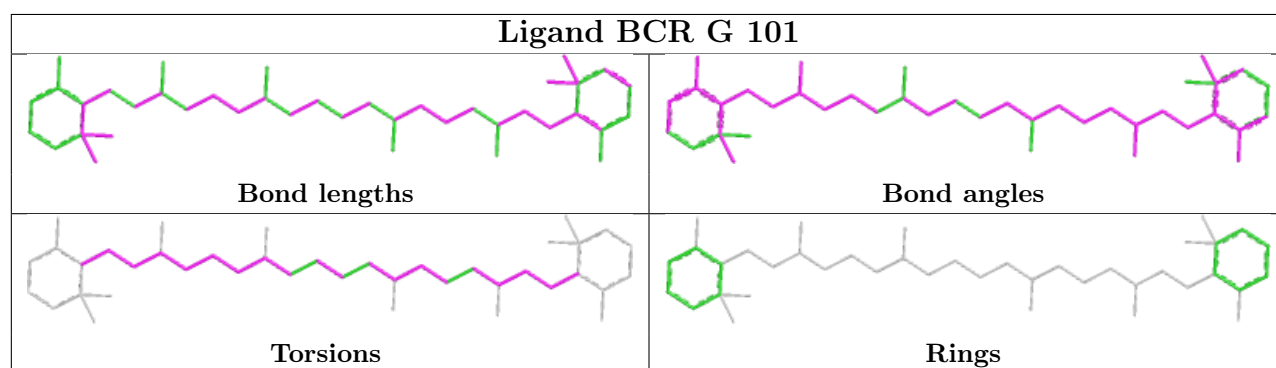
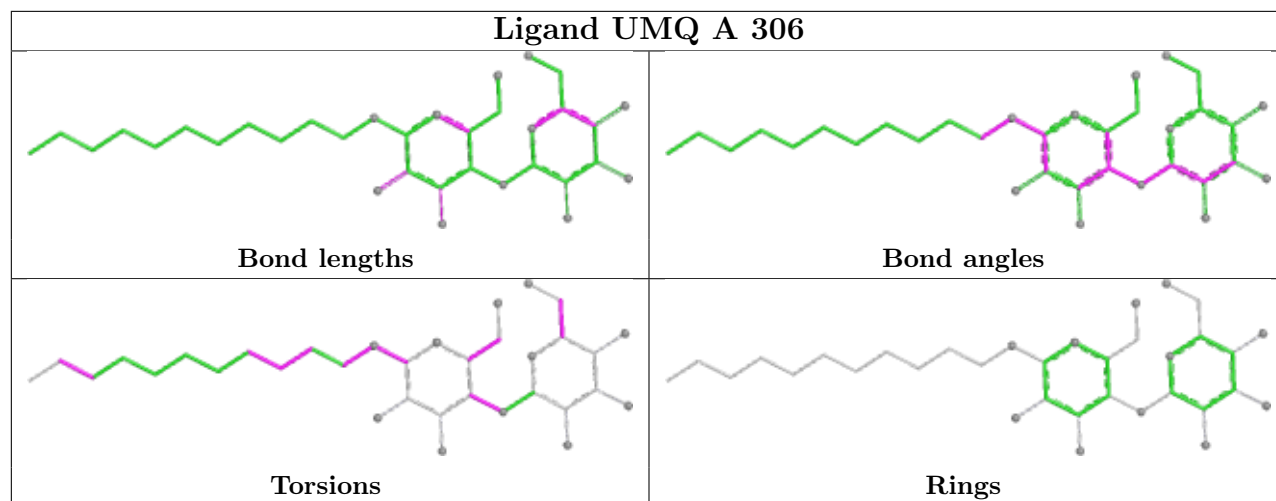


