



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:27 PM UTC

PDB ID : 4H13 / pdb_00004h13
Title : Crystal Structure of the Cytochrome b6f Complex from *Mastigocladus laminosus* with TDS
Authors : Hasan, S.S.; Yamashita, E.; Baniulis, D.; Cramer, W.A.
Deposited on : 2012-09-10
Resolution : 3.07 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:

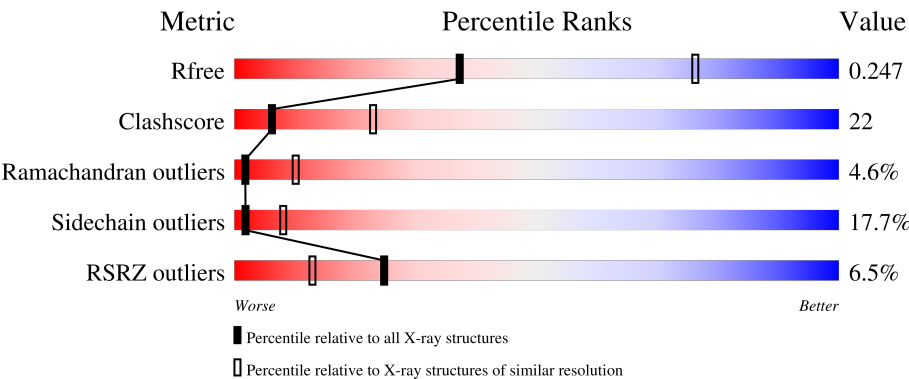
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.07 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.



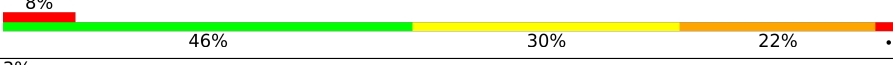
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2010 (3.10-3.06)
Clashscore	190562	2102 (3.10-3.06)
Ramachandran outliers	187476	1982 (3.10-3.06)
Sidechain outliers	187428	1981 (3.10-3.06)
RSRZ outliers	180081	2010 (3.10-3.06)

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% 65%27%9%
2	B	160	2% 58%38%. .
3	C	289	10% 47%39%12%
4	D	179	8% 45%39%9%. 6%
5	E	32	6% 59%28%12%

Continued on next page...

Continued from previous page...

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
14	UMQ	A	308	X	-	-	-
14	UMQ	B	202	X	-	-	-
16	CLA	B	203	X	-	-	-
18	SQD	D	201	X	-	-	-

2 Entry composition

There are 22 unique types of molecules in this entry. The entry contains 16526 atoms, of which 8399 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	H	N	O	S	0	0	0
			3449	1140	1738	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	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	288	Total	C	H	N	O	S	0	0	0
			4451	1415	2235	369	424	8			

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	168	Total	C	H	N	O	S	0	0	0
			2563	823	1275	221	237	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	31	Total	C	H	N	O	S	0	0	0
			483	160	249	34	39	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	H	N	O	S	0	0	0
			572	188	289	44	50	1			

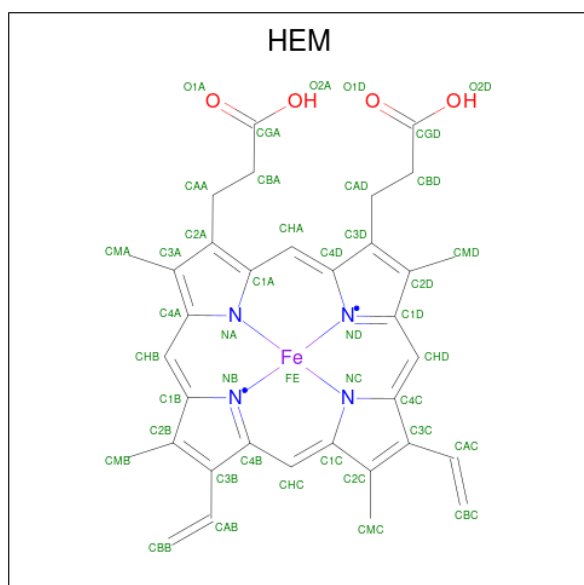
- Molecule 8 is a protein called Cytochrome b6-f complex subunit 8.

