



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 09:52 PM EDT

PDB ID : 2ZT9 / pdb_00002zt9
Title : Crystal Structure of the Cytochrome b6f Complex from Nostoc sp. PCC 7120
Authors : Craner, W.A.; Baniulis, D.; Yamashita, E.
Deposited on : 2008-09-27
Resolution : 3.00 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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

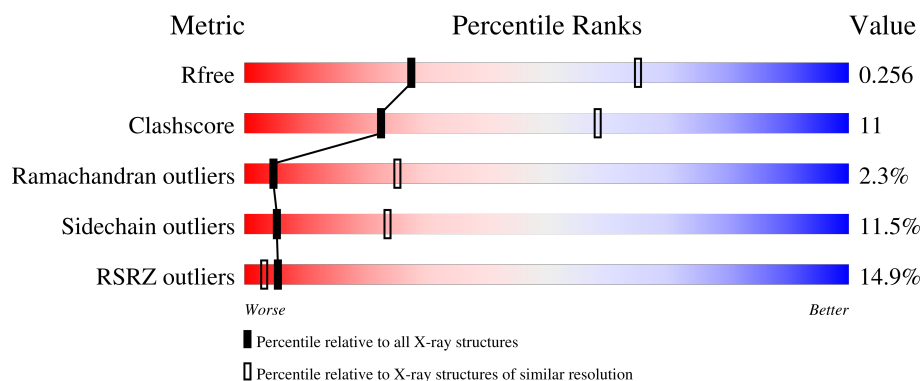
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	
2	B	160	
3	C	289	
4	D	179	
5	E	31	

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Mol	Chain	Length	Quality of chain
6	F	34	
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
10	UMQ	A	304	X	-	-	-
10	UMQ	A	305	X	-	-	-
10	UMQ	A	306	X	-	-	-
11	CLA	B	201	X	-	-	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 7912 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 b6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1715	1144	272	288	11			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	160	Total	C	N	O	S	0	0	0
			1239	830	195	208	6			

- Molecule 3 is a protein called Apocytochrome f.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	289	Total	C	N	O	S	0	0	0
			2195	1396	364	429	6			

- Molecule 4 is a protein called Cytochrome b6-f complex iron-sulfur subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	166	Total	C	N	O	S	0	0	0
			1249	791	213	239	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	31	Total	C	N	O	S	0	0	0
			227	157	35	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	N	O	S	0	0	0
			231	156	36	38	1			

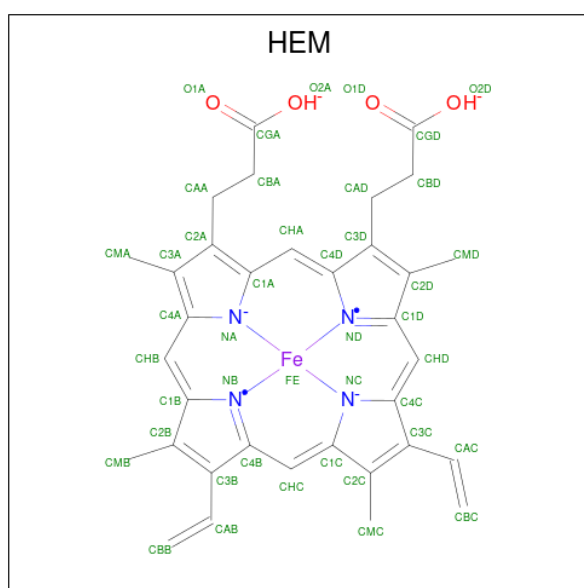
- Molecule 7 is a protein called Cytochrome b6-f complex subunit 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	37	Total	C	N	O	S	0	0	0
			281	188	44	48	1			

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

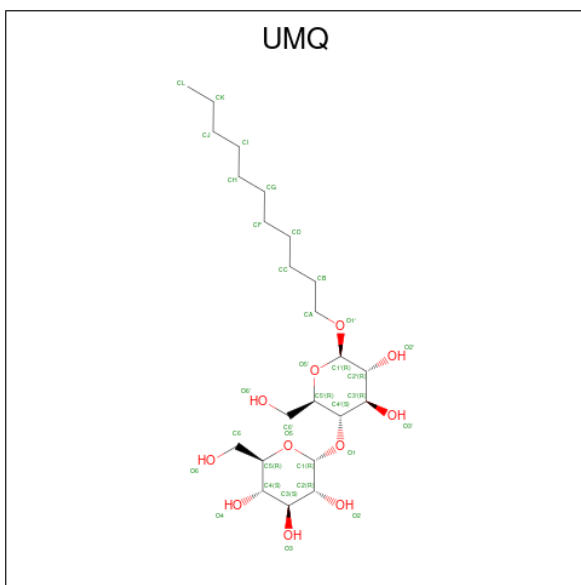
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	29	Total	C	N	O	S	0	0	0
			227	155	36	34	2			

- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



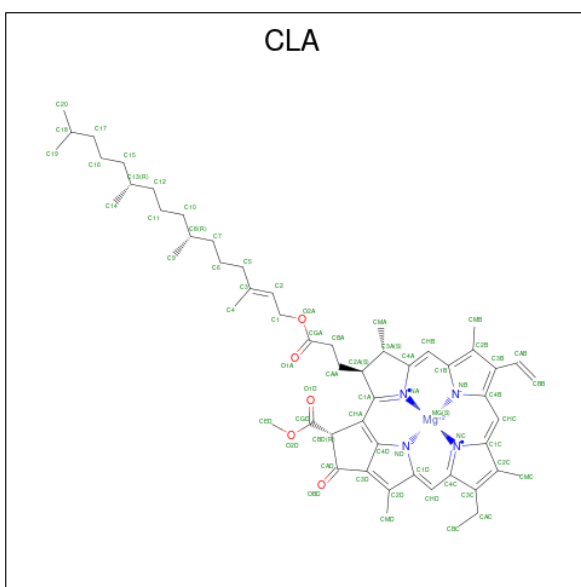
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 10 is UNDECYL-MALTOSIDE (CCD ID: UMQ) (formula: $C_{23}H_{44}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total 34	C 23	O 11	0	0
10	A	1	Total 34	C 23	O 11	0	0
10	A	1	Total 34	C 23	O 11	0	0

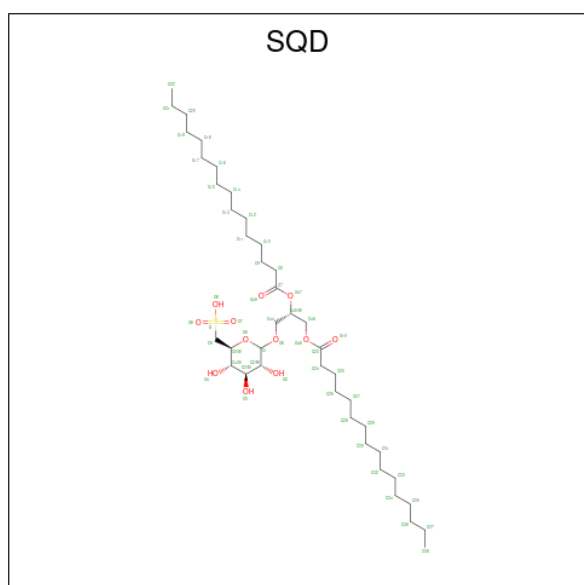
- Molecule 11 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

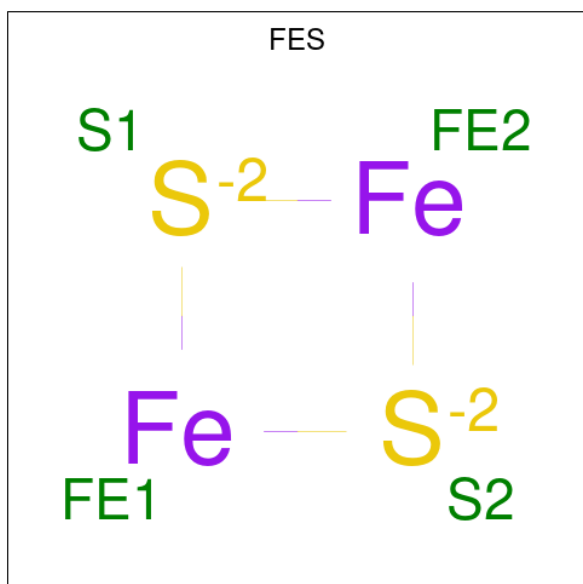
- # OPC

- Molecule 13 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



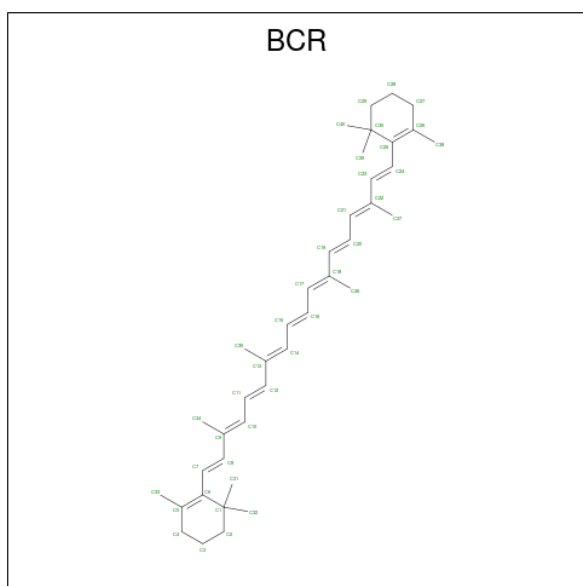
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	B	1	Total	C	O	S	0	0
			54	41	12	1		

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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

- Molecule 15 is BETA-CAROTENE (CCD ID: BCR) (formula: $\text{C}_{40}\text{H}_{56}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	G	1	Total C 40 40	0	0

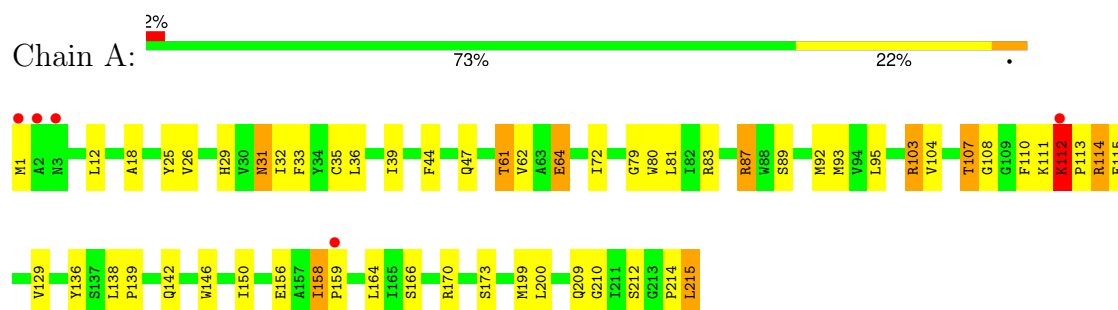
- Molecule 16 is water.

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

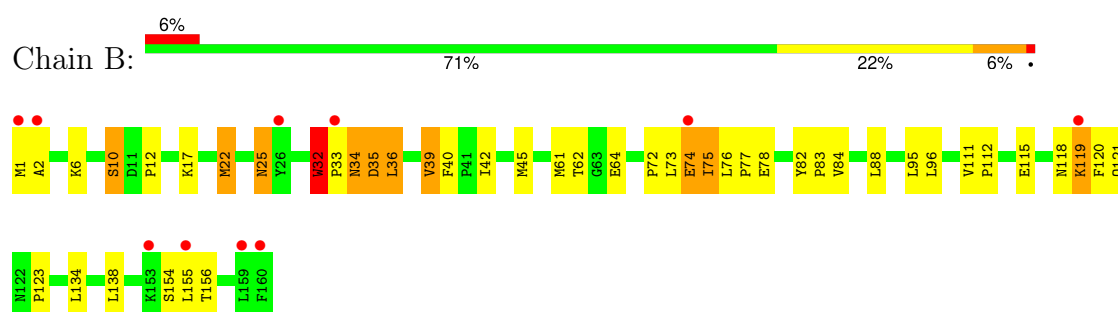
3 Residue-property plots [i](#)

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.

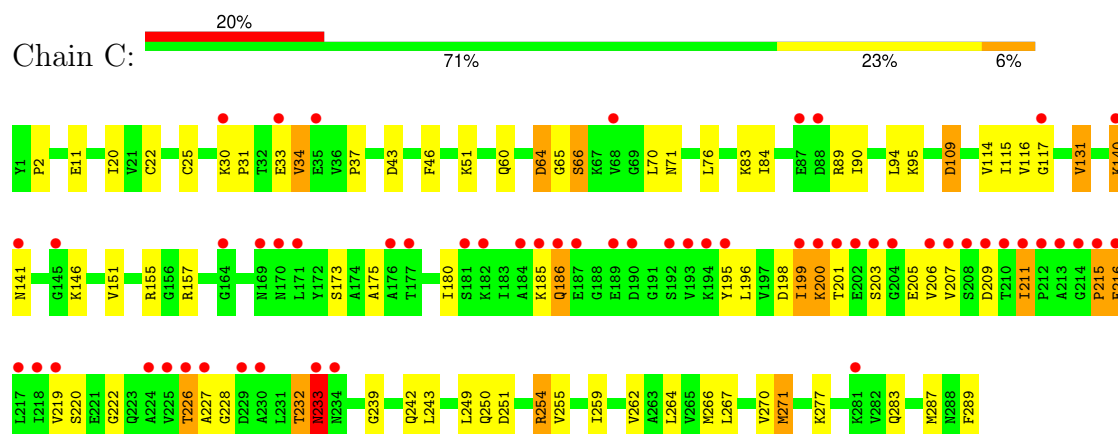
• Molecule 1: Cytochrome b6



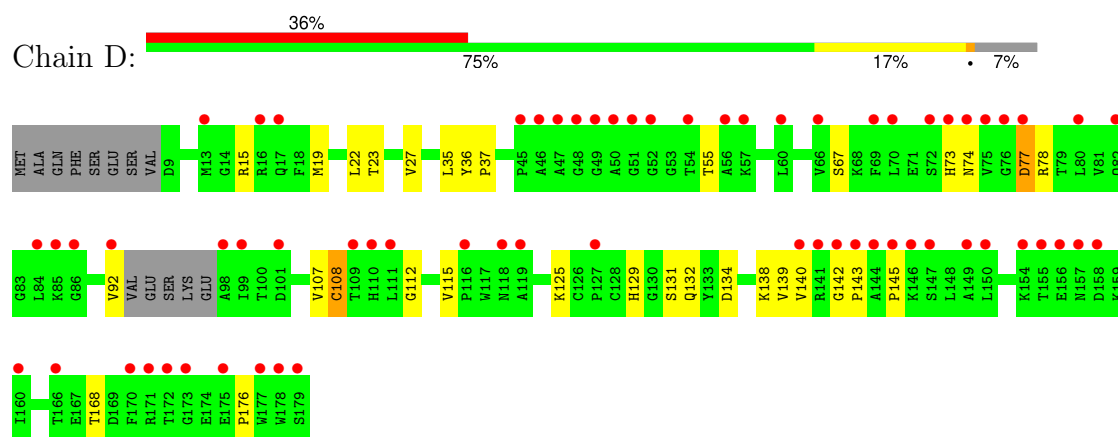
• Molecule 2: Cytochrome b6-f complex subunit 4