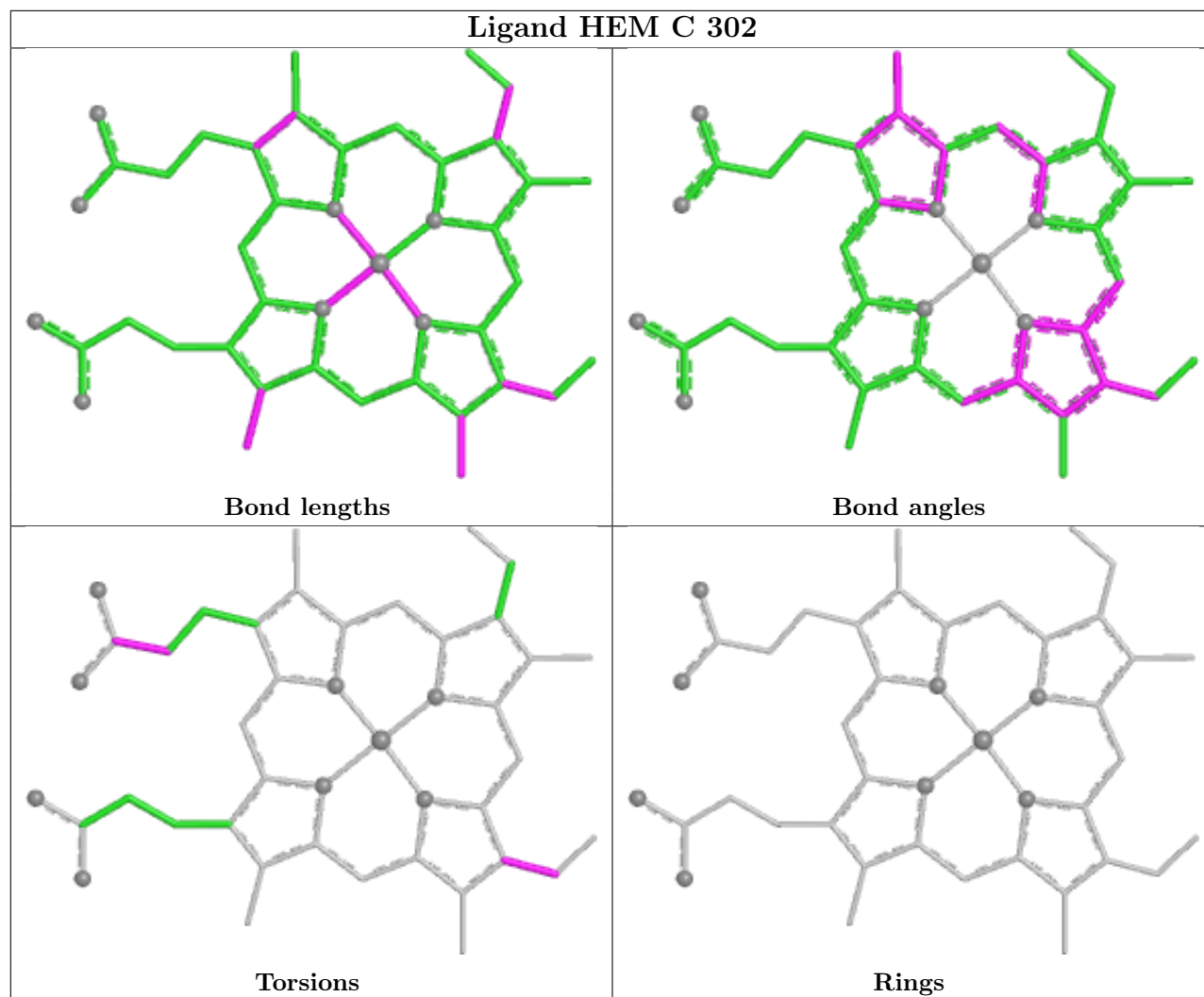
Ligand HEM A 303

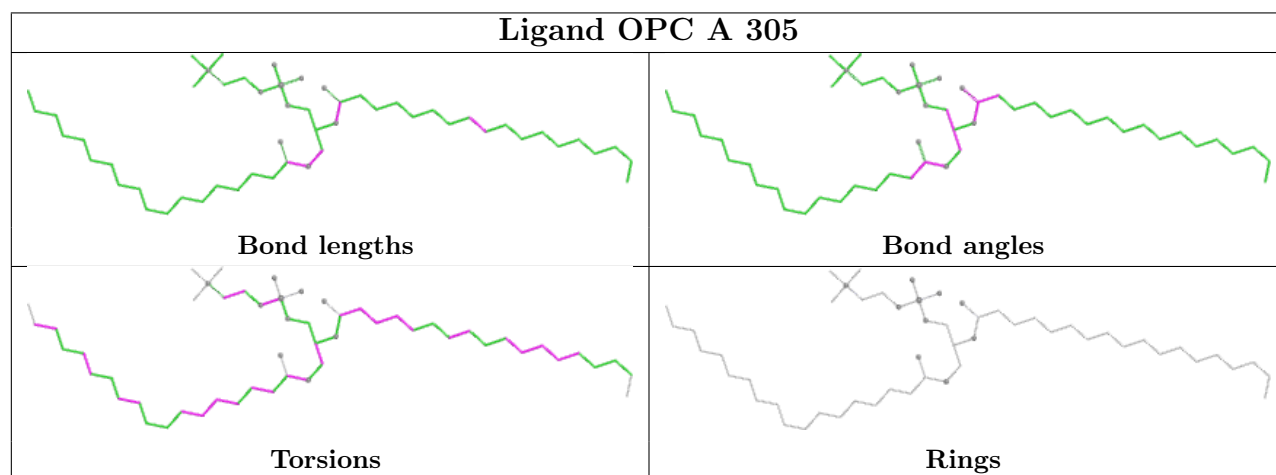
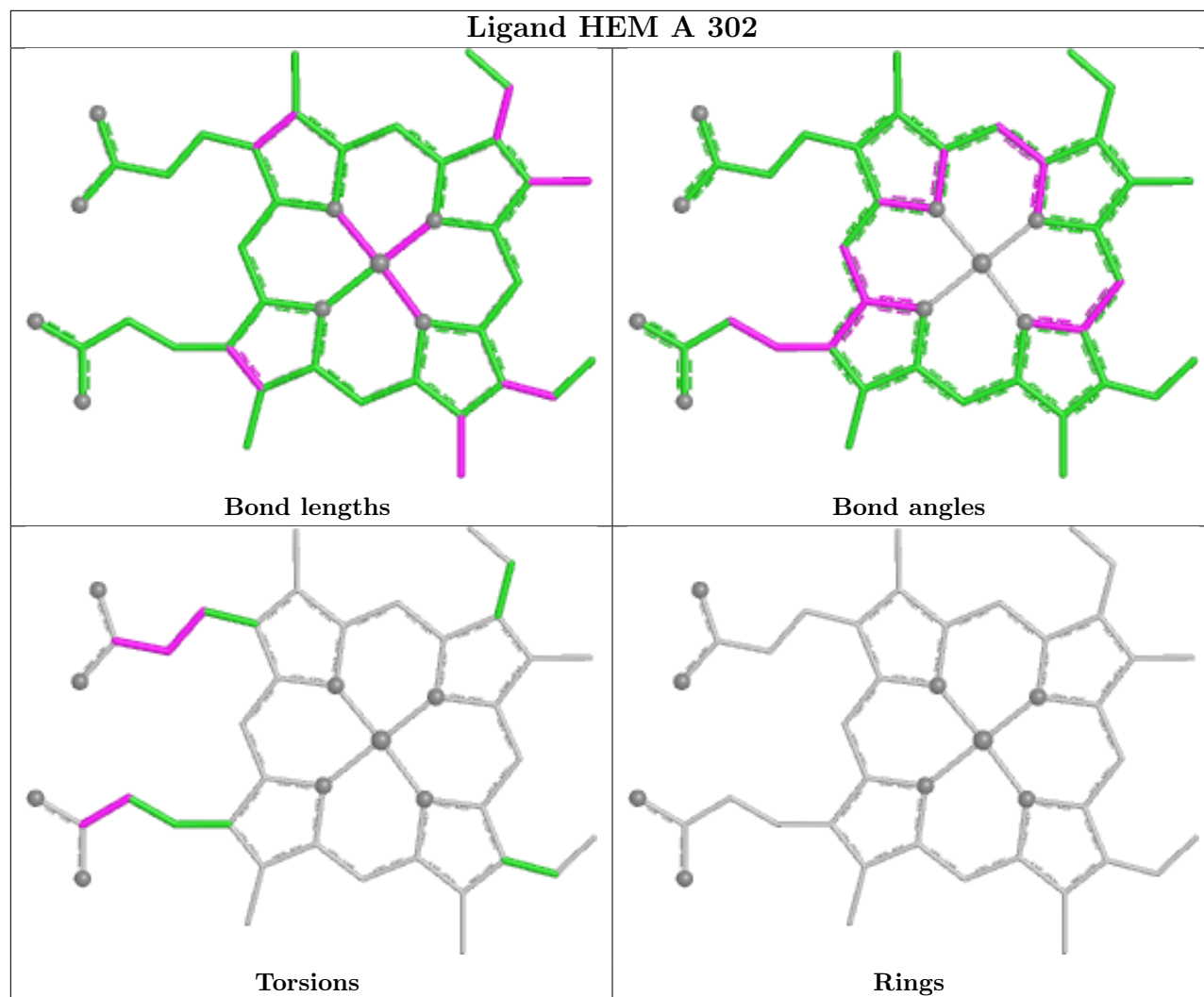