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).

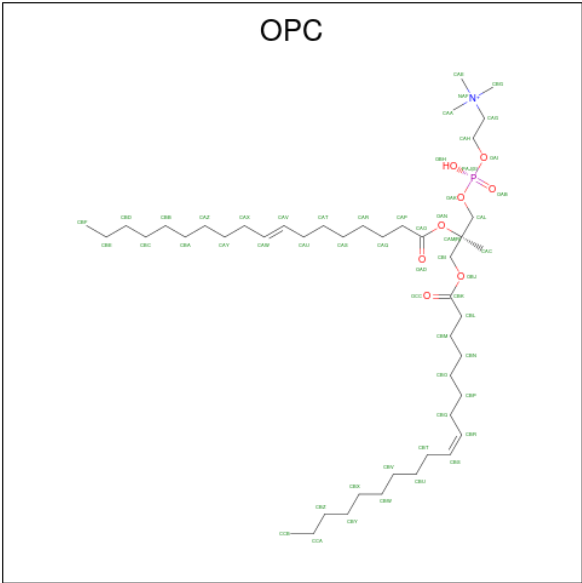
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Cd	0	0
			1	1		

- Molecule 10 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



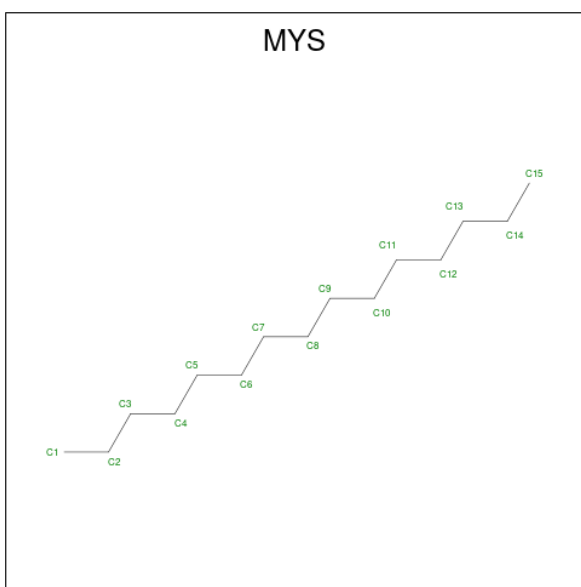
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
10	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
10	A	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
10	C	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

- 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).



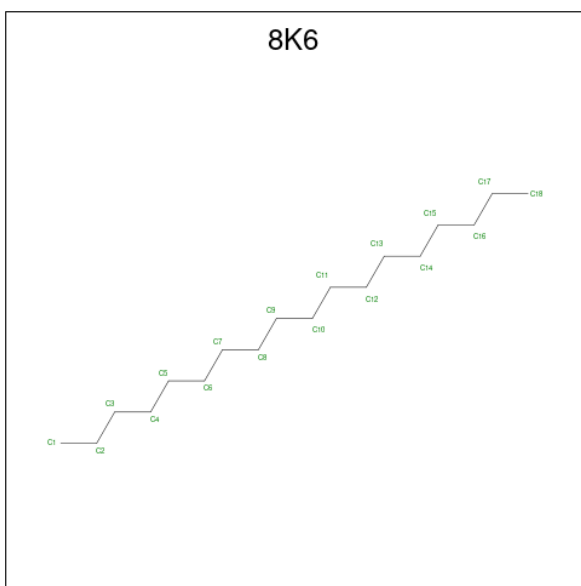
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
11	A	1	Total	C	H	N	O	P	0	0
			137	44	83	1	8	1		
11	B	1	Total	C	H	N	O	P	0	0
			137	44	83	1	8	1		

- Molecule 12 is PENTADECANE (CCD ID: MYS) (formula: C₁₅H₃₂).