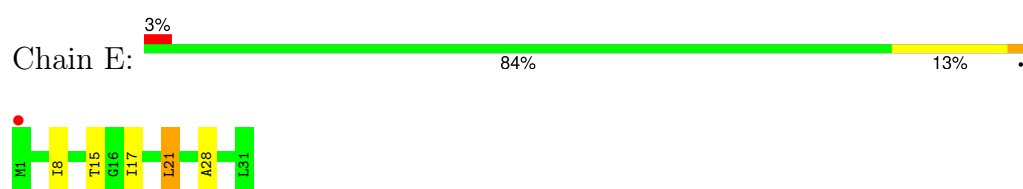
• Molecule 3: Apocytochrome f



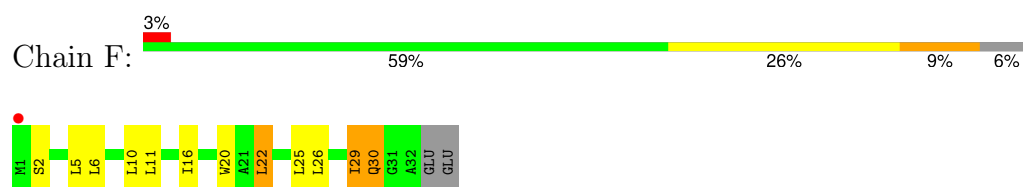
• Molecule 4: Cytochrome b6-f complex iron-sulfur subunit 1



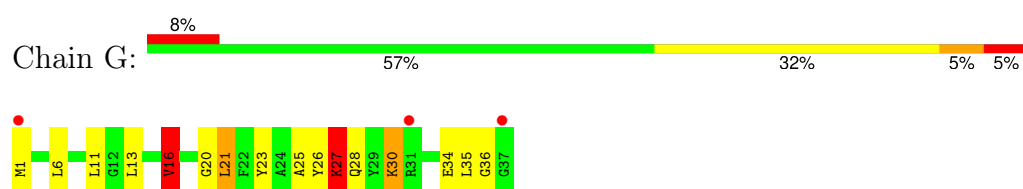
- Molecule 5: Cytochrome b6-f complex subunit 6



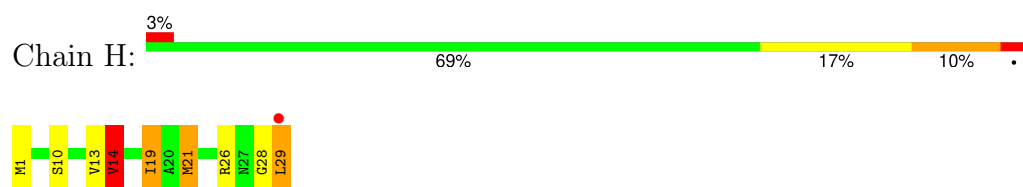
- Molecule 6: Cytochrome b6-f complex subunit 7



- 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	159.22Å 159.22Å 365.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.69 – 3.00 45.69 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (45.69-3.00) 98.5 (45.69-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.87 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.230 , 0.259 0.228 , 0.256	Depositor DCC
R_{free} test set	2770 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	75.0	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7912	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: OPC, HEM, BCR, FES, SQD, CLA, UMQ

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	0.63	0/1768	1.02	5/2411 (0.2%)
2	B	0.62	1/1278 (0.1%)	0.97	3/1752 (0.2%)
3	C	0.58	0/2241	0.89	0/3053
4	D	0.53	0/1280	0.89	1/1745 (0.1%)
5	E	0.57	0/230	0.93	0/309
6	F	0.50	0/234	0.91	0/315
7	G	0.63	0/286	1.08	1/387 (0.3%)
8	H	0.61	0/233	1.03	1/319 (0.3%)
All	All	0.59	1/7550 (0.0%)	0.95	11/10291 (0.1%)

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	111	VAL	CA-CB	5.22	1.56	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	LYS	CA-C-N	-10.15	109.31	119.56
1	A	112	LYS	C-N-CA	-10.15	109.31	119.56
1	A	158	ILE	CA-C-N	9.07	128.67	119.24
1	A	158	ILE	C-N-CA	9.07	128.67	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	16	VAL	CB-CA-C	-6.21	103.90	112.04
2	B	32	TRP	CA-C-N	-6.15	112.15	119.84
2	B	32	TRP	C-N-CA	-6.15	112.15	119.84
1	A	114	ARG	N-CA-C	5.39	119.84	112.88
4	D	77	ASP	N-CA-C	5.31	117.73	110.24
8	H	14	VAL	N-CA-CB	5.08	117.45	110.54
2	B	73	LEU	N-CA-C	-5.06	101.45	109.96

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	32	TRP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1715	0	1734	49	0
2	B	1239	0	1290	40	0
3	C	2195	0	2183	56	0
4	D	1249	0	1208	17	0
5	E	227	0	257	3	0
6	F	231	0	252	6	0
7	G	281	0	303	12	0
8	H	227	0	243	13	0
9	A	129	0	90	8	0
9	C	43	0	30	6	0
10	A	102	0	123	4	0
11	B	65	0	72	1	0
12	B	54	0	83	0	0
12	H	54	0	83	5	0
13	B	54	0	78	1	0
14	D	4	0	0	1	0
15	G	40	0	53	7	0
16	A	1	0	0	0	0
16	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7912	0	8082	168	0

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

All (168) 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)
1:A:35:CYS:SG	9:A:303:HEM:CAB	2.17	1.32
1:A:35:CYS:HG	9:A:303:HEM:CAB	1.43	1.32
1:A:35:CYS:SG	9:A:303:HEM:HAB	1.79	1.22
3:C:25:CYS:SG	9:C:301:HEM:CAC	2.37	1.13
3:C:25:CYS:SG	9:C:301:HEM:HAC	1.93	1.09
2:B:34:ASN:HD22	2:B:34:ASN:H	1.13	0.96
3:C:251:ASP:HB3	3:C:254:ARG:HD3	1.45	0.96
3:C:22:CYS:HB2	9:C:301:HEM:HAB	1.46	0.95
3:C:250:GLN:HE21	3:C:251:ASP:H	0.99	0.92
9:A:303:HEM:HHA	9:A:303:HEM:HBD1	1.55	0.87
3:C:232:THR:O	3:C:233:ASN:HB3	1.75	0.87
1:A:32:ILE:HD11	15:G:101:BCR:H322	1.60	0.82
1:A:103:ARG:NH1	1:A:104:VAL:HA	1.95	0.81
1:A:146:TRP:HB3	2:B:75:ILE:HD11	1.67	0.75
1:A:39:ILE:HD11	15:G:101:BCR:H312	1.70	0.74
8:H:28:GLY:C	8:H:29:LEU:HG	2.12	0.74
3:C:250:GLN:HE21	3:C:251:ASP:N	1.81	0.73
2:B:22:MET:O	2:B:22:MET:HG2	1.88	0.73
4:D:131:SER:HA	4:D:142:GLY:HA3	1.71	0.73
1:A:83:ARG:NH1	9:A:301:HEM:O1D	2.21	0.72
2:B:32:TRP:O	2:B:33:PRO:C	2.32	0.71
2:B:34:ASN:H	2:B:34:ASN:ND2	1.84	0.70
3:C:60:GLN:HE22	3:C:157:ARG:H	1.38	0.70
1:A:112:LYS:O	1:A:115:GLU:OE1	2.10	0.70
2:B:118:ASN:HD22	2:B:120:PHE:H	1.39	0.68
2:B:17:LYS:HB3	2:B:22:MET:O	1.93	0.68
1:A:103:ARG:O	1:A:107:THR:HB	1.94	0.67
2:B:45:MET:HE3	4:D:27:VAL:HG13	1.77	0.67
3:C:226:THR:HG22	3:C:227:ALA:H	1.60	0.67
1:A:47:GLN:NE2	1:A:89:SER:HB3	2.09	0.67
1:A:103:ARG:HH11	1:A:104:VAL:HA	1.58	0.66
3:C:270:VAL:HG22	8:H:21:MET:HE2	1.79	0.64
2:B:32:TRP:CD1	2:B:33:PRO:HD3	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:PRO:HD2	7:G:25:ALA:HB1	1.80	0.64
5:E:17:ILE:O	5:E:21:LEU:HB2	1.98	0.64
1:A:209:GLN:HB3	2:B:22:MET:HE2	1.81	0.63
1:A:32:ILE:N	8:H:29:LEU:HD13	2.14	0.62
3:C:84:ILE:HD11	3:C:114:VAL:HG11	1.82	0.62
3:C:20:ILE:HD12	3:C:242:GLN:HG2	1.83	0.60
4:D:108:CYS:HB3	4:D:115:VAL:CG2	2.31	0.60
2:B:119:LYS:O	2:B:119:LYS:HG2	2.02	0.59
1:A:39:ILE:CD1	15:G:101:BCR:H312	2.33	0.59
10:A:304:UMQ:HB1	3:C:254:ARG:HA	1.85	0.58
4:D:108:CYS:HB3	4:D:115:VAL:HG22	1.86	0.57
4:D:15:ARG:NH1	5:E:28:ALA:O	2.37	0.56
2:B:34:ASN:HD21	3:C:283:GLN:HE22	1.51	0.56
3:C:262:VAL:HG13	8:H:14:VAL:HG13	1.86	0.56
8:H:1:MET:HE3	12:H:30:OPC:HAE3	1.87	0.56
3:C:175:ALA:HB2	3:C:209:ASP:OD2	2.06	0.56
3:C:200:LYS:HG3	3:C:206:VAL:HG22	1.86	0.56
3:C:262:VAL:HG12	3:C:266:MET:HE2	1.87	0.56
3:C:30:LYS:HG2	3:C:239:GLY:HA3	1.87	0.56
3:C:155:ARG:HD2	3:C:155:ARG:H	1.72	0.55
6:F:20:TRP:CZ3	15:G:101:BCR:H19C	2.41	0.55
3:C:31:PRO:O	3:C:155:ARG:NH2	2.41	0.54
2:B:22:MET:O	2:B:22:MET:CG	2.54	0.54
1:A:29:HIS:HB2	7:G:28:GLN:HE22	1.72	0.54
1:A:114:ARG:NH1	1:A:210:GLY:O	2.41	0.54
2:B:45:MET:CE	4:D:27:VAL:HG13	2.37	0.54
4:D:131:SER:CA	4:D:142:GLY:HA3	2.37	0.53
1:A:87:ARG:NH1	2:B:78:GLU:OE1	2.40	0.53
12:H:30:OPC:HAP2	12:H:30:OPC:HBL1	1.91	0.53
4:D:107:VAL:HG12	4:D:112:GLY:HA2	1.91	0.52
3:C:34:VAL:HG23	3:C:243:LEU:HD12	1.92	0.52
3:C:173:SER:HB2	3:C:228:GLY:HA2	1.90	0.52
3:C:255:VAL:O	3:C:259:ILE:HG12	2.09	0.52
1:A:32:ILE:H	8:H:29:LEU:HD13	1.72	0.52
1:A:83:ARG:HD2	9:A:301:HEM:O1A	2.09	0.52
1:A:111:LYS:O	1:A:113:PRO:HD2	2.09	0.52
1:A:146:TRP:HB3	2:B:75:ILE:CD1	2.38	0.52
3:C:22:CYS:HB2	9:C:301:HEM:CAB	2.31	0.51
8:H:10:SER:O	8:H:14:VAL:HG22	2.10	0.51
1:A:44:PHE:HB2	1:A:93:MET:HE3	1.92	0.51
3:C:64:ASP:CG	3:C:65:GLY:H	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:MET:HG3	3:C:146:LYS:HD3	1.93	0.50
3:C:140:LYS:N	3:C:140:LYS:HD3	2.25	0.50
4:D:131:SER:CB	4:D:142:GLY:HA3	2.41	0.50
1:A:31:ASN:HD22	1:A:33:PHE:H	1.58	0.50
2:B:25:ASN:H	2:B:25:ASN:ND2	2.08	0.50
4:D:36:TYR:HB3	4:D:37:PRO:HD3	1.94	0.50
10:A:305:UMQ:HB2	13:B:203:SQD:O10	2.12	0.49
3:C:266:MET:O	3:C:270:VAL:HG23	2.12	0.49
7:G:20:GLY:N	15:G:101:BCR:H363	2.26	0.49
1:A:215:LEU:HG	7:G:28:GLN:OE1	2.12	0.49
8:H:1:MET:HB3	12:H:30:OPC:HAE1	1.95	0.49
8:H:28:GLY:O	8:H:29:LEU:HG	2.13	0.49
3:C:199:ILE:O	3:C:200:LYS:CB	2.61	0.49
8:H:26:ARG:HH11	8:H:29:LEU:HD11	1.77	0.49
1:A:80:TRP:CH2	3:C:254:ARG:HG2	2.48	0.48
7:G:26:TYR:CE2	7:G:30:LYS:HE2	2.49	0.48
1:A:142:GLN:HG3	2:B:72:PRO:HG3	1.95	0.48
3:C:250:GLN:NE2	3:C:251:ASP:H	1.85	0.48
4:D:77:ASP:OD2	4:D:77:ASP:N	2.46	0.48
6:F:11:LEU:HD21	12:H:30:OPC:HAV	1.96	0.48
1:A:25:TYR:OH	3:C:289:PHE:O	2.24	0.47
2:B:10:SER:O	2:B:12:PRO:HD3	2.14	0.47
4:D:129:HIS:HB2	14:D:200:FES:S1	2.54	0.47
1:A:129:VAL:HG21	11:B:201:CLA:H43	1.96	0.47
2:B:154:SER:C	2:B:156:THR:H	2.23	0.47
3:C:46:PHE:CE2	3:C:131:VAL:HG22	2.49	0.47
7:G:23:TYR:OH	7:G:27:LYS:HE3	2.15	0.47
3:C:22:CYS:CB	9:C:301:HEM:HAB	2.32	0.47
1:A:150:ILE:HD11	2:B:75:ILE:HG12	1.97	0.46
1:A:72:ILE:O	1:A:79:GLY:HA3	2.16	0.46
9:A:303:HEM:HBD1	9:A:303:HEM:CHA	2.32	0.46
1:A:115:GLU:OE1	1:A:115:GLU:N	2.45	0.46
15:G:101:BCR:H20C	15:G:101:BCR:H361	1.65	0.46
3:C:271:MET:HG3	4:D:23:THR:HA	1.96	0.46
4:D:168:THR:HA	4:D:176:PRO:HD3	1.98	0.46
2:B:32:TRP:O	2:B:34:ASN:N	2.49	0.46
1:A:29:HIS:CB	7:G:28:GLN:HE22	2.30	0.45
4:D:134:ASP:HB2	4:D:138:LYS:H	1.81	0.45
3:C:155:ARG:HD2	3:C:155:ARG:N	2.31	0.45
3:C:270:VAL:HA	8:H:21:MET:CE	2.46	0.45
6:F:26:LEU:HA	6:F:29:ILE:HG23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33:GLU:HB2	3:C:51:LYS:HB2	1.97	0.45
1:A:138:LEU:N	1:A:139:PRO:CD	2.79	0.45
2:B:36:LEU:O	2:B:40:PHE:HB2	2.16	0.45
2:B:82:TYR:HB2	2:B:83:PRO:HD3	1.98	0.45
3:C:186:GLN:HE21	3:C:196:LEU:HG	1.82	0.45
2:B:22:MET:HE3	2:B:22:MET:HB3	1.91	0.45
2:B:1:MET:HB3	2:B:2:ALA:H	1.61	0.45
3:C:37:PRO:HB3	12:H:30:OPC:HAH1	1.97	0.45
3:C:76:LEU:HD12	3:C:151:VAL:HG22	1.99	0.45
2:B:74:GLU:OE1	7:G:1:MET:HA	2.17	0.45
3:C:199:ILE:O	3:C:200:LYS:HB2	2.16	0.45
1:A:61:THR:HG22	1:A:64:GLU:H	1.82	0.44
3:C:30:LYS:HB3	3:C:31:PRO:HD2	1.98	0.44
3:C:232:THR:O	3:C:233:ASN:CB	2.57	0.44
1:A:92:MET:HA	1:A:92:MET:HE2	1.99	0.44
7:G:34:GLU:HG2	7:G:35:LEU:HG	1.99	0.44
15:G:101:BCR:H323	8:H:19:ILE:HG12	1.98	0.44
3:C:71:ASN:N	9:C:301:HEM:O2A	2.45	0.44
2:B:39:VAL:HA	2:B:42:ILE:HD12	1.99	0.44
2:B:35:ASP:HA	2:B:39:VAL:HG13	2.00	0.43
3:C:43:ASP:CG	3:C:89:ARG:HH12	2.27	0.43
7:G:13:LEU:HA	7:G:16:VAL:HG23	2.00	0.43
3:C:109:ASP:OD2	3:C:109:ASP:C	2.61	0.43
1:A:108:GLY:HA3	2:B:121:GLN:HA	2.00	0.43
1:A:199:MET:HE2	9:A:302:HEM:HBB2	2.00	0.43
1:A:110:PHE:HD1	2:B:112:PRO:HB3	1.83	0.43
3:C:266:MET:SD	8:H:13:VAL:HG12	2.59	0.43
1:A:1:MET:HE2	1:A:1:MET:H1	1.84	0.43
3:C:215:PRO:HB2	3:C:216:GLU:H	1.70	0.42
1:A:114:ARG:NH2	1:A:212:SER:HA	2.35	0.42
3:C:195:TYR:HB2	3:C:211:ILE:HG13	2.01	0.42
7:G:21:LEU:HD12	7:G:21:LEU:HA	1.91	0.42
6:F:5:LEU:HD21	7:G:11:LEU:HD12	2.00	0.42
4:D:78:ARG:HG2	4:D:92:VAL:HG22	2.02	0.42
3:C:90:ILE:O	3:C:95:LYS:NZ	2.53	0.42
4:D:131:SER:HB3	4:D:143:PRO:HD2	2.00	0.42
3:C:180:ILE:HA	3:C:198:ASP:O	2.20	0.42
1:A:209:GLN:O	2:B:22:MET:HB2	2.19	0.42
2:B:25:ASN:ND2	2:B:25:ASN:N	2.68	0.42
1:A:113:PRO:HB2	2:B:22:MET:CE	2.50	0.41
2:B:118:ASN:ND2	2:B:120:PHE:HD1	2.17	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:SER:HB3	1:A:170:ARG:NH2	2.35	0.41
1:A:29:HIS:CD2	1:A:214:PRO:HA	2.55	0.41
1:A:136:TYR:CE1	2:B:78:GLU:HG3	2.55	0.41
3:C:199:ILE:HD12	3:C:207:VAL:HG23	2.02	0.41
1:A:158:ILE:HA	1:A:159:PRO:HD3	1.81	0.41
3:C:2:PRO:HG2	3:C:117:GLY:HA2	2.01	0.41
6:F:30:GLN:HE21	6:F:30:GLN:HB2	1.61	0.41
1:A:111:LYS:HE2	2:B:115:GLU:O	2.22	0.40
10:A:306:UMQ:HA2	2:B:32:TRP:NE1	2.36	0.40
5:E:15:THR:OG1	6:F:22:LEU:HD21	2.21	0.40
1:A:18:ALA:CB	10:A:306:UMQ:H6'1	2.52	0.40
3:C:180:ILE:O	3:C:222:GLY:HA2	2.21	0.40