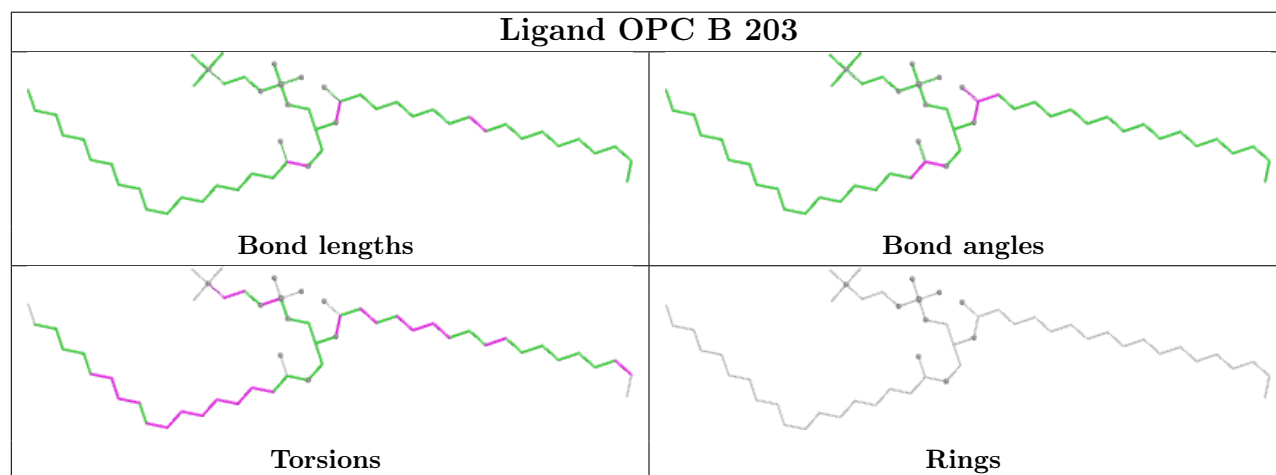
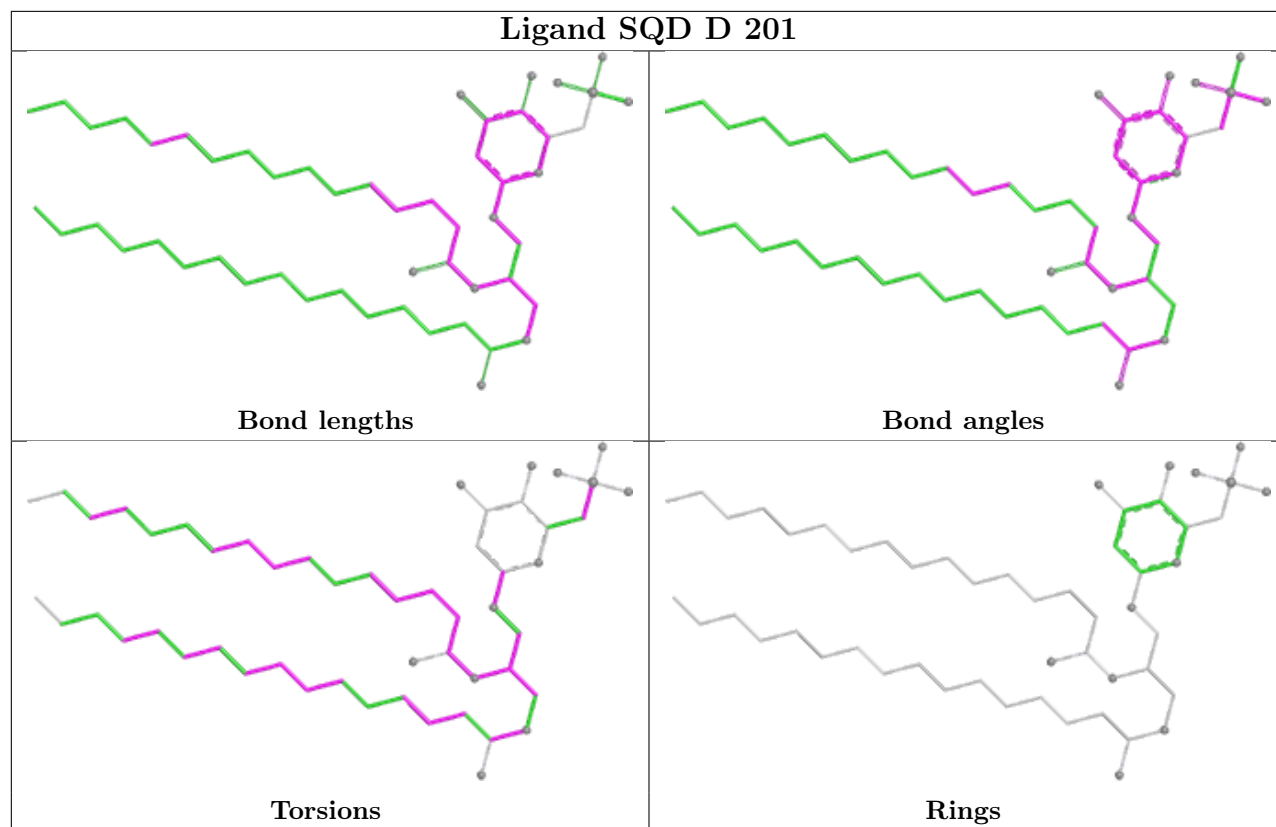
Ligand UMQ C 301

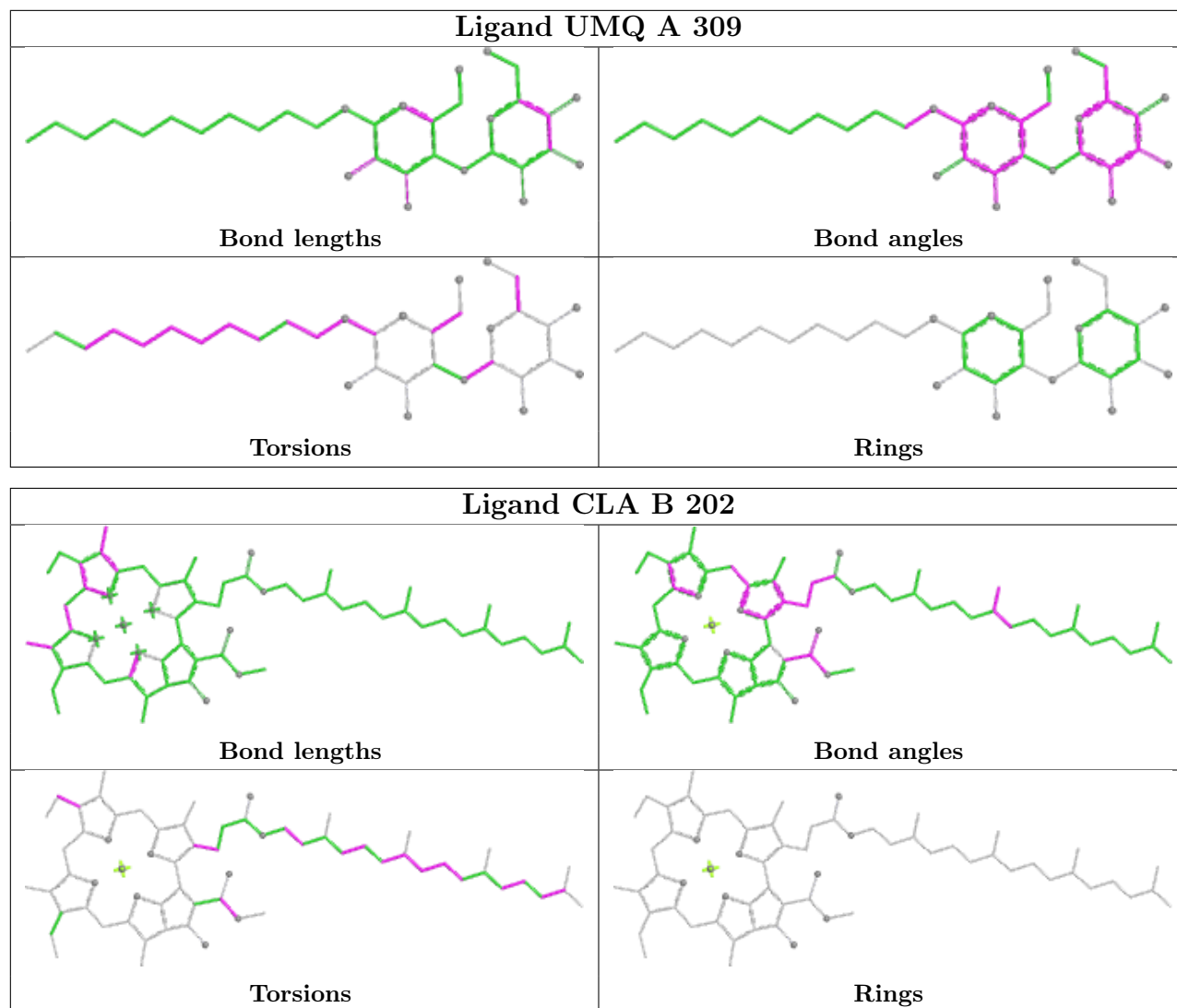


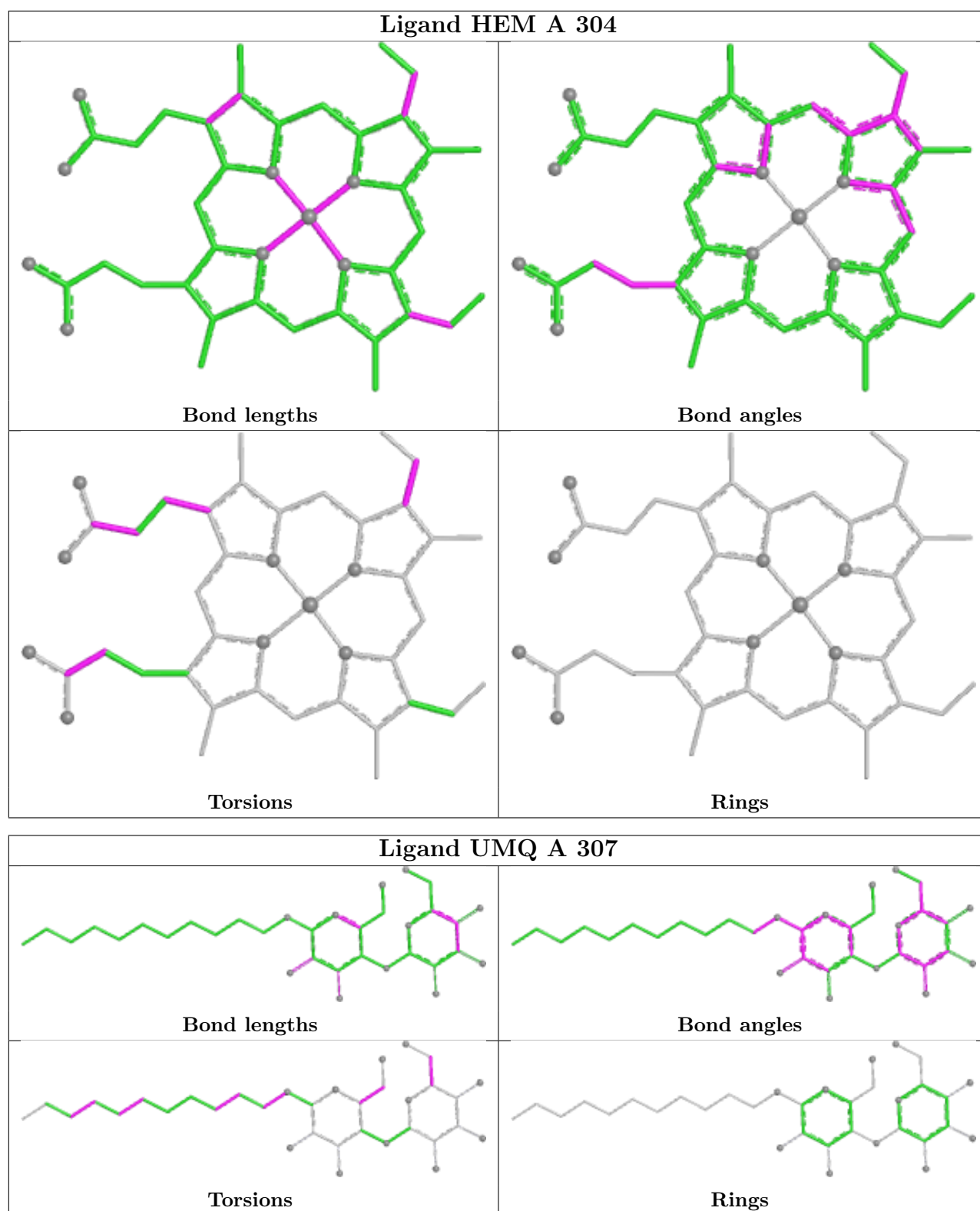












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	213/215 (99%)	-0.17	6 (2%)	55	36	46, 69, 101, 156	0
2	B	160/160 (100%)	0.28	9 (5%)	30	20	57, 88, 138, 167	0
3	C	286/289 (98%)	0.68	42 (14%)	6	5	57, 101, 206, 233	1 (0%)
4	D	161/179 (89%)	1.32	39 (24%)	2	2	59, 156, 199, 216	0
5	E	32/32 (100%)	0.66	4 (12%)	8	7	77, 103, 139, 170	0
6	F	32/35 (91%)	0.91	5 (15%)	5	4	72, 93, 157, 167	0
7	G	37/37 (100%)	0.89	7 (18%)	3	3	64, 87, 167, 173	0
8	H	29/29 (100%)	0.37	3 (10%)	12	10	70, 84, 120, 147	0
All	All	950/976 (97%)	0.54	115 (12%)	8	7	46, 92, 190, 233	1 (0%)

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	G	37	GLY	8.5
3	C	88	GLU	7.6
4	D	145	PRO	6.8
4	D	160	ILE	6.1
4	D	144	ALA	6.0
8	H	1	MET	5.7
6	F	1	MET	4.9
4	D	146	LEU	4.8
5	E	2	ILE	4.7
5	E	1	MET	4.7
4	D	46	SER	4.6
3	C	193	VAL	4.6
4	D	70	LEU	4.3
4	D	125	LYS	4.3
7	G	27	GLN	4.3
2	B	74	GLU	4.3

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Mol	Chain	Res	Type	RSRZ
4	D	170	PHE	4.2
2	B	75	ILE	4.2
7	G	32	PRO	4.1
4	D	135	GLU	4.1
3	C	286	GLU	4.0
4	D	168	THR	4.0
4	D	169	ASP	3.8
4	D	172	THR	3.7
4	D	179	VAL	3.7
4	D	85	LYS	3.6
4	D	73	HIS	3.6
3	C	90	ILE	3.6
6	F	32	ALA	3.5
3	C	86	PRO	3.5
3	C	89	ARG	3.4
4	D	165	TRP	3.4
4	D	143	PRO	3.4
3	C	68	VAL	3.4
7	G	36	GLY	3.4
3	C	87	GLU	3.3
8	H	29	LEU	3.3
3	C	241	GLY	3.2
4	D	149	ALA	3.2
3	C	218	ILE	3.2
4	D	91	ILE	3.2
3	C	256	LYS	3.1
3	C	165	GLU	3.1
1	A	215	LEU	3.1
3	C	183	ILE	3.1
3	C	190	TYR	3.0
4	D	75	ALA	3.0
3	C	226	LYS	3.0
4	D	177	TRP	3.0
1	A	136	TYR	3.0
3	C	125	GLN	3.0
2	B	2	ALA	2.9
4	D	69	PHE	2.9
3	C	60	GLN	2.9
3	C	199	ILE	2.9
4	D	123	LYS	2.9
4	D	142	GLY	2.9
4	D	176	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
4	D	147	SER	2.8
3	C	192	ASN	2.8
7	G	33	ASN	2.8
3	C	220	SER	2.7
3	C	95	LYS	2.7
4	D	120	ALA	2.7
2	B	160	PHE	2.7
4	D	173	GLY	2.7
3	C	217	LEU	2.7
6	F	19	GLY	2.6
7	G	26	TYR	2.6
4	D	77	ASP	2.6
4	D	122	ASN	2.6
2	B	115	GLU	2.6
2	B	116	ASN	2.5
3	C	222	GLY	2.5
4	D	171	ARG	2.4
3	C	230	ALA	2.4
3	C	176	ALA	2.3
3	C	207	VAL	2.3
3	C	215	PRO	2.3
3	C	85	ALA	2.3
2	B	155	LEU	2.3
4	D	64	VAL	2.3
3	C	108	GLU	2.3
7	G	1	MET	2.3
4	D	65	LYS	2.3
3	C	214	GLY	2.3
1	A	10	GLU	2.2
5	E	32	ILE	2.2
4	D	68	LYS	2.2
3	C	257	TRP	2.2
4	D	166	THR	2.2
6	F	29	ILE	2.2
6	F	6	LEU	2.2
3	C	195	TYR	2.2
3	C	6	GLN	2.2
1	A	108	GLY	2.2
3	C	59	GLN	2.1
3	C	225	VAL	2.1
4	D	99	ILE	2.1
3	C	57	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
4	D	119	ALA	2.1
4	D	52	GLY	2.1
3	C	234	ASN	2.1
3	C	253	ASN	2.1
2	B	6	LYS	2.1
5	E	3	LEU	2.1
1	A	112	LYS	2.1
4	D	175	LYS	2.1
3	C	56	THR	2.1
3	C	281	LYS	2.0
8	H	6	LEU	2.0
2	B	72	PRO	2.0
3	C	119	LEU	2.0
3	C	231	LEU	2.0
1	A	173	SER	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.