There are no symmetry-related clashes.

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	213/215 (99%)	200 (94%)	12 (6%)	1 (0%)	24	60
2	B	158/160 (99%)	143 (90%)	10 (6%)	5 (3%)	3	18
3	C	287/289 (99%)	245 (85%)	31 (11%)	11 (4%)	2	15
4	D	162/179 (90%)	144 (89%)	16 (10%)	2 (1%)	10	40
5	E	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
6	F	30/34 (88%)	28 (93%)	1 (3%)	1 (3%)	3	17
7	G	35/37 (95%)	32 (91%)	1 (3%)	2 (6%)	1	8
8	H	27/29 (93%)	27 (100%)	0	0	100	100
All	All	941/974 (97%)	847 (90%)	72 (8%)	22 (2%)	5	25

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	LYS
2	B	32	TRP
3	C	64	ASP
3	C	66	SER
3	C	200	LYS
3	C	215	PRO
3	C	233	ASN
4	D	145	PRO
3	C	220	SER
6	F	2	SER
2	B	74	GLU
2	B	155	LEU
3	C	199	ILE
3	C	216	GLU
3	C	201	THR
3	C	205	GLU
7	G	27	LYS
3	C	203	SER
4	D	74	ASN
2	B	75	ILE
7	G	36	GLY
2	B	77	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	184/184 (100%)	167 (91%)	17 (9%)	8	33
2	B	134/134 (100%)	116 (87%)	18 (13%)	4	18
3	C	238/238 (100%)	212 (89%)	26 (11%)	6	26
4	D	133/145 (92%)	122 (92%)	11 (8%)	10	37
5	E	21/21 (100%)	19 (90%)	2 (10%)	8	31
6	F	22/24 (92%)	15 (68%)	7 (32%)	0	1
7	G	29/29 (100%)	24 (83%)	5 (17%)	2	11
8	H	24/24 (100%)	20 (83%)	4 (17%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	785/799 (98%)	695 (88%)	90 (12%)	5 24

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	26	VAL
1	A	31	ASN
1	A	36	LEU
1	A	61	THR
1	A	62	VAL
1	A	64	GLU
1	A	81	LEU
1	A	87	ARG
1	A	95	LEU
1	A	103	ARG
1	A	107	THR
1	A	156	GLU
1	A	164	LEU
1	A	173	SER
1	A	200	LEU
1	A	215	LEU
2	B	6	LYS
2	B	10	SER
2	B	22	MET
2	B	25	ASN
2	B	34	ASN
2	B	35	ASP
2	B	36	LEU
2	B	39	VAL
2	B	62	THR
2	B	64	GLU
2	B	76	LEU
2	B	84	VAL
2	B	88	LEU
2	B	95	LEU
2	B	96	LEU
2	B	119	LYS
2	B	134	LEU
2	B	138	LEU
3	C	11	GLU
3	C	34	VAL

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Mol	Chain	Res	Type
3	C	66	SER
3	C	70	LEU
3	C	83	LYS
3	C	94	LEU
3	C	109	ASP
3	C	115	ILE
3	C	116	VAL
3	C	131	VAL
3	C	140	LYS
3	C	141	ASN
3	C	185	LYS
3	C	186	GLN
3	C	211	ILE
3	C	219	VAL
3	C	226	THR
3	C	232	THR
3	C	233	ASN
3	C	249	LEU
3	C	254	ARG
3	C	264	LEU
3	C	267	LEU
3	C	271	MET
3	C	277	LYS
3	C	287	MET
4	D	19	MET
4	D	22	LEU
4	D	35	LEU
4	D	55	THR
4	D	67	SER
4	D	73	HIS
4	D	108	CYS
4	D	125	LYS
4	D	132	GLN
4	D	139	VAL
4	D	140	VAL
5	E	8	ILE
5	E	21	LEU
6	F	6	LEU
6	F	10	LEU
6	F	16	ILE
6	F	22	LEU
6	F	25	LEU

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Mol	Chain	Res	Type
6	F	29	ILE
6	F	30	GLN
7	G	6	LEU
7	G	16	VAL
7	G	21	LEU
7	G	27	LYS
7	G	30	LYS
8	H	14	VAL
8	H	19	ILE
8	H	21	MET
8	H	29	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	47	GLN
1	A	77	ASN
2	B	25	ASN
2	B	34	ASN
2	B	93	ASN
2	B	118	ASN
2	B	122	ASN
3	C	60	GLN
3	C	123	GLN
3	C	250	GLN
3	C	288	ASN
6	F	30	GLN
7	G	28	GLN
7	G	33	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	UMQ	A	306	-	35,35,35	1.49	3 (8%)	46,46,46	2.26	11 (23%)
10	UMQ	A	305	-	35,35,35	1.47	3 (8%)	46,46,46	2.18	7 (15%)
15	BCR	G	101	-	41,41,41	2.47	11 (26%)	56,56,56	5.56	16 (28%)
9	HEM	A	302	1	50,50,50	1.84	10 (20%)	67,82,82	1.04	2 (2%)
11	CLA	B	201	16	69,73,73	1.93	17 (24%)	82,113,113	2.48	27 (32%)
9	HEM	A	301	1	50,50,50	1.83	7 (14%)	67,82,82	1.45	11 (16%)
14	FES	D	200	4	0,4,4	-	-	-	-	-
9	HEM	C	301	3	50,50,50	1.85	10 (20%)	67,82,82	1.28	4 (5%)
12	OPC	B	202	-	53,53,54	2.09	14 (26%)	59,61,64	2.30	15 (25%)
10	UMQ	A	304	-	35,35,35	1.41	3 (8%)	46,46,46	2.14	8 (17%)
12	OPC	H	30	-	53,53,54	2.07	14 (26%)	59,61,64	2.30	16 (27%)
9	HEM	A	303	16	50,50,50	1.99	8 (16%)	67,82,82	1.36	5 (7%)
13	SQD	B	203	-	52,54,54	1.02	2 (3%)	62,65,65	3.11	15 (24%)

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
10	UMQ	A	306	-	2/2/10/10	7/20/60/60	0/2/2/2
10	UMQ	A	305	-	2/2/10/10	13/20/60/60	0/2/2/2
15	BCR	G	101	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	B	201	16	1/1/15/20	13/39/115/115	-
9	HEM	A	302	1	-	8/14/54/54	-
9	HEM	A	301	1	-	5/14/54/54	-
14	FES	D	200	4	-	-	0/1/1/1
9	HEM	C	301	3	-	6/14/54/54	-
12	OPC	B	202	-	-	22/57/57/60	-
10	UMQ	A	304	-	2/2/10/10	13/20/60/60	0/2/2/2
12	OPC	H	30	-	-	33/57/57/60	-
9	HEM	A	303	16	-	5/14/54/54	-
13	SQD	B	203	-	-	30/49/69/69	0/1/1/1

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	G	101	BCR	C8-C9	-8.30	1.28	1.46
15	G	101	BCR	C23-C22	-8.17	1.28	1.46
9	C	301	HEM	C3D-C2D	7.91	1.53	1.36
9	A	302	HEM	C3D-C2D	7.84	1.53	1.36
9	A	303	HEM	C3D-C2D	7.51	1.53	1.36
9	A	301	HEM	C3D-C2D	7.35	1.52	1.36
10	A	306	UMQ	C1'-C2'	-6.43	1.33	1.52
10	A	305	UMQ	C1'-C2'	-6.27	1.34	1.52
9	A	303	HEM	FE-ND	6.06	2.13	1.94
10	A	304	UMQ	C1'-C2'	-6.00	1.34	1.52
9	A	303	HEM	FE-NC	5.75	2.14	1.95
12	B	202	OPC	CAG-CAH	-5.75	1.33	1.51
12	H	30	OPC	CAG-CAH	-5.35	1.35	1.51
12	B	202	OPC	CAQ-CAP	-5.15	1.33	1.52
12	H	30	OPC	CAQ-CAP	-5.14	1.33	1.52
12	B	202	OPC	OBJ-CBK	5.05	1.48	1.33
11	B	201	CLA	C3C-C2C	4.82	1.47	1.36
11	B	201	CLA	C3D-C4D	-4.74	1.33	1.44
15	G	101	BCR	C24-C25	-4.68	1.29	1.45
11	B	201	CLA	O2D-CGD	4.63	1.44	1.33
13	B	203	SQD	O47-C7	4.63	1.47	1.34
11	B	201	CLA	CHC-C1C	4.59	1.47	1.38
12	H	30	OPC	CBP-CBQ	-4.50	1.33	1.52
13	B	203	SQD	O48-C23	4.46	1.46	1.33
11	B	201	CLA	O2A-CGA	4.44	1.46	1.33
9	C	301	HEM	FE-NB	4.41	2.08	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	30	OPC	OBJ-CBK	4.41	1.46	1.33
15	G	101	BCR	C12-C13	-4.40	1.36	1.46
9	A	301	HEM	FE-NC	4.36	2.09	1.95
12	H	30	OPC	OAN-CAO	4.33	1.46	1.34
9	A	301	HEM	FE-NB	4.32	2.08	1.94
15	G	101	BCR	C19-C18	-4.23	1.36	1.46
12	B	202	OPC	OAN-CAO	4.11	1.45	1.34
12	B	202	OPC	CBP-CBQ	-4.06	1.35	1.52
9	A	302	HEM	FE-ND	4.05	2.07	1.94
11	B	201	CLA	CHD-C4C	3.95	1.48	1.39
10	A	306	UMQ	O2'-C2'	-3.90	1.33	1.43
12	B	202	OPC	CAV-CAW	3.87	1.53	1.31
12	H	30	OPC	CBP-CBO	-3.83	1.32	1.51
9	C	301	HEM	FE-ND	3.81	2.06	1.94
11	B	201	CLA	CHD-C1D	3.79	1.45	1.38
12	H	30	OPC	CAV-CAW	3.78	1.53	1.31
10	A	305	UMQ	O2'-C2'	-3.78	1.33	1.43
15	G	101	BCR	C7-C6	-3.78	1.32	1.45
9	A	302	HEM	FE-NC	3.78	2.07	1.95
10	A	305	UMQ	O1'-C1'	3.74	1.46	1.40
10	A	304	UMQ	O2'-C2'	-3.70	1.33	1.43
12	H	30	OPC	CAQ-CAR	-3.68	1.33	1.51
10	A	306	UMQ	O1'-C1'	3.61	1.46	1.40
12	B	202	OPC	CAQ-CAR	-3.60	1.33	1.51
9	A	302	HEM	FE-NB	3.59	2.05	1.94
9	A	301	HEM	FE-NA	3.59	2.07	1.95
12	B	202	OPC	CAR-CAS	-3.55	1.34	1.51
12	H	30	OPC	CAR-CAS	-3.55	1.34	1.51
11	B	201	CLA	OBD-CAD	3.54	1.28	1.22
12	H	30	OPC	CBB-CBC	-3.54	1.34	1.51
12	B	202	OPC	CBC-CBD	-3.53	1.34	1.51
12	B	202	OPC	CBB-CBC	-3.50	1.34	1.51
12	B	202	OPC	CBP-CBO	-3.48	1.34	1.51
11	B	201	CLA	CHC-C4B	3.47	1.47	1.39
12	H	30	OPC	CBC-CBD	-3.46	1.34	1.51
10	A	304	UMQ	O1'-C1'	3.38	1.45	1.40
9	A	301	HEM	CAC-C3C	3.33	1.56	1.47
15	G	101	BCR	C24-C23	-3.28	1.23	1.33
11	B	201	CLA	CHB-C1B	3.25	1.46	1.39
9	A	303	HEM	CAC-C3C	3.22	1.56	1.47
9	C	301	HEM	CAB-C3B	3.12	1.55	1.47
12	H	30	OPC	CBQ-CBR	-3.00	1.33	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	H	30	OPC	CBT-CBS	-2.96	1.33	1.50
9	A	301	HEM	CAB-C3B	2.95	1.55	1.47
9	A	302	HEM	CAB-C3B	2.90	1.55	1.47
9	A	303	HEM	CAB-C3B	2.89	1.55	1.47
11	B	201	CLA	C3D-C2D	2.87	1.46	1.39
12	B	202	OPC	CBT-CBS	-2.86	1.34	1.50
9	C	301	HEM	FE-NC	2.85	2.04	1.95
12	B	202	OPC	CBQ-CBR	-2.85	1.34	1.50
9	C	301	HEM	CAC-C3C	2.82	1.54	1.47
12	B	202	OPC	CAG-NAF	-2.73	1.43	1.51
9	A	302	HEM	CAC-C3C	2.70	1.54	1.47
11	B	201	CLA	C1B-C2B	2.65	1.49	1.43
11	B	201	CLA	C4C-C3C	2.57	1.49	1.45
11	B	201	CLA	C1C-C2C	2.52	1.49	1.44
9	A	303	HEM	FE-NB	2.44	2.02	1.94
9	A	303	HEM	CMA-C3A	2.43	1.55	1.50
15	G	101	BCR	C11-C10	-2.41	1.35	1.43
12	H	30	OPC	CAG-NAF	-2.39	1.44	1.51
11	B	201	CLA	C1D-C2D	2.37	1.50	1.45
9	A	302	HEM	CMA-C3A	2.35	1.55	1.50
15	G	101	BCR	C20-C21	-2.30	1.36	1.43
9	C	301	HEM	CMC-C2C	2.25	1.55	1.50
9	A	302	HEM	CMC-C2C	2.25	1.55	1.50
9	A	302	HEM	CMD-C2D	2.24	1.55	1.50
9	A	301	HEM	CMC-C2C	2.22	1.55	1.50
15	G	101	BCR	C15-C14	-2.20	1.36	1.43
15	G	101	BCR	C16-C17	-2.20	1.36	1.43
9	C	301	HEM	CMD-C2D	2.13	1.55	1.50
11	B	201	CLA	C1B-NB	-2.13	1.35	1.37
9	A	303	HEM	CMD-C2D	2.13	1.55	1.50
9	C	301	HEM	CMA-C3A	2.10	1.55	1.50
9	A	302	HEM	CMB-C2B	2.09	1.55	1.50
9	C	301	HEM	CMB-C2B	2.07	1.55	1.50
11	B	201	CLA	C1D-ND	-2.05	1.35	1.37