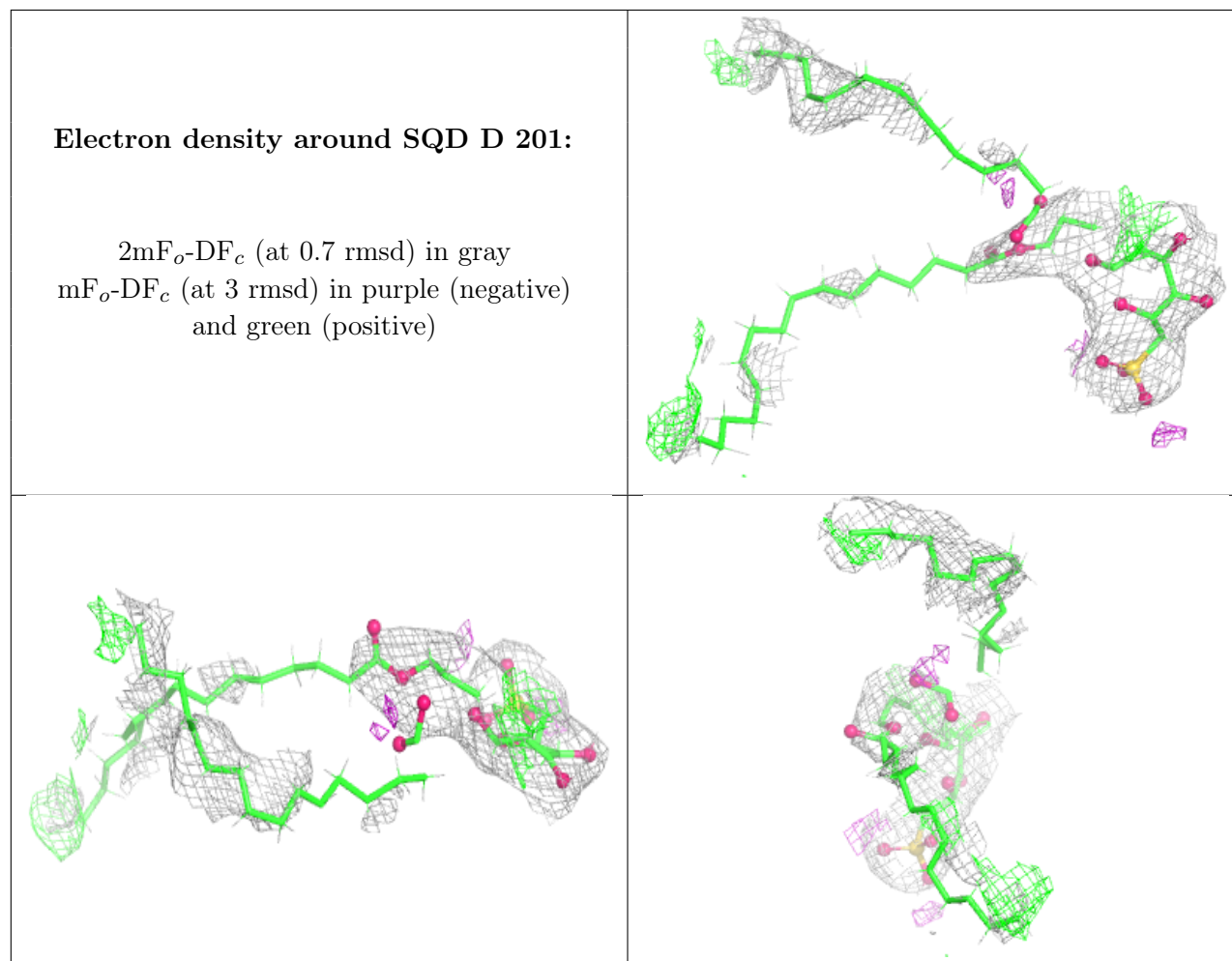
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	SQD	D	201	53/54	0.76	0.28	83,150,191,196	1
12	UMQ	A	306	34/34	0.81	0.23	61,148,192,198	0
12	UMQ	C	301	34/34	0.84	0.24	51,119,203,224	0
12	UMQ	A	309	34/34	0.87	0.19	87,162,229,238	0
13	QNO	A	308	21/21	0.89	0.24	83,113,154,167	0
11	OPC	B	203	54/55	0.91	0.21	66,126,180,198	0
11	OPC	A	305	54/55	0.91	0.22	62,118,206,229	0
17	BCR	G	101	40/40	0.91	0.20	51,97,180,199	0

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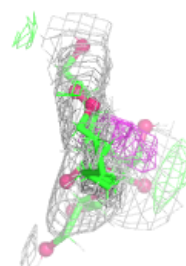
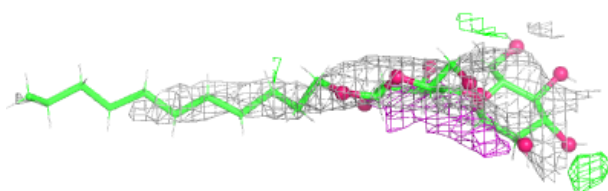
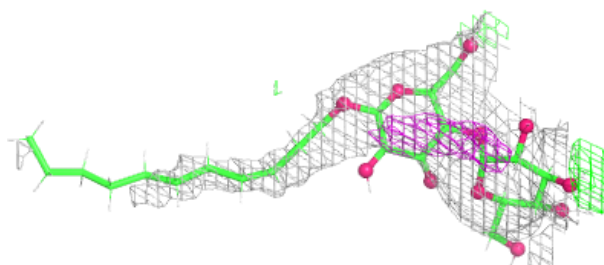
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	UMQ	A	307	34/34	0.92	0.15	81,138,182,186	0
15	FES	D	200	4/4	0.96	0.11	108,129,130,138	0
9	CD	B	201	1/1	0.96	0.06	186,186,186,186	0
14	CLA	B	202	65/65	0.96	0.12	59,90,133,153	0
10	HEM	A	304	43/43	0.97	0.12	54,80,107,112	0
10	HEM	C	302	43/43	0.98	0.11	52,81,118,122	0
10	HEM	A	303	43/43	0.98	0.10	39,58,82,83	0
9	CD	A	301	1/1	0.99	0.07	83,83,83,83	0
10	HEM	A	302	43/43	0.99	0.09	35,58,79,112	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.