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	G	101	BCR	C24-C23-C22	30.25	170.99	126.23
15	G	101	BCR	C7-C8-C9	19.21	154.66	126.23
15	G	101	BCR	C23-C24-C25	15.75	169.08	127.00
13	B	203	SQD	O9-S-C6	-11.90	88.99	106.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	203	SQD	O8-S-O9	-11.36	82.97	111.40
13	B	203	SQD	O9-S-O7	-10.15	80.82	113.82
10	A	305	UMQ	O1'-C1'-C2'	8.63	121.38	108.27
12	H	30	OPC	CAA-NAF-CAE	-8.58	86.43	108.98
12	H	30	OPC	CAA-NAF-CBG	-8.56	86.49	108.98
10	A	304	UMQ	O1'-C1'-C2'	8.51	121.20	108.27
12	B	202	OPC	CAA-NAF-CBG	-8.38	86.96	108.98
12	B	202	OPC	CAA-NAF-CAE	-8.27	87.26	108.98
11	B	201	CLA	CMD-C2D-C1D	8.16	139.09	124.73
13	B	203	SQD	O8-S-C6	7.92	121.27	105.97
10	A	306	UMQ	O1'-C1'-C2'	7.66	119.91	108.27
15	G	101	BCR	C8-C7-C6	7.19	146.21	127.00
13	B	203	SQD	O7-S-C6	6.45	116.39	106.76
11	B	201	CLA	C2C-C1C-NC	6.44	116.75	109.98
11	B	201	CLA	C2B-C1B-NB	6.36	116.92	110.33
11	B	201	CLA	O2D-CGD-CBD	6.02	121.75	111.23
12	B	202	OPC	CAA-NAF-CAG	-5.65	87.46	109.91
9	C	301	HEM	C4D-ND-C1D	5.61	111.85	105.21
11	B	201	CLA	C3B-C2B-C1B	-5.60	100.57	107.17
12	H	30	OPC	CAA-NAF-CAG	-5.34	88.70	109.91
10	A	305	UMQ	CA-O1'-C1'	5.21	122.58	113.68
9	A	303	HEM	C4D-ND-C1D	5.21	111.38	105.21
9	A	301	HEM	C4D-ND-C1D	5.09	111.24	105.21
11	B	201	CLA	C3D-C2D-C1D	-5.02	98.98	105.83
10	A	306	UMQ	O5'-C1'-C2'	4.89	120.41	110.37
10	A	306	UMQ	C1'-C2'-C3'	4.79	120.08	110.01
15	G	101	BCR	C30-C25-C26	-4.76	116.14	122.64
10	A	306	UMQ	CA-O1'-C1'	4.73	121.76	113.68
10	A	304	UMQ	C1'-C2'-C3'	4.73	119.95	110.01
9	A	302	HEM	C4D-ND-C1D	4.72	110.79	105.21
10	A	304	UMQ	O5'-C1'-C2'	4.68	119.98	110.37
13	B	203	SQD	O47-C7-C8	4.65	121.54	111.48
15	G	101	BCR	C8-C9-C10	4.61	126.27	119.01
10	A	305	UMQ	C1'-C2'-C3'	4.53	119.54	110.01
11	B	201	CLA	C3C-C4C-NC	4.52	116.22	110.43
11	B	201	CLA	C1C-C2C-C3C	-4.51	102.24	106.98
10	A	305	UMQ	O2'-C2'-C1'	4.48	120.76	110.08
11	B	201	CLA	C3B-C4B-NB	4.39	114.45	110.53
10	A	304	UMQ	O2'-C2'-C1'	4.35	120.43	110.08
10	A	305	UMQ	O5'-C1'-O1'	4.29	120.19	110.04
9	A	301	HEM	CBD-CAD-C3D	-4.27	100.73	112.53
12	B	202	OPC	OAN-CAO-CAP	4.26	120.71	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	306	UMQ	O2'-C2'-C1'	4.25	120.20	110.08
12	B	202	OPC	CBG-NAF-CAE	4.10	119.75	108.98
10	A	306	UMQ	O5'-C1'-O1'	4.08	119.68	110.04
11	B	201	CLA	CHD-C1D-ND	-3.98	119.20	124.80
10	A	306	UMQ	O2'-C2'-C3'	3.96	119.72	110.38
10	A	305	UMQ	O2'-C2'-C3'	3.96	119.70	110.38
11	B	201	CLA	CHD-C4C-C3C	-3.93	119.04	124.77
10	A	305	UMQ	O5'-C1'-C2'	3.93	118.44	110.37
10	A	304	UMQ	O2'-C2'-C3'	3.92	119.61	110.38
13	B	203	SQD	O6-C44-C45	-3.85	101.46	110.82
12	H	30	OPC	CBG-NAF-CAE	3.84	119.05	108.98
13	B	203	SQD	O6-C1-C2	3.80	114.04	108.27
15	G	101	BCR	C34-C9-C10	-3.79	116.68	122.82
10	A	304	UMQ	CA-O1'-C1'	3.78	120.14	113.68
10	A	304	UMQ	O5'-C1'-O1'	3.71	118.81	110.04
9	A	301	HEM	CHC-C4B-NB	3.60	128.30	124.42
12	B	202	OPC	CAR-CAQ-CAP	3.40	125.62	113.13
12	H	30	OPC	CAH-CAG-NAF	3.36	126.61	115.82
10	A	306	UMQ	C1-O5-C5	3.34	120.23	113.72
12	H	30	OPC	OAN-CAO-CAP	3.33	118.68	111.48
11	B	201	CLA	C2D-C1D-ND	3.33	113.42	110.13
15	G	101	BCR	C27-C26-C25	-3.27	118.29	122.70
11	B	201	CLA	C1D-ND-C4D	-3.21	104.06	106.31
13	B	203	SQD	O8-S-O7	3.19	119.37	111.40
9	A	303	HEM	CAD-C3D-C4D	3.15	130.19	124.70
11	B	201	CLA	CAA-CBA-CGA	-3.10	104.39	113.21
10	A	306	UMQ	O5-C5-C4	3.10	115.28	109.70
11	B	201	CLA	O2A-CGA-CBA	3.05	121.14	111.83
12	H	30	OPC	CAE-NAF-CAG	3.01	121.88	109.91
11	B	201	CLA	CAC-C3C-C4C	2.97	128.65	124.79
12	H	30	OPC	OAI-CAH-CAG	2.94	123.78	109.65
12	B	202	OPC	OBJ-CBK-CBL	2.93	120.76	111.83
11	B	201	CLA	C3D-C4D-ND	2.91	114.71	109.99
9	A	301	HEM	C1D-C2D-C3D	-2.90	103.93	106.98
15	G	101	BCR	C38-C26-C27	2.88	119.74	113.60
12	H	30	OPC	OBJ-CBK-CBL	2.88	120.61	111.83
9	A	301	HEM	CAD-CBD-CGD	-2.83	106.16	113.67
13	B	203	SQD	O48-C23-C24	2.82	120.43	111.83
11	B	201	CLA	CMC-C2C-C1C	2.81	129.42	125.03
11	B	201	CLA	C4C-C3C-C2C	-2.79	102.83	106.89
10	A	306	UMQ	O5'-C5'-C4'	2.78	115.47	109.72
11	B	201	CLA	CAA-C2A-C3A	-2.74	105.58	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	H	30	OPC	CBP-CBQ-CBR	2.72	127.83	112.60
13	B	203	SQD	O5-C1-C2	-2.68	104.86	110.37
9	A	303	HEM	CMD-C2D-C1D	2.67	129.20	125.03
11	B	201	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
15	G	101	BCR	C30-C25-C24	2.65	122.83	115.65
12	B	202	OPC	CBO-CBP-CBQ	2.60	126.35	113.86
12	B	202	OPC	CBP-CBQ-CBR	2.57	126.98	112.60
12	B	202	OPC	CBU-CBT-CBS	2.54	126.83	112.60
11	B	201	CLA	CMD-C2D-C3D	-2.51	121.93	127.69
11	B	201	CLA	O1D-CGD-CBD	-2.51	119.56	124.52
9	A	301	HEM	CHA-C4D-ND	2.51	127.47	124.37
12	B	202	OPC	CAE-NAF-CAG	2.49	119.82	109.91
15	G	101	BCR	C32-C1-C6	-2.48	106.35	110.24
12	B	202	OPC	CBG-NAF-CAG	2.47	119.73	109.91
12	H	30	OPC	CAR-CAS-CAT	2.43	126.66	114.37
12	H	30	OPC	CBO-CBP-CBQ	2.41	125.44	113.86
13	B	203	SQD	C1-O5-C5	-2.38	109.06	113.72
15	G	101	BCR	C20-C21-C22	-2.38	123.95	127.28
12	B	202	OPC	CAM-OAN-CAO	-2.37	112.11	117.80
15	G	101	BCR	C38-C26-C25	-2.34	121.94	124.48
10	A	306	UMQ	C1'-O5'-C5'	2.32	118.25	113.72
15	G	101	BCR	C28-C27-C26	-2.32	109.92	114.06
13	B	203	SQD	O47-C7-O49	-2.30	118.32	123.70
11	B	201	CLA	CHC-C1C-C2C	-2.29	120.44	126.95
12	H	30	OPC	OBJ-CBK-OCC	-2.28	117.91	123.63
11	B	201	CLA	CMB-C2B-C1B	2.28	128.89	125.42
12	B	202	OPC	OAN-CAO-OAD	-2.25	118.45	123.70
11	B	201	CLA	CHB-C1B-NB	-2.24	120.68	124.05
12	H	30	OPC	CAQ-CAR-CAS	2.24	125.70	114.37
9	A	301	HEM	C1B-NB-C4B	2.20	107.81	105.21
9	A	301	HEM	C3D-C4D-ND	-2.20	107.76	110.17
9	A	301	HEM	O1D-CGD-CBD	-2.19	116.15	123.09
11	B	201	CLA	C4B-C3B-C2B	-2.19	104.58	107.30
15	G	101	BCR	C11-C10-C9	2.16	130.30	127.28
9	C	301	HEM	CAD-CBD-CGD	-2.15	107.97	113.67
9	A	302	HEM	C1D-C2D-C3D	-2.14	104.73	106.98
12	H	30	OPC	CBG-NAF-CAG	2.13	118.36	109.91
15	G	101	BCR	C2-C1-C6	2.13	113.53	110.44
9	C	301	HEM	C1B-NB-C4B	2.13	107.72	105.21
10	A	304	UMQ	C1'-O5'-C5'	-2.12	109.59	113.72
12	H	30	OPC	CBU-CBT-CBS	2.11	124.42	112.60
9	A	301	HEM	C3B-C2B-C1B	2.09	107.98	106.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	303	HEM	O1D-CGD-CBD	-2.08	116.51	123.09
13	B	203	SQD	C45-O47-C7	-2.07	112.83	117.80
9	A	301	HEM	C2B-C1B-NB	-2.05	107.48	109.84
9	A	303	HEM	C2A-C1A-NA	-2.04	107.89	110.15
13	B	203	SQD	C1-C2-C3	-2.04	105.72	110.01
9	C	301	HEM	C1D-C2D-C3D	-2.02	104.85	106.98
12	B	202	OPC	CAR-CAS-CAT	2.00	124.48	114.37

All (7) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	A	304	UMQ	C2'
10	A	304	UMQ	C1'
10	A	305	UMQ	C2'
10	A	305	UMQ	C1'
10	A	306	UMQ	C2'
10	A	306	UMQ	C1'
11	B	201	CLA	C8

All (165) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	301	HEM	C2B-C3B-CAB-CBB
10	A	304	UMQ	C2'-C1'-O1'-CA
11	B	201	CLA	C1A-C2A-CAA-CBA
11	B	201	CLA	C3A-C2A-CAA-CBA
12	B	202	OPC	CAL-OAK-PAJ-OAI
12	B	202	OPC	NAF-CAG-CAH-OAI
12	B	202	OPC	CBO-CBP-CBQ-CBR
12	H	30	OPC	CAM-CAL-OAK-PAJ
12	H	30	OPC	CAL-OAK-PAJ-OAI
12	H	30	OPC	NAF-CAG-CAH-OAI
12	H	30	OPC	CBO-CBP-CBQ-CBR
13	B	203	SQD	C2-C1-O6-C44
13	B	203	SQD	O49-C7-O47-C45
13	B	203	SQD	C8-C7-O47-C45
13	B	203	SQD	C5-C6-S-O8
15	G	101	BCR	C1-C6-C7-C8
15	G	101	BCR	C5-C6-C7-C8
15	G	101	BCR	C22-C23-C24-C25
12	H	30	OPC	OAD-CAO-OAN-CAM
12	H	30	OPC	CAP-CAO-OAN-CAM