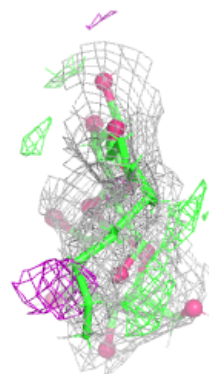
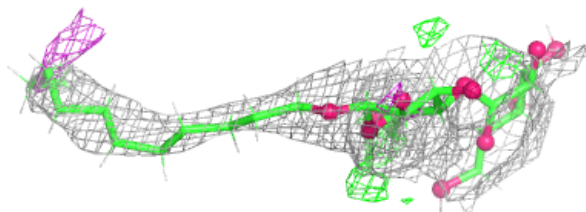
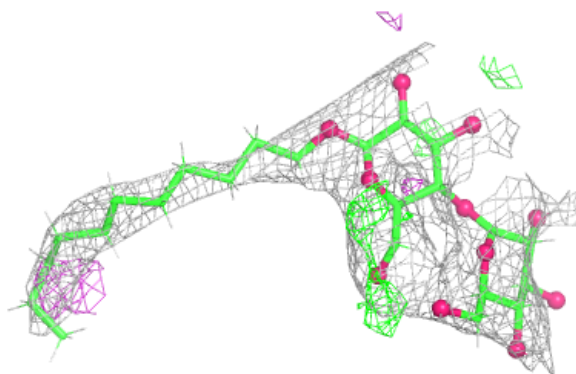


Electron density around UMQ A 306:

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

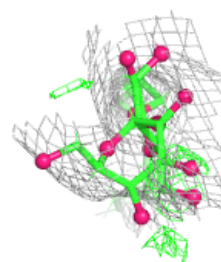
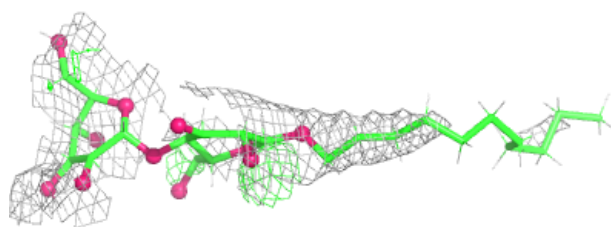
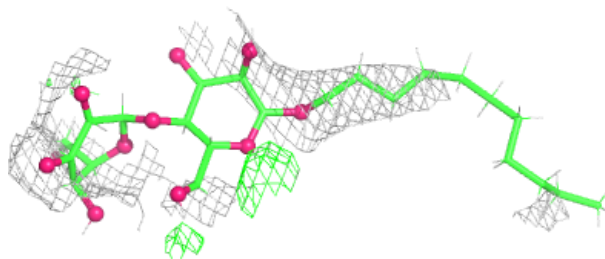
**Electron density around UMQ C 301:**

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

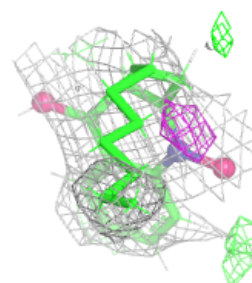
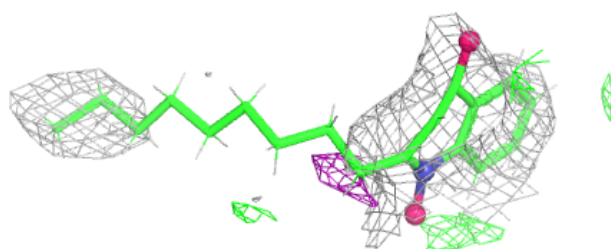
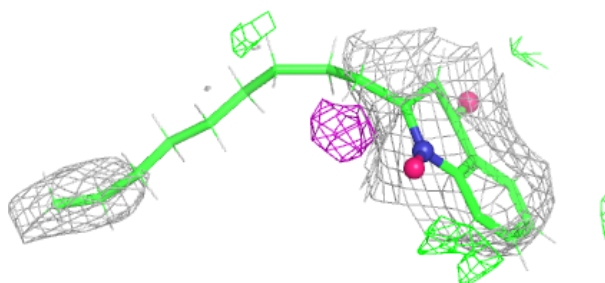


Electron density around UMQ A 309:

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

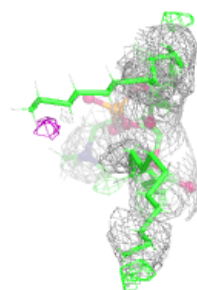
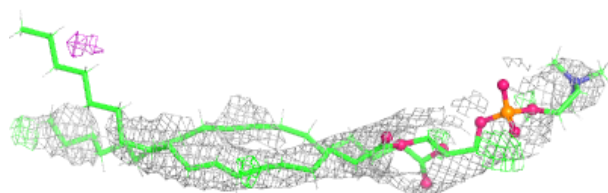
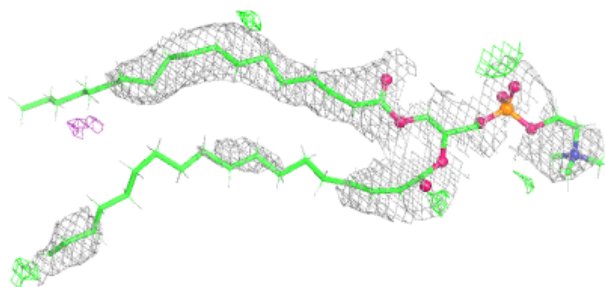
**Electron density around QNO A 308:**

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

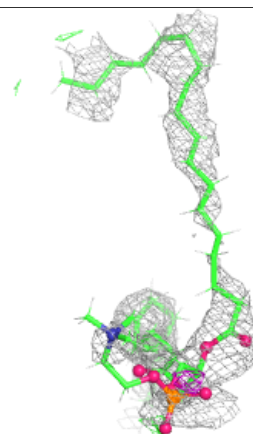
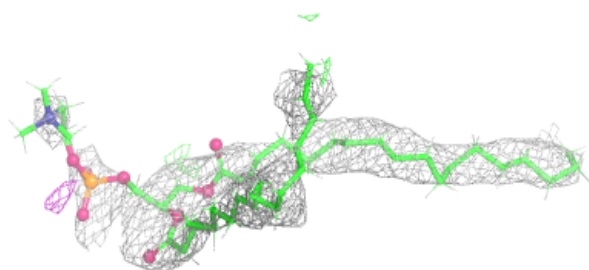
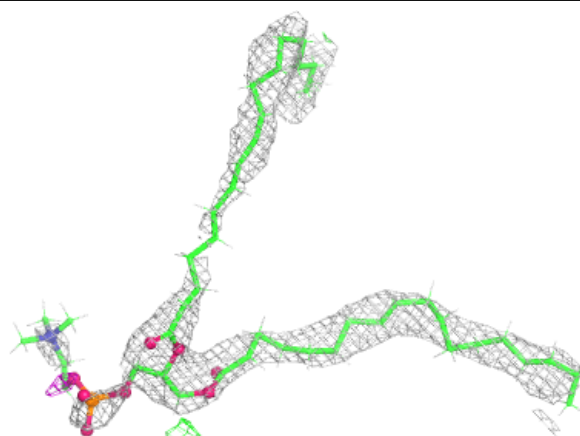


Electron density around OPC B 203:

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

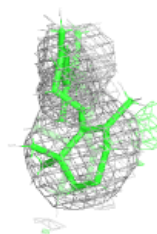
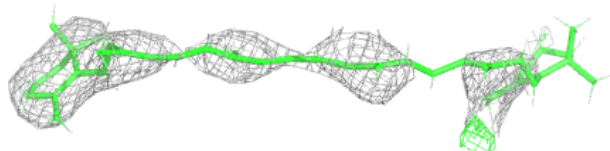
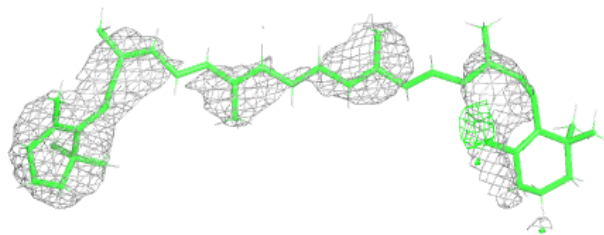
**Electron density around OPC A 305:**

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

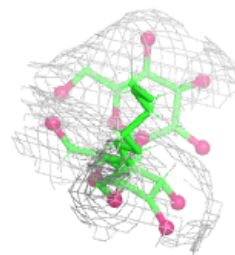
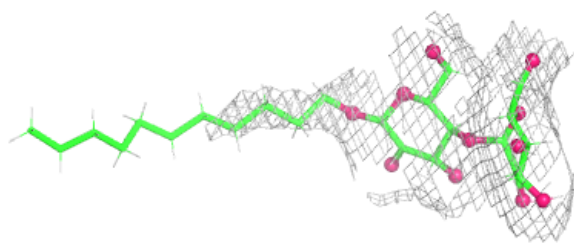
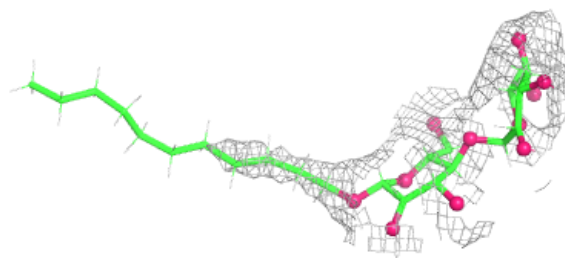


Electron density around BCR G 101:

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

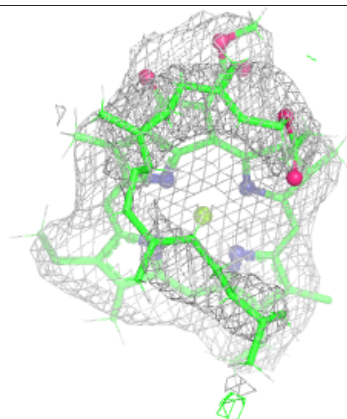
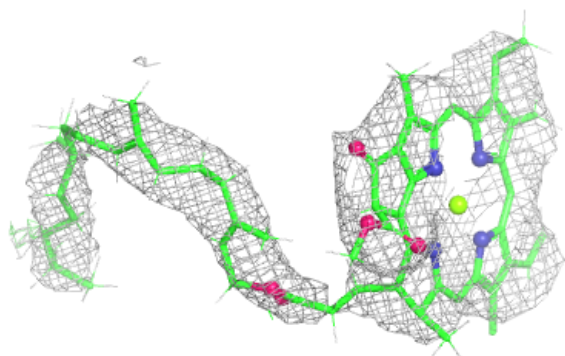
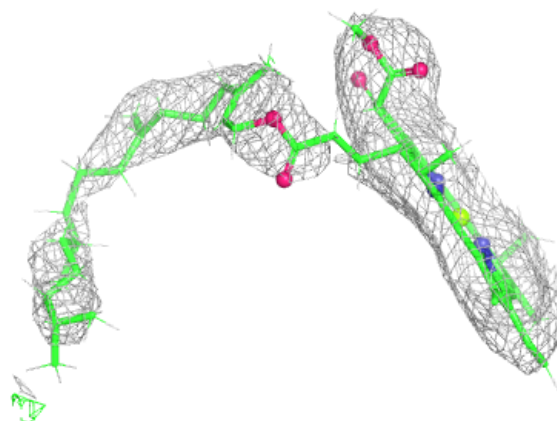
**Electron density around UMQ A 307:**

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



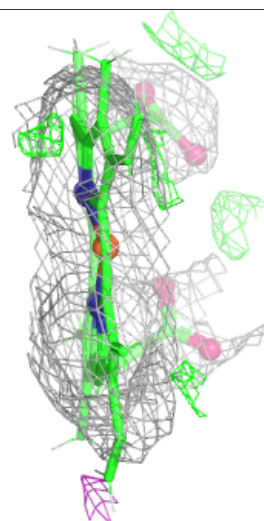
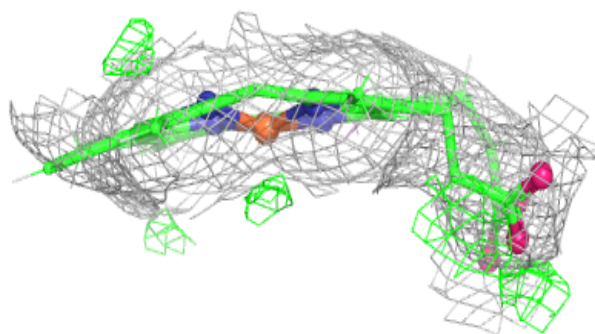
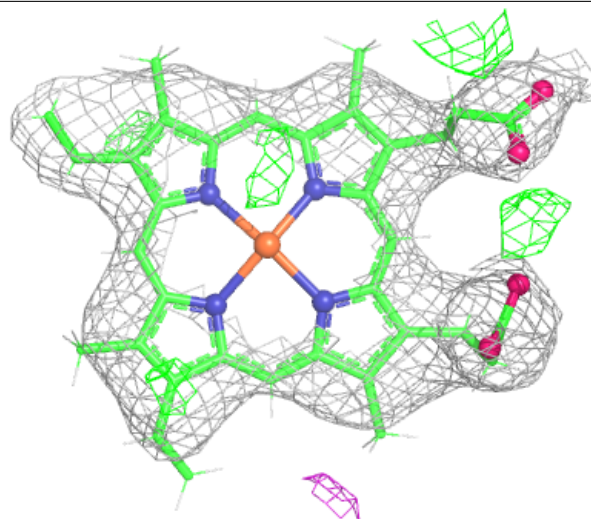
Electron density around CLA B 202:

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



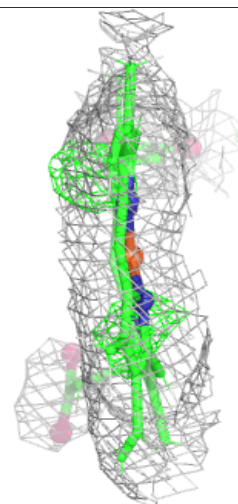
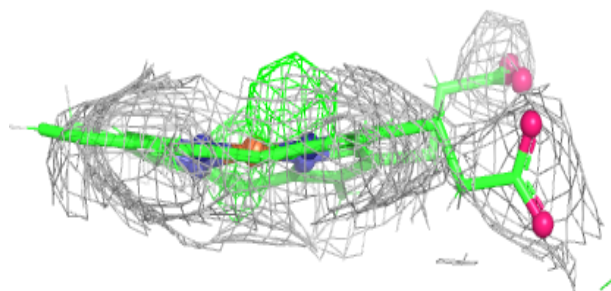
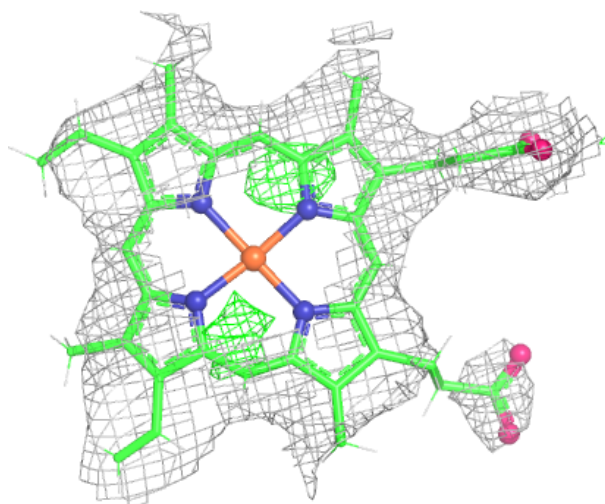
Electron density around HEM A 304:

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



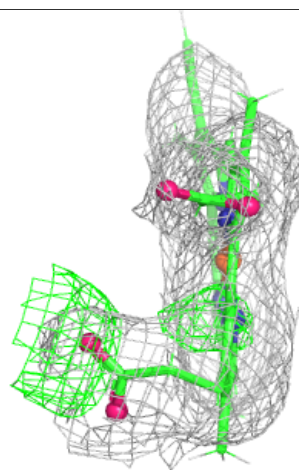
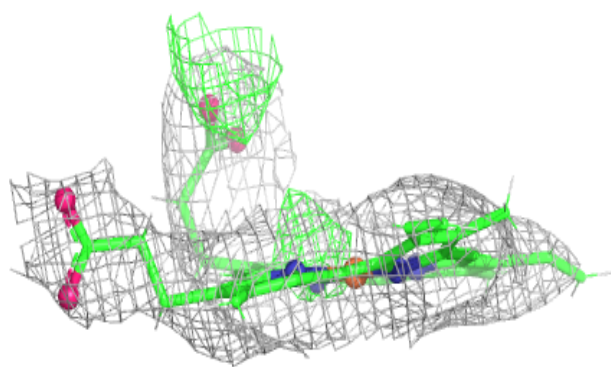
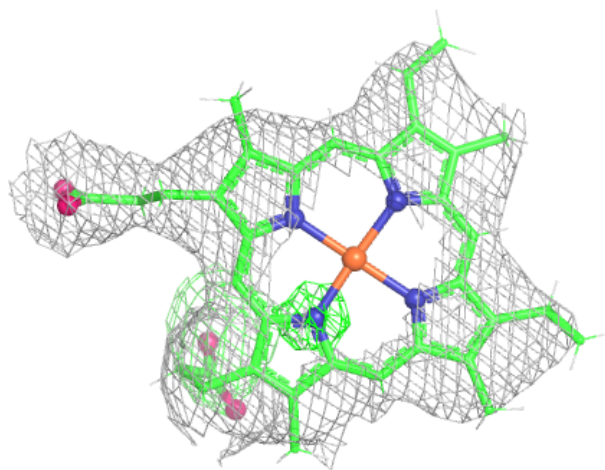
Electron density around HEM C 302:

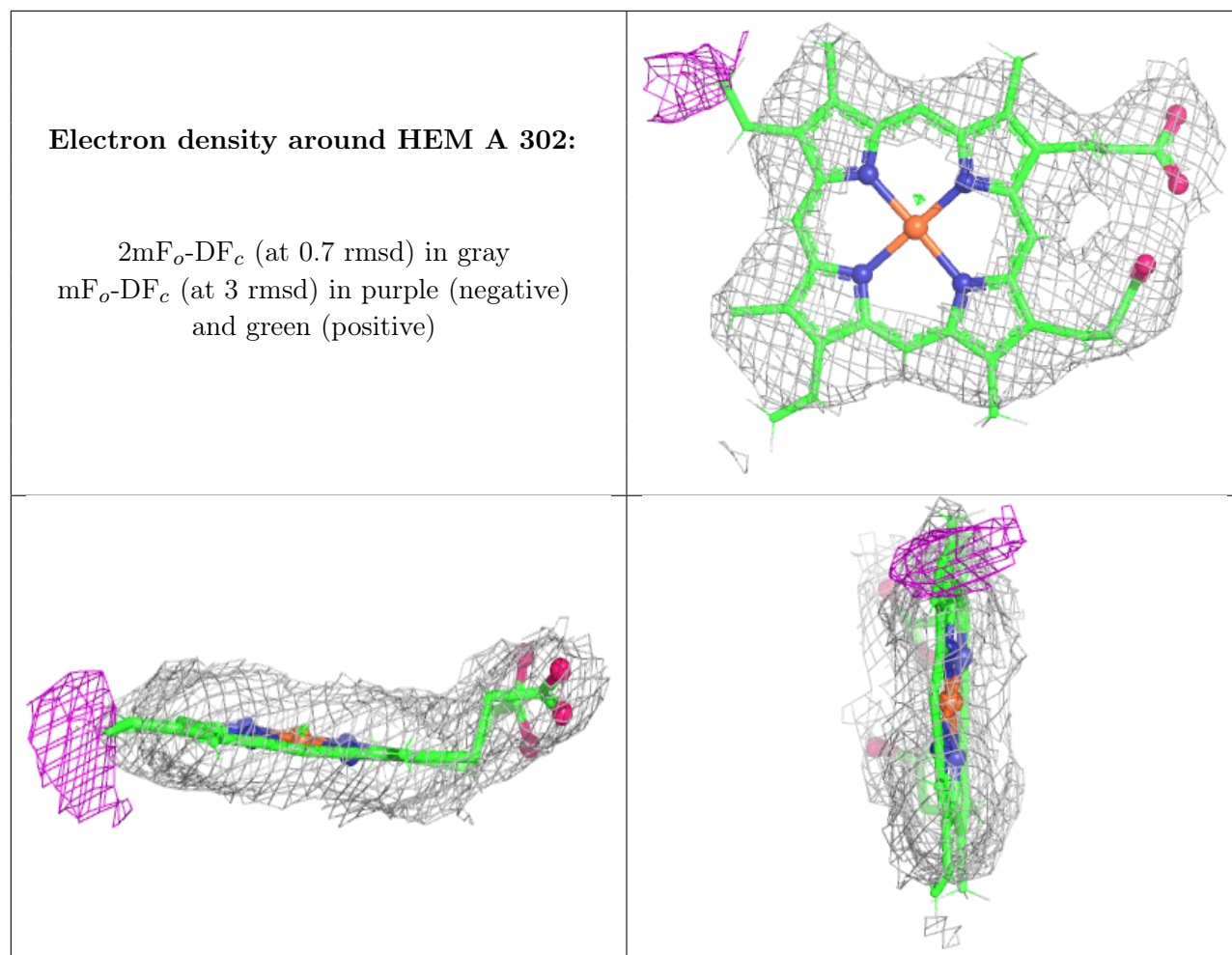
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 303:

$2mF_o-DF_c$ (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.