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Mol	Chain	Res	Type	Atoms
9	A	303	HEM	C2D-C3D-CAD-CBD
12	H	30	OPC	CBB-CBC-CBD-CBE
9	A	303	HEM	C4D-C3D-CAD-CBD
12	H	30	OPC	CAQ-CAR-CAS-CAT
10	A	304	UMQ	O5-C5-C6-O6
10	A	305	UMQ	O5-C5-C6-O6
13	B	203	SQD	O5-C1-O6-C44
10	A	304	UMQ	O5'-C5'-C6'-O6'
10	A	306	UMQ	O5'-C5'-C6'-O6'
10	A	305	UMQ	O5'-C5'-C6'-O6'
10	A	305	UMQ	C4'-C5'-C6'-O6'
12	H	30	OPC	CBL-CBK-OBJ-CBI
13	B	203	SQD	C24-C23-O48-C46
10	A	306	UMQ	C4'-C5'-C6'-O6'
10	A	304	UMQ	C4-C5-C6-O6
10	A	305	UMQ	C4-C5-C6-O6
15	G	101	BCR	C37-C22-C23-C24
15	G	101	BCR	C21-C22-C23-C24
13	B	203	SQD	C7-C8-C9-C10
12	H	30	OPC	OCC-CBK-OBJ-CBI
13	B	203	SQD	O10-C23-O48-C46
10	A	304	UMQ	C4'-C5'-C6'-O6'
12	B	202	OPC	CAP-CAO-OAN-CAM
12	B	202	OPC	CBK-CBL-CBM-CBN
13	B	203	SQD	C23-C24-C25-C26
11	B	201	CLA	C8-C10-C11-C12
12	B	202	OPC	OAD-CAO-OAN-CAM
12	B	202	OPC	CAH-CAG-NAF-CBG
11	B	201	CLA	C10-C11-C12-C13
10	A	306	UMQ	C2'-C1'-O1'-CA
12	H	30	OPC	CAH-CAG-NAF-CAA
10	A	304	UMQ	CF-CG-CH-CI
12	B	202	OPC	CAR-CAS-CAT-CAU
13	B	203	SQD	C28-C29-C30-C31
13	B	203	SQD	C30-C31-C32-C33
13	B	203	SQD	C9-C10-C11-C12
11	B	201	CLA	C4B-C3B-CAB-CBB
10	A	306	UMQ	CH-CI-CJ-CK
12	H	30	OPC	CBV-CBW-CBX-CBY
10	A	305	UMQ	CH-CI-CJ-CK
12	B	202	OPC	CBV-CBW-CBX-CBY
11	B	201	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
12	H	30	OPC	CBX-CBY-CBZ-CCA
13	B	203	SQD	C11-C12-C13-C14
10	A	304	UMQ	CA-CB-CC-CD
10	A	304	UMQ	CD-CF-CG-CH
10	A	306	UMQ	CF-CG-CH-CI
11	B	201	CLA	C2B-C3B-CAB-CBB
15	G	101	BCR	C23-C24-C25-C30
10	A	305	UMQ	CA-CB-CC-CD
12	H	30	OPC	CAZ-CBA-CBB-CBC
10	A	305	UMQ	CG-CH-CI-CJ
13	B	203	SQD	C24-C25-C26-C27
10	A	305	UMQ	O5'-C1'-O1'-CA
12	H	30	OPC	CAY-CAZ-CBA-CBB
9	A	302	HEM	C2C-C3C-CAC-CBC
12	B	202	OPC	CAY-CAZ-CBA-CBB
10	A	305	UMQ	O1'-CA-CB-CC
9	A	302	HEM	C4C-C3C-CAC-CBC
9	C	301	HEM	C4B-C3B-CAB-CBB
12	B	202	OPC	CAS-CAT-CAU-CAV
12	H	30	OPC	CBS-CBT-CBU-CBV
13	B	203	SQD	C27-C28-C29-C30
12	B	202	OPC	CBW-CBX-CBY-CBZ
13	B	203	SQD	C33-C34-C35-C36
13	B	203	SQD	C31-C32-C33-C34
12	H	30	OPC	CBU-CBV-CBW-CBX
10	A	304	UMQ	CG-CH-CI-CJ
12	B	202	OPC	CBT-CBU-CBV-CBW
11	B	201	CLA	O2A-C1-C2-C3
13	B	203	SQD	C14-C15-C16-C17
12	H	30	OPC	CBY-CBZ-CCA-CCB
10	A	304	UMQ	CI-CJ-CK-CL
12	H	30	OPC	CBW-CBX-CBY-CBZ
13	B	203	SQD	C12-C13-C14-C15
12	H	30	OPC	CBM-CBN-CBO-CBP
11	B	201	CLA	C4-C3-C5-C6
13	B	203	SQD	C44-C45-C46-O48
15	G	101	BCR	C23-C24-C25-C26
13	B	203	SQD	C25-C26-C27-C28
13	B	203	SQD	O6-C44-C45-O47
11	B	201	CLA	C2-C3-C5-C6
13	B	203	SQD	C13-C14-C15-C16
15	G	101	BCR	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
12	B	202	OPC	CBL-CBM-CBN-CBO
9	A	301	HEM	C2A-CAA-CBA-CGA
9	A	303	HEM	C2B-C3B-CAB-CBB
10	A	304	UMQ	CB-CC-CD-CF
13	B	203	SQD	C16-C17-C18-C19
13	B	203	SQD	O6-C44-C45-C46
10	A	304	UMQ	CC-CD-CF-CG
10	A	305	UMQ	CD-CF-CG-CH
10	A	305	UMQ	C2'-C1'-O1'-CA
10	A	305	UMQ	CF-CG-CH-CI
12	H	30	OPC	OAK-CAL-CAM-CBI
12	B	202	OPC	CBC-CBD-CBE-CBF
12	B	202	OPC	CBP-CBQ-CBR-CBS
12	H	30	OPC	CBP-CBQ-CBR-CBS
12	H	30	OPC	OAK-CAL-CAM-OAN
9	A	302	HEM	C3D-CAD-CBD-CGD
9	A	302	HEM	C2D-C3D-CAD-CBD
12	B	202	OPC	CAL-OAK-PAJ-OAB
12	H	30	OPC	CAL-OAK-PAJ-OAB
11	B	201	CLA	C11-C12-C13-C15
11	B	201	CLA	C2A-CAA-CBA-CGA
10	A	306	UMQ	CI-CJ-CK-CL
13	B	203	SQD	C29-C30-C31-C32
10	A	304	UMQ	CB-CA-O1'-C1'
12	B	202	OPC	CAZ-CBA-CBB-CBC
11	B	201	CLA	C6-C7-C8-C10
9	A	302	HEM	C4D-C3D-CAD-CBD
10	A	306	UMQ	O5'-C1'-O1'-CA
15	G	101	BCR	C11-C10-C9-C34
9	A	302	HEM	C2A-CAA-CBA-CGA
9	A	303	HEM	C2A-CAA-CBA-CGA
9	C	301	HEM	CAD-CBD-CGD-O1D
12	H	30	OPC	CAR-CAS-CAT-CAU
9	C	301	HEM	CAD-CBD-CGD-O2D
12	H	30	OPC	CAH-CAG-NAF-CBG
15	G	101	BCR	C11-C10-C9-C8
12	H	30	OPC	CBC-CBD-CBE-CBF
9	A	301	HEM	CAD-CBD-CGD-O2D
9	A	301	HEM	CAD-CBD-CGD-O1D
9	A	303	HEM	C4B-C3B-CAB-CBB
9	C	301	HEM	C4C-C3C-CAC-CBC
10	A	305	UMQ	CI-CJ-CK-CL

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Mol	Chain	Res	Type	Atoms
12	B	202	OPC	CBM-CBN-CBO-CBP
9	A	301	HEM	CAA-CBA-CGA-O1A
12	H	30	OPC	OAN-CAO-CAP-CAQ
12	H	30	OPC	OBJ-CBK-CBL-CBM
12	B	202	OPC	OAN-CAO-CAP-CAQ
13	B	203	SQD	O48-C23-C24-C25
9	A	302	HEM	CAA-CBA-CGA-O1A
9	A	302	HEM	CAA-CBA-CGA-O2A
12	H	30	OPC	CAH-CAG-NAF-CAE
13	B	203	SQD	C35-C36-C37-C38
13	B	203	SQD	C17-C18-C19-C20
12	B	202	OPC	OAD-CAO-CAP-CAQ
12	H	30	OPC	OAD-CAO-CAP-CAQ
12	H	30	OPC	OCC-CBK-CBL-CBM
13	B	203	SQD	O10-C23-C24-C25
12	B	202	OPC	CBR-CBS-CBT-CBU
9	A	301	HEM	CAA-CBA-CGA-O2A
9	C	301	HEM	C2C-C3C-CAC-CBC
12	H	30	OPC	CBR-CBS-CBT-CBU

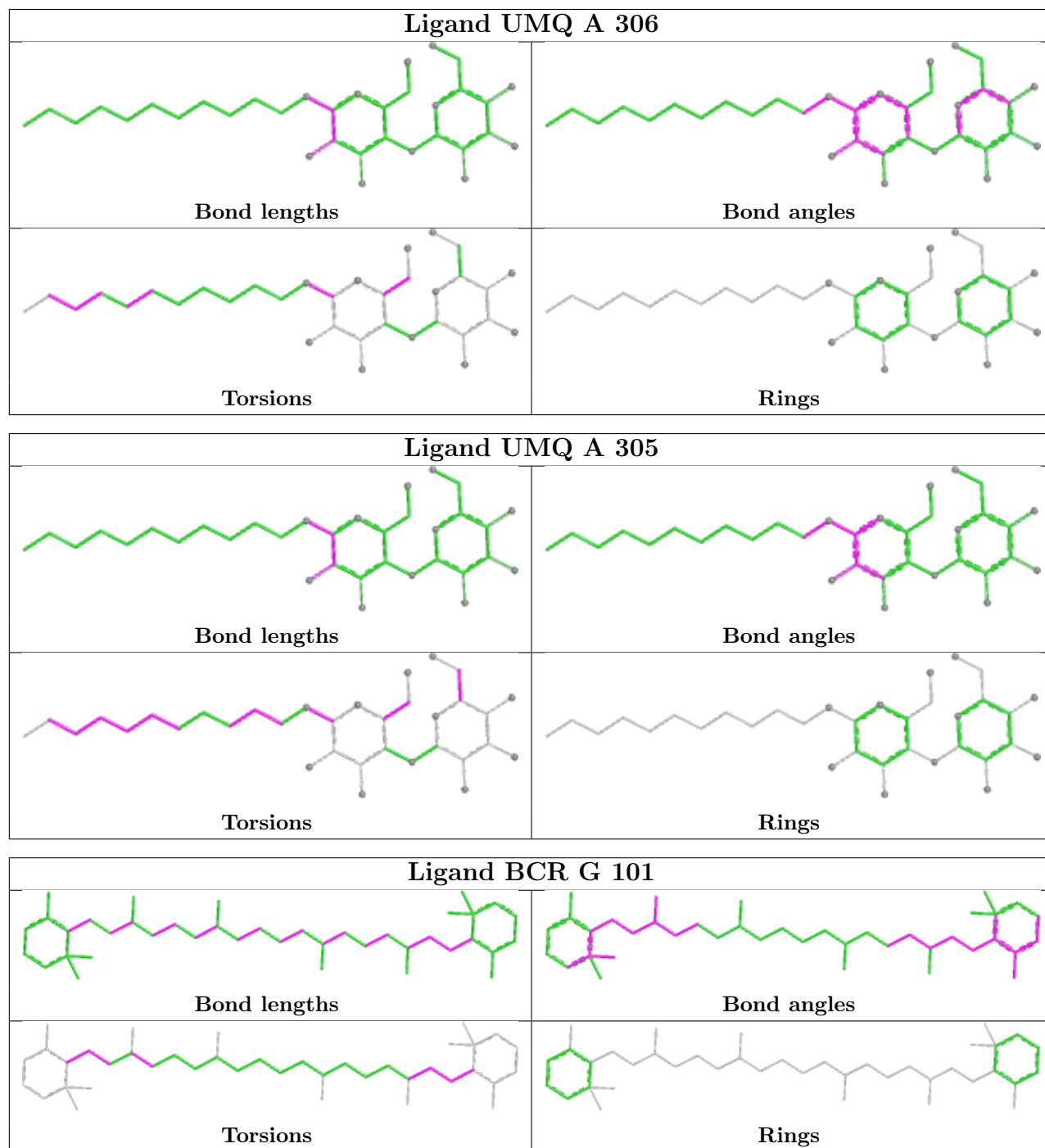
There are no ring outliers.

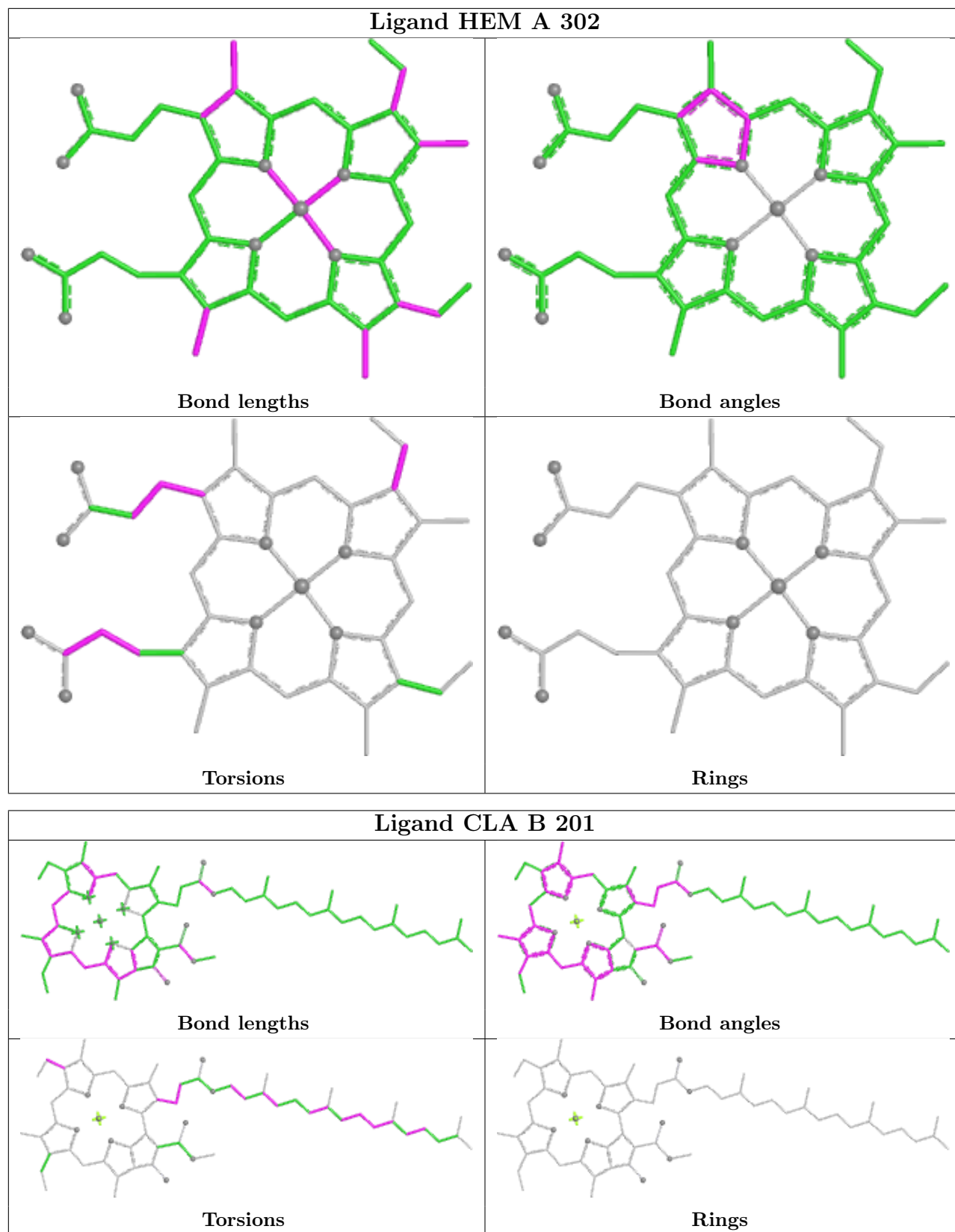
12 monomers are involved in 32 short contacts:

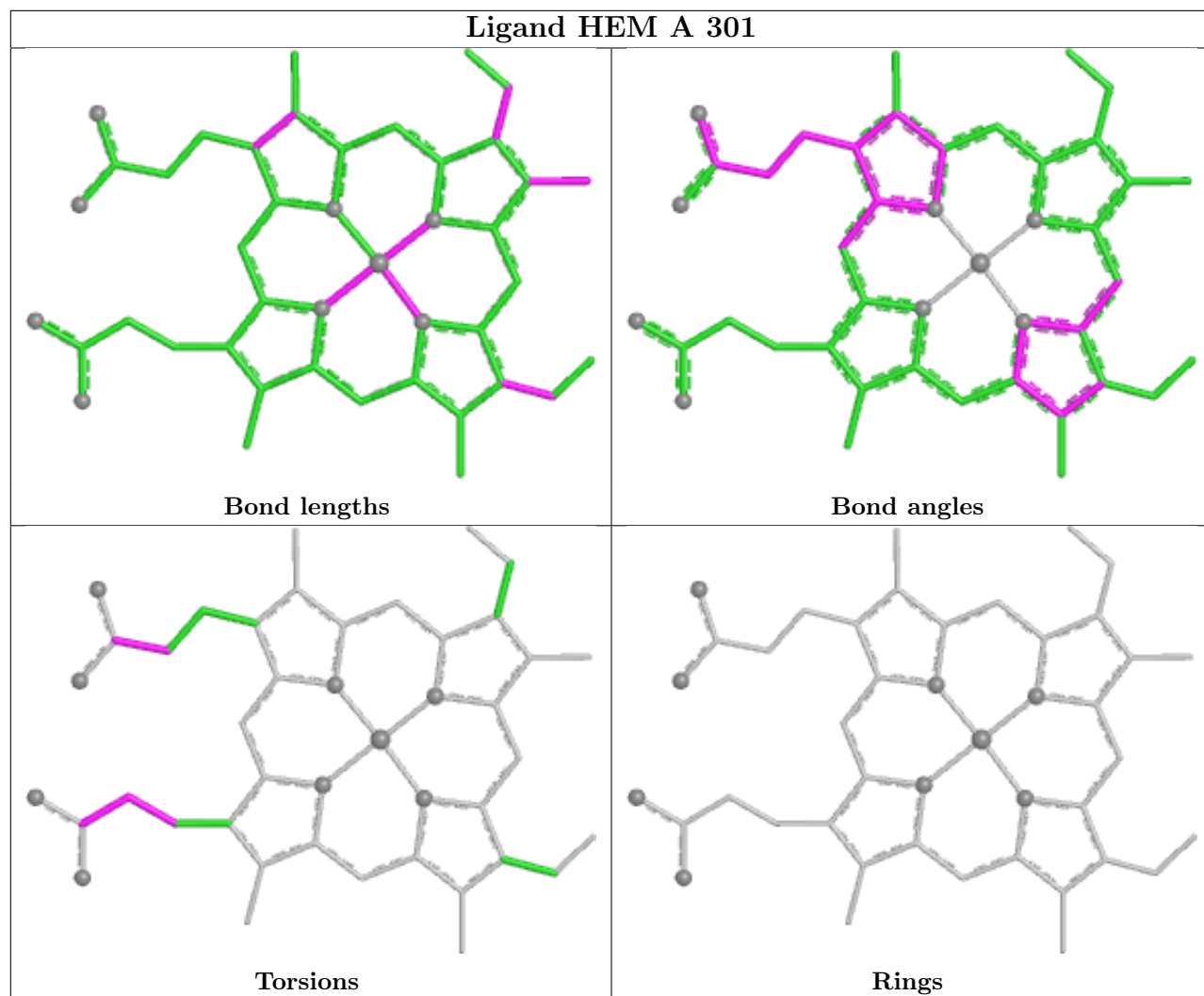
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	306	UMQ	2	0
10	A	305	UMQ	1	0
15	G	101	BCR	7	0
9	A	302	HEM	1	0
11	B	201	CLA	1	0
9	A	301	HEM	2	0
14	D	200	FES	1	0
9	C	301	HEM	6	0
10	A	304	UMQ	1	0
12	H	30	OPC	5	0
9	A	303	HEM	5	0
13	B	203	SQD	1	0

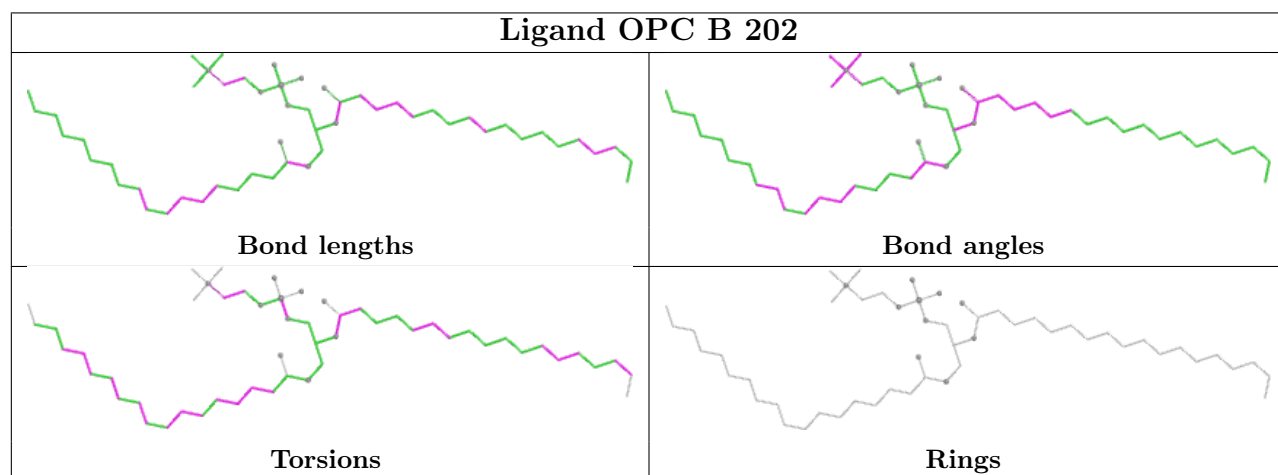
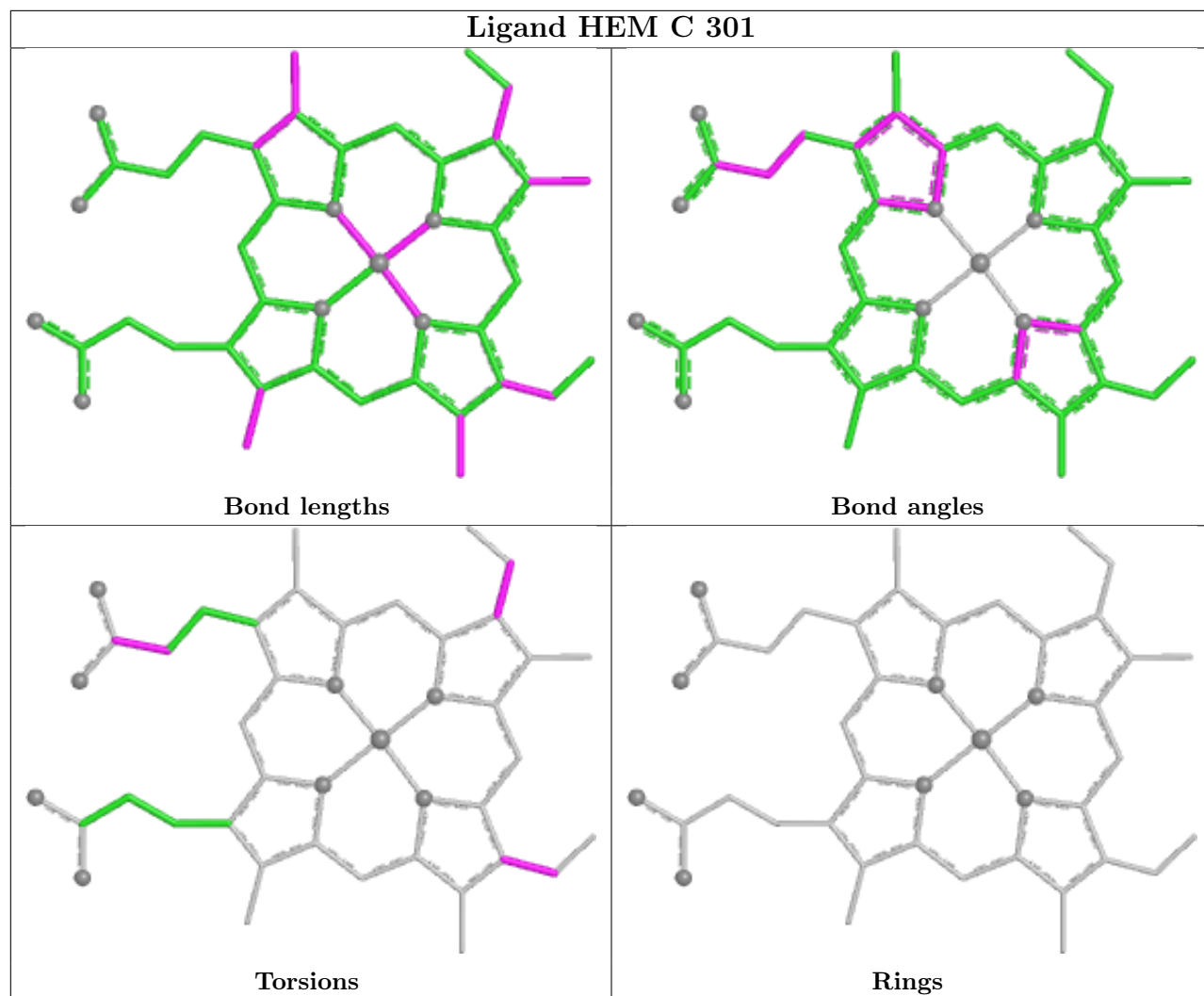
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

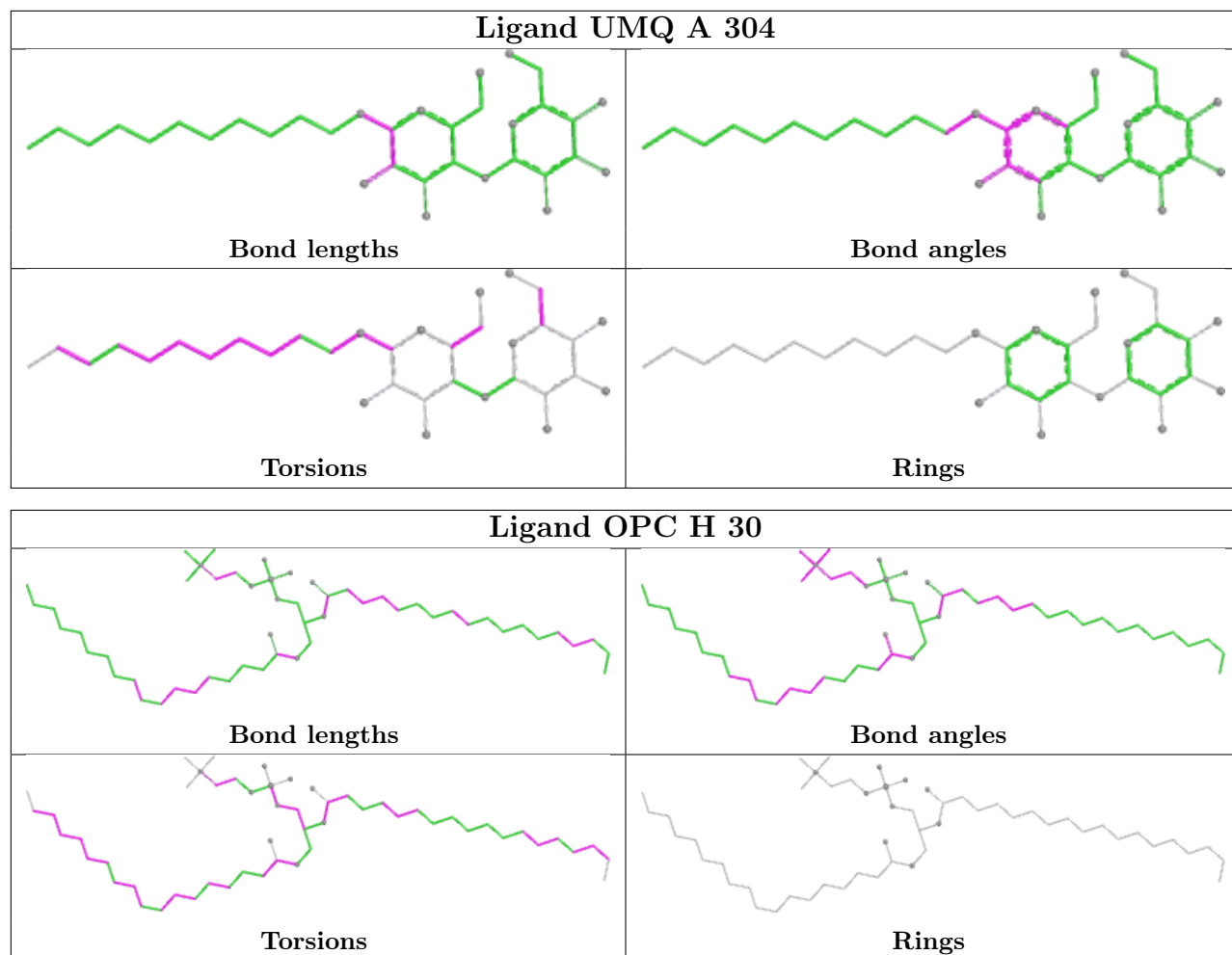
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

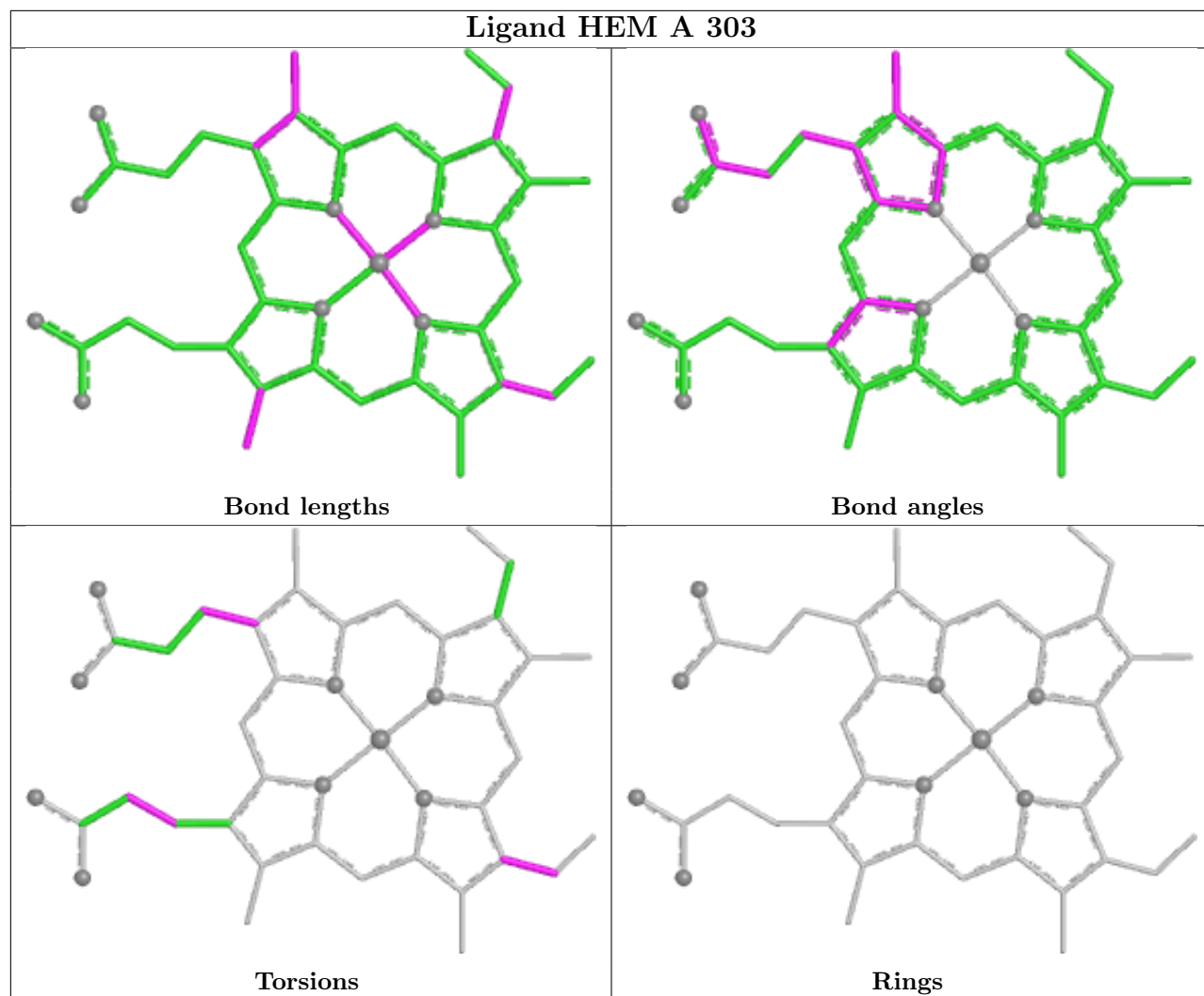


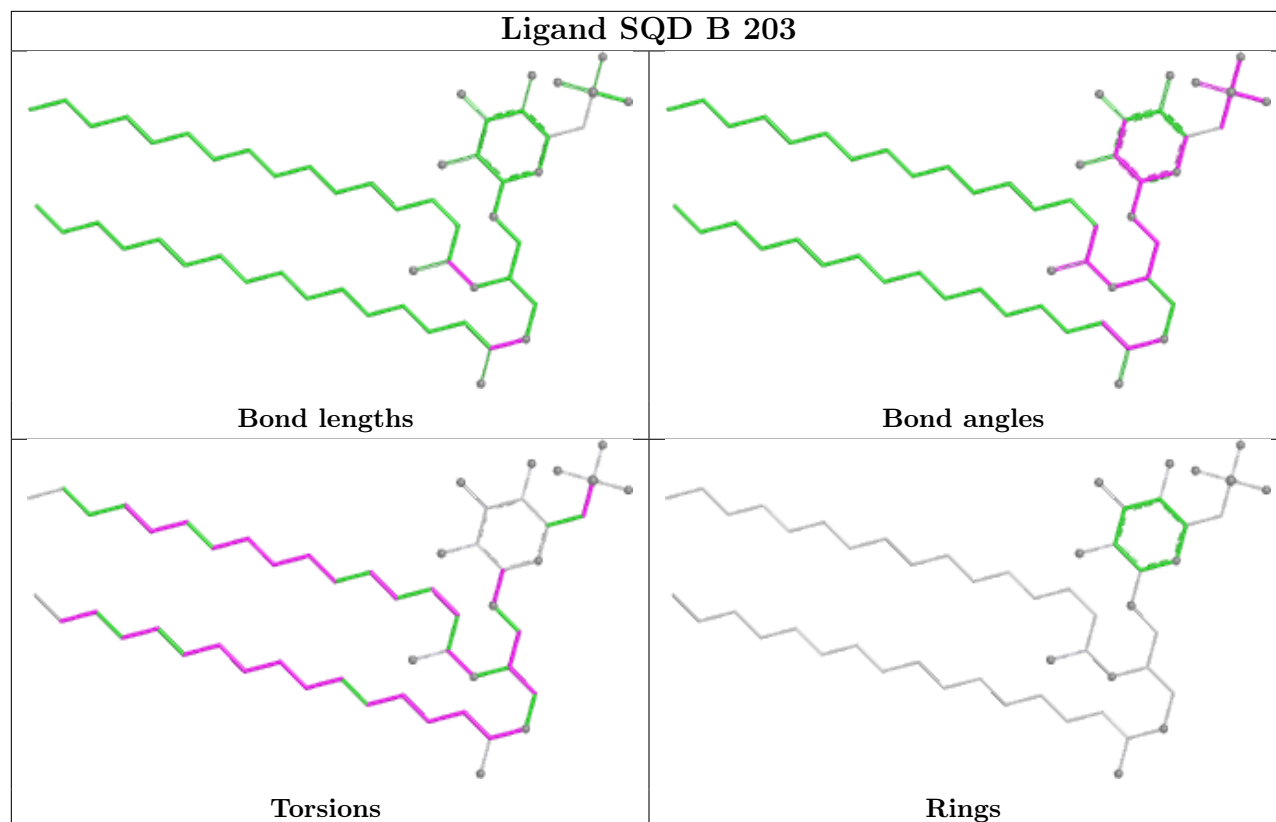












5.7 Other polymers [i](#)

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	215/215 (100%)	-0.20	5 (2%) 61 38	34, 47, 75, 102	0
2	B	160/160 (100%)	0.33	10 (6%) 26 13	46, 63, 96, 108	0
3	C	289/289 (100%)	1.19	57 (19%) 3 2	48, 64, 136, 139	0
4	D	166/179 (92%)	2.06	65 (39%) 1 1	48, 111, 140, 143	0
5	E	31/31 (100%)	0.41	1 (3%) 50 29	72, 78, 94, 95	0
6	F	32/34 (94%)	0.50	1 (3%) 51 30	60, 71, 88, 95	0
7	G	37/37 (100%)	0.44	3 (8%) 18 9	52, 63, 98, 99	0
8	H	29/29 (100%)	0.00	1 (3%) 48 27	57, 60, 69, 77	0
All	All	959/974 (98%)	0.77	143 (14%) 5 3	34, 64, 135, 143	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	156	GLU	8.1
7	G	37	GLY	7.2
4	D	75	VAL	6.6
6	F	1	MET	6.6
4	D	50	ALA	6.6
4	D	47	ALA	6.3
4	D	49	GLY	6.3
4	D	145	PRO	6.2
4	D	48	GLY	5.9
4	D	142	GLY	5.9
2	B	1	MET	5.5
4	D	98	ALA	5.4
3	C	206	VAL	5.2
4	D	155	THR	5.2
4	D	143	PRO	5.1
4	D	73	HIS	5.1

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Mol	Chain	Res	Type	RSRZ
3	C	224	ALA	5.0
4	D	140	VAL	4.9
1	A	2	ALA	4.9
3	C	208	SER	4.8
3	C	193	VAL	4.7
3	C	192	SER	4.7
1	A	1	MET	4.7
4	D	144	ALA	4.6
3	C	207	VAL	4.5
4	D	170	PHE	4.5
4	D	179	SER	4.4
4	D	85	LYS	4.4
3	C	218	ILE	4.4
4	D	72	SER	4.4
3	C	177	THR	4.3
4	D	157	ASN	4.2
4	D	74	ASN	4.1
3	C	226	THR	4.1
3	C	214	GLY	4.1
4	D	141	ARG	4.1
4	D	177	TRP	4.0
4	D	77	ASP	4.0
3	C	200	LYS	3.9
3	C	203	SER	3.9
4	D	99	ILE	3.8
3	C	194	LYS	3.8
3	C	199	ILE	3.8
3	C	184	ALA	3.7
2	B	155	LEU	3.6
4	D	17	GLN	3.6
2	B	26	TYR	3.5
4	D	52	GLY	3.5
3	C	213	ALA	3.5
3	C	215	PRO	3.5
4	D	109	THR	3.5
3	C	195	TYR	3.4
4	D	70	LEU	3.4
3	C	117	GLY	3.4
4	D	57	LYS	3.4
3	C	230	ALA	3.4
3	C	217	LEU	3.3
4	D	160	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
3	C	189	GLU	3.2
3	C	186	GLN	3.2
4	D	146	LYS	3.2
3	C	219	VAL	3.2
2	B	74	GLU	3.2
4	D	110	HIS	3.2
8	H	29	LEU	3.1
4	D	119	ALA	3.0
3	C	201	THR	3.0
4	D	69	PHE	3.0
3	C	227	ALA	3.0
4	D	172	THR	3.0
1	A	159	PRO	3.0
4	D	166	THR	3.0
3	C	181	SER	2.9
3	C	185	LYS	2.9
2	B	160	PHE	2.9
3	C	212	PRO	2.9
3	C	204	GLY	2.9
3	C	225	VAL	2.8
4	D	111	LEU	2.8
4	D	56	ALA	2.8
4	D	92	VAL	2.8
4	D	54	THR	2.8
4	D	175	GLU	2.8
3	C	211	ILE	2.8
2	B	2	ALA	2.7
3	C	176	ALA	2.7
4	D	150	LEU	2.7
4	D	82	GLN	2.7
4	D	154	LYS	2.7
1	A	3	ASN	2.6
3	C	234	ASN	2.6
5	E	1	MET	2.6
7	G	1	MET	2.6
4	D	60	LEU	2.5
3	C	35	GLU	2.5
3	C	87	GLU	2.5
3	C	233	ASN	2.5
4	D	127	PRO	2.5
4	D	51	GLY	2.5
3	C	202	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
4	D	101	ASP	2.5
4	D	86	GLY	2.4
3	C	281	LYS	2.4
3	C	209	ASP	2.4
4	D	46	ALA	2.4
3	C	33	GLU	2.4
3	C	68	VAL	2.4
4	D	149	ALA	2.3
3	C	190	ASP	2.3
3	C	140	LYS	2.3
3	C	88	ASP	2.3
3	C	182	LYS	2.3
4	D	173	GLY	2.3
7	G	31	ARG	2.3
3	C	145	GLY	2.3
4	D	16	ARG	2.3
1	A	112	LYS	2.2
4	D	147	SER	2.2
3	C	141	ASN	2.2
4	D	158	ASP	2.2
2	B	159	LEU	2.2
3	C	164	GLY	2.2
4	D	171	ARG	2.2
4	D	84	LEU	2.2
3	C	210	THR	2.2
2	B	153	LYS	2.1
3	C	187	GLU	2.1
4	D	116	PRO	2.1
3	C	30	LYS	2.1
4	D	45	PRO	2.1
4	D	118	ASN	2.1
4	D	66	VAL	2.1
3	C	171	LEU	2.1
4	D	13	MET	2.1
2	B	33	PRO	2.1
3	C	216	GLU	2.1
3	C	169	ASN	2.1
4	D	76	GLY	2.1
3	C	170	ASN	2.1
4	D	178	TRP	2.1
4	D	80	LEU	2.0
3	C	229	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	119	LYS	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](#)

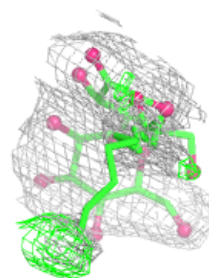
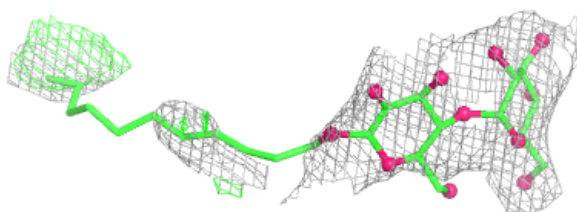
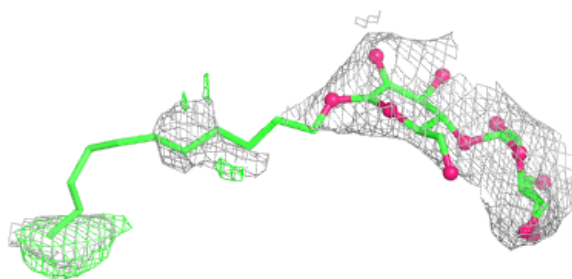
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
10	UMQ	A	305	34/34	0.70	0.27	135,137,140,141	0
12	OPC	H	30	54/55	0.84	0.30	81,109,134,134	0
13	SQD	B	203	54/54	0.84	0.26	79,105,121,121	0
10	UMQ	A	304	34/34	0.85	0.23	72,103,110,111	0
15	BCR	G	101	40/40	0.85	0.21	57,66,76,77	0
12	OPC	B	202	54/55	0.87	0.23	75,82,110,111	0
10	UMQ	A	306	34/34	0.87	0.19	95,100,104,104	0
11	CLA	B	201	65/65	0.93	0.14	59,64,88,89	0
14	FES	D	200	4/4	0.97	0.08	105,106,106,107	0
9	HEM	C	301	43/43	0.97	0.10	52,55,63,64	0
9	HEM	A	302	43/43	0.98	0.08	40,43,52,54	0
9	HEM	A	303	43/43	0.98	0.09	54,56,60,64	0
9	HEM	A	301	43/43	0.99	0.07	38,40,44,45	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.

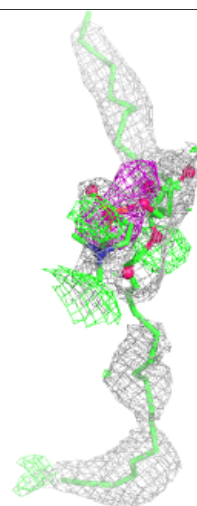
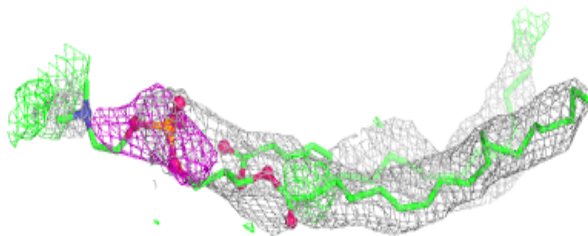
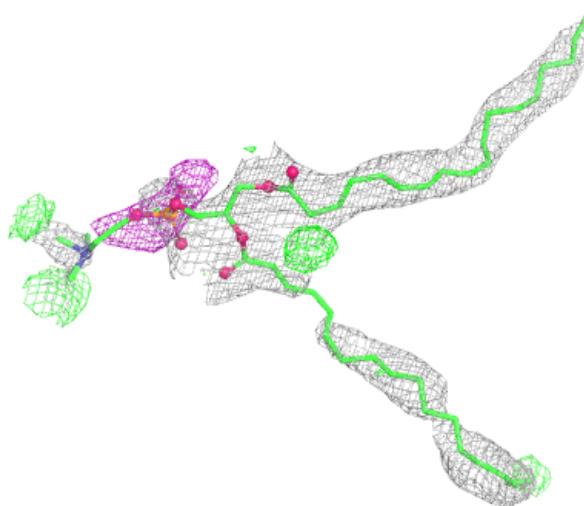
Electron density around UMQ A 305:

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



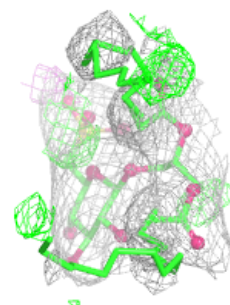
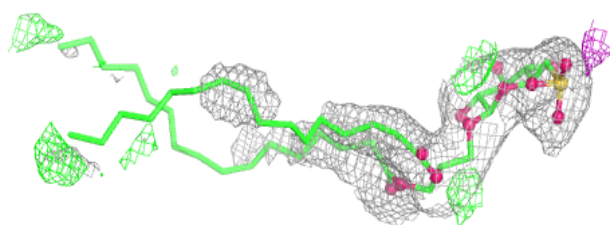
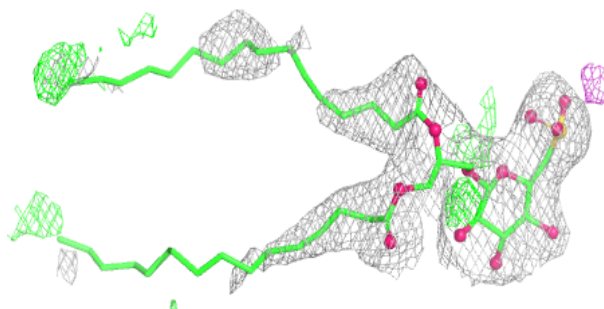
Electron density around OPC H 30:

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

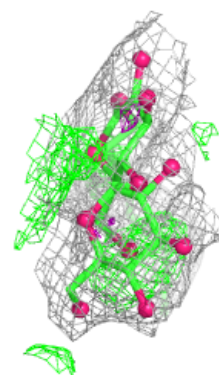
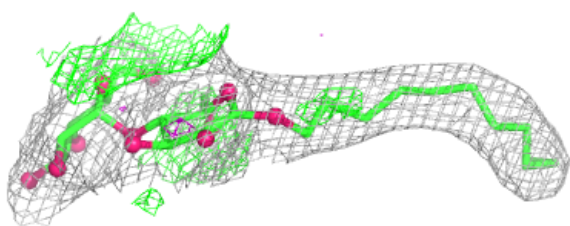
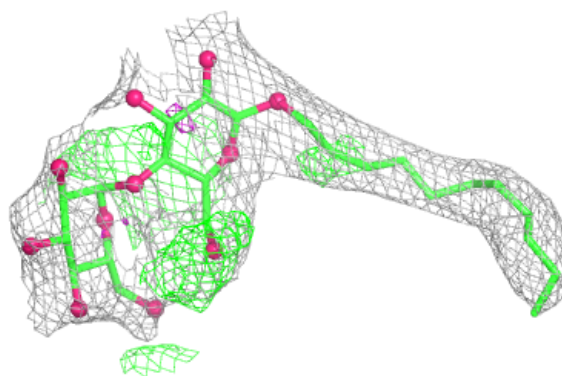


Electron density around SQD B 203:

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

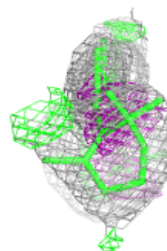
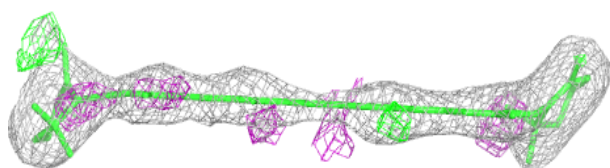
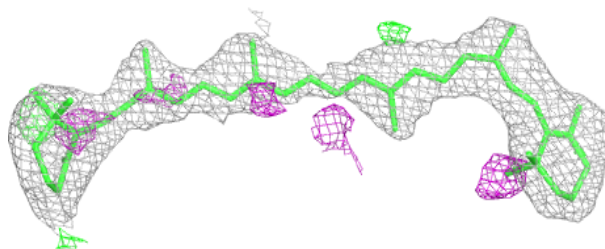
**Electron density around UMQ A 304:**

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

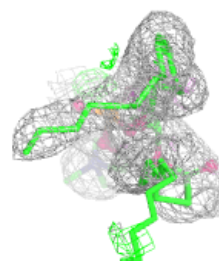
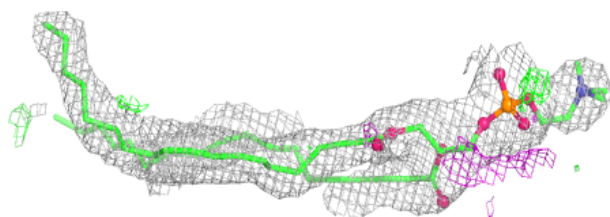
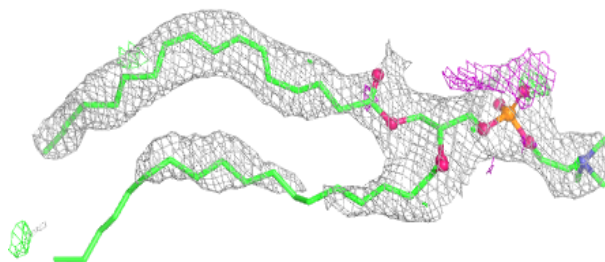


Electron density around BCR G 101:

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

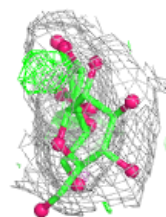
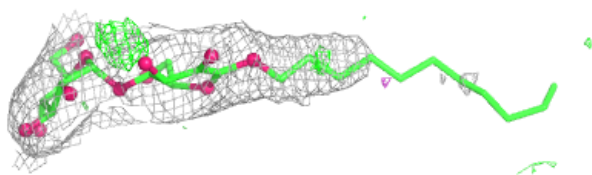
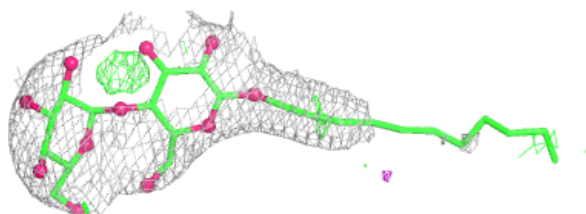
**Electron density around OPC B 202:**

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

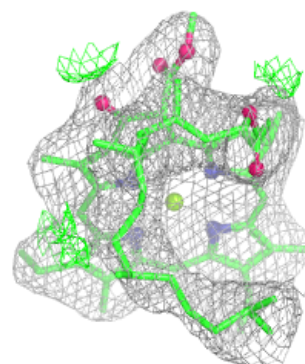
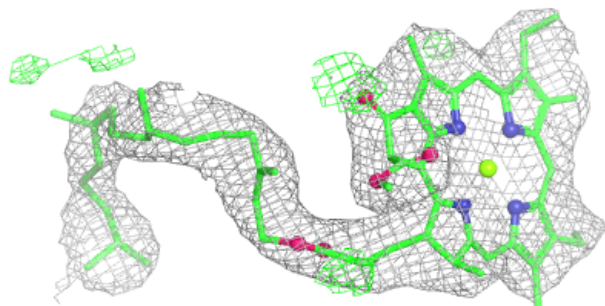
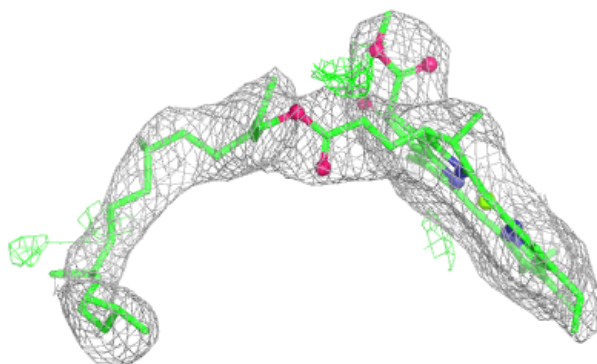


Electron density around UMQ A 306:

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

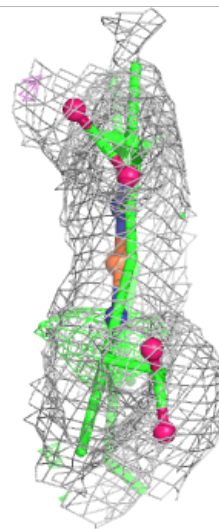
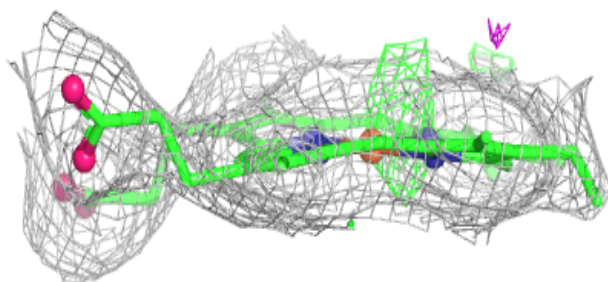
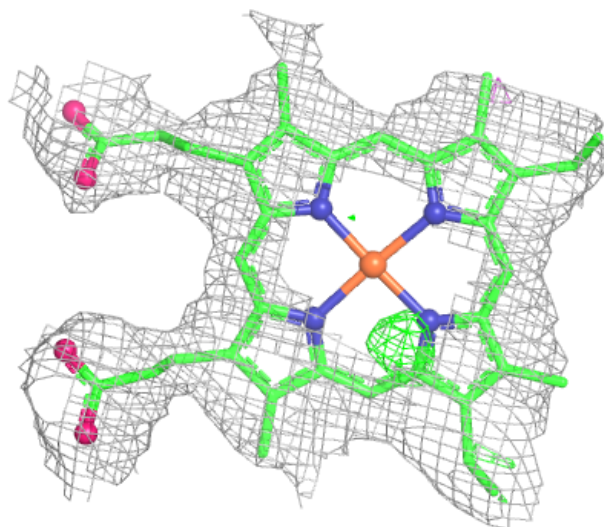
**Electron density around CLA B 201:**

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



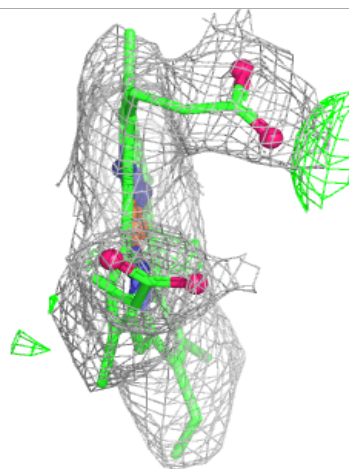
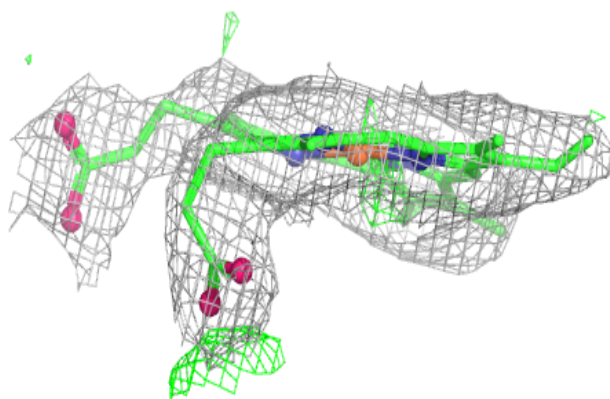
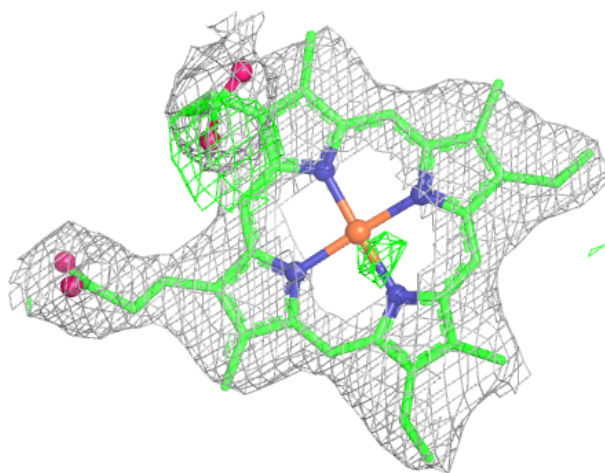
Electron density around HEM C 301:

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



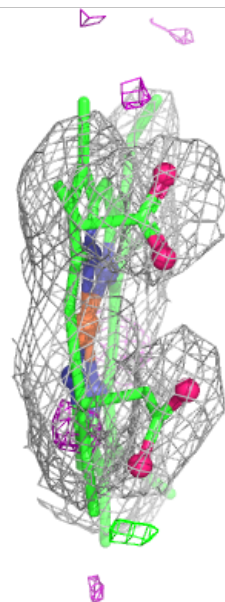
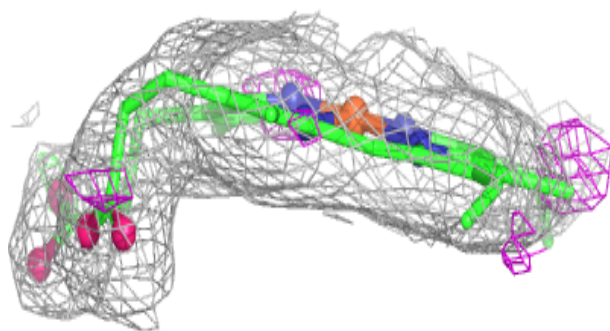
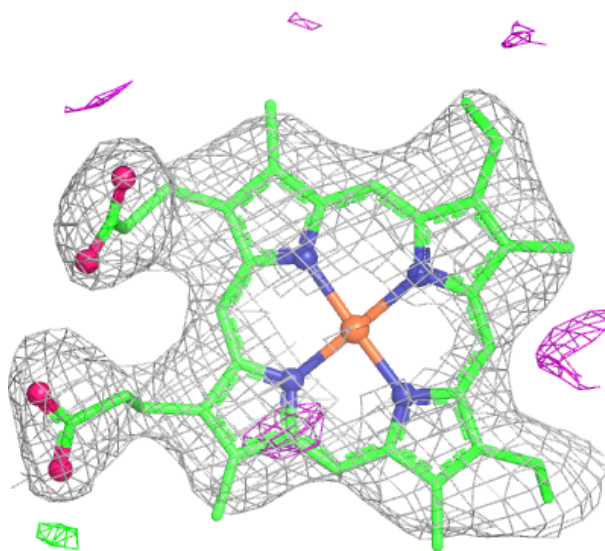
Electron density around HEM A 302:

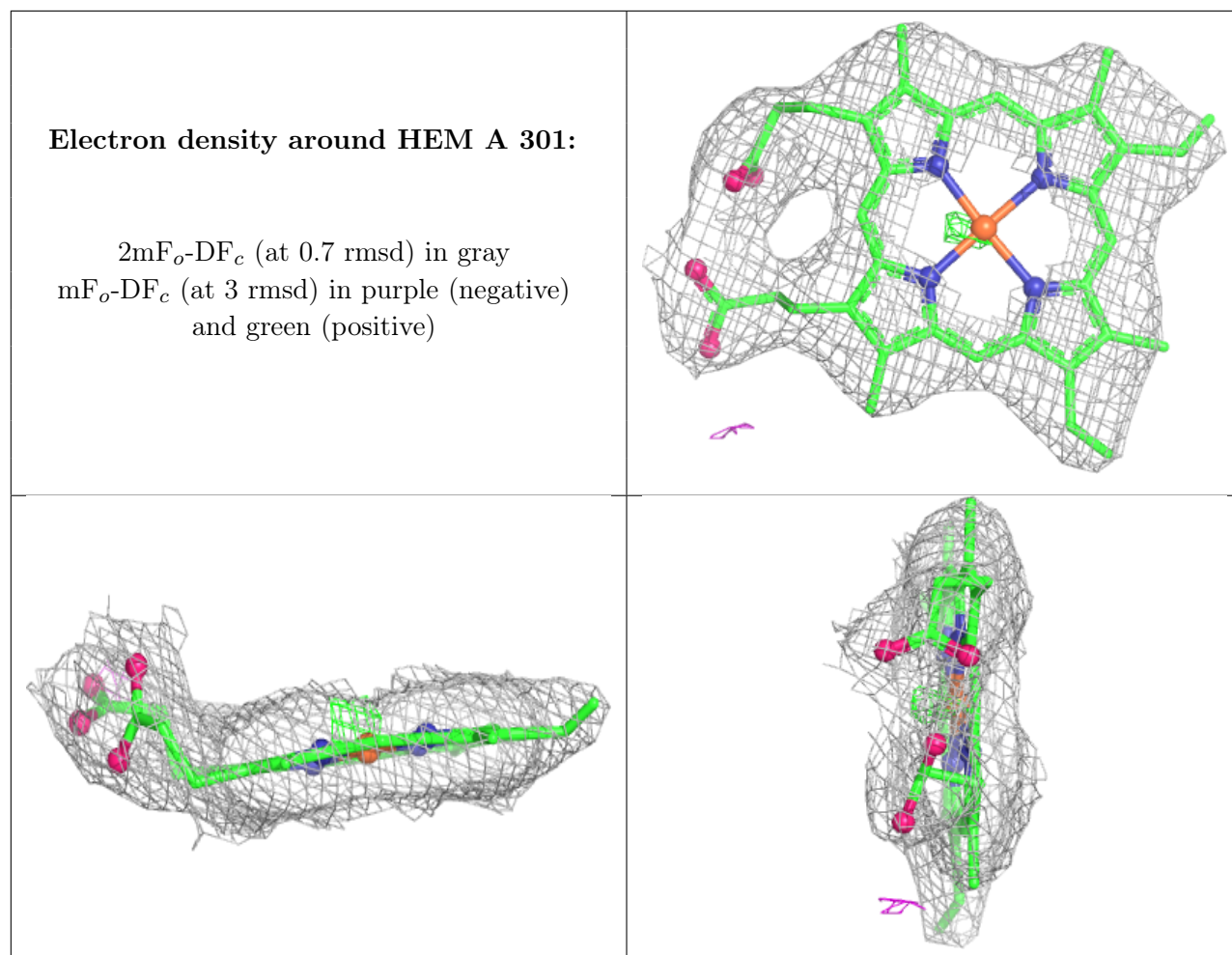
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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.