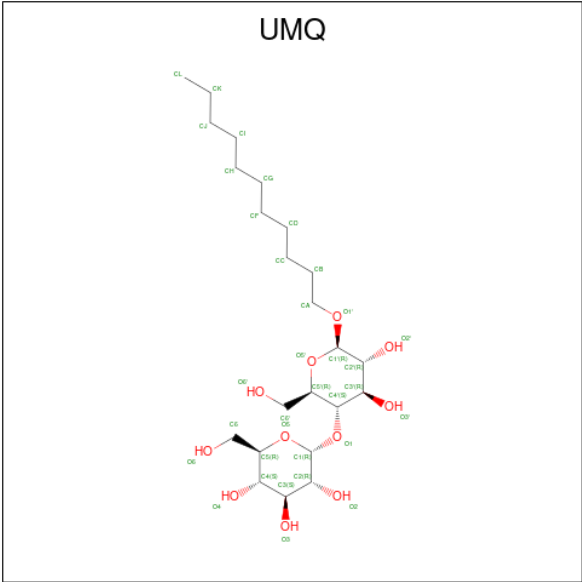
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	H	0	0
			47	15	32		

- Molecule 13 is Octadecane (CCD ID: 8K6) (formula: $C_{18}H_{38}$).



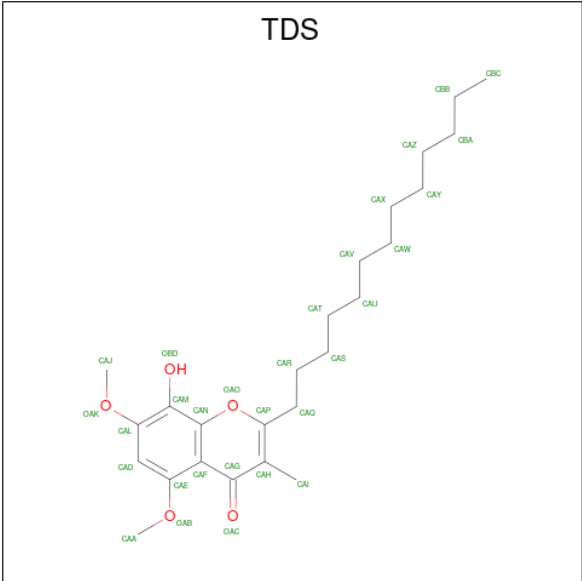
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	A	1	Total	C	H	0	0
			56	18	38		

- Molecule 14 is UNDECYL-MALTOSIDE (CCD ID: UMQ) (formula: $C_{23}H_{44}O_{11}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	A	1	Total	C	H	O	0	0
			77	23	43	11		
14	B	1	Total	C	H	O	0	0
			77	23	43	11		

- Molecule 15 is 8-HYDROXY-5,7-DIMETHOXY-3-METHYL-2-TRIDECYL-4H-CHROME N-4-ONE (CCD ID: TDS) (formula: C₂₅H₃₈O₅).



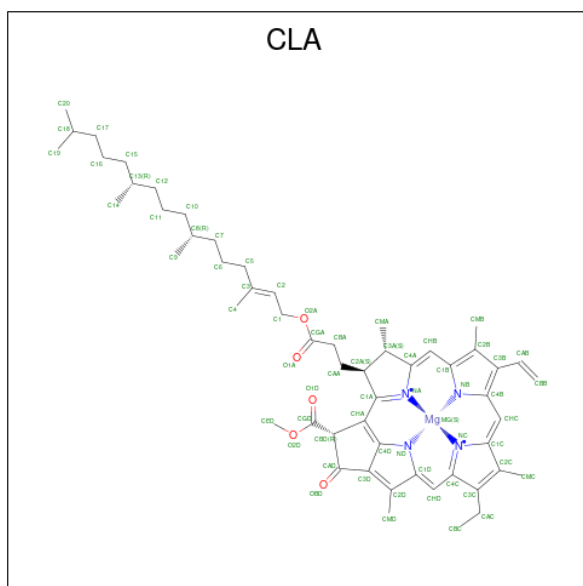
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	A	1	Total	C	H	O	0	0
			68	25	38	5		

Continued on next page...

Continued from previous page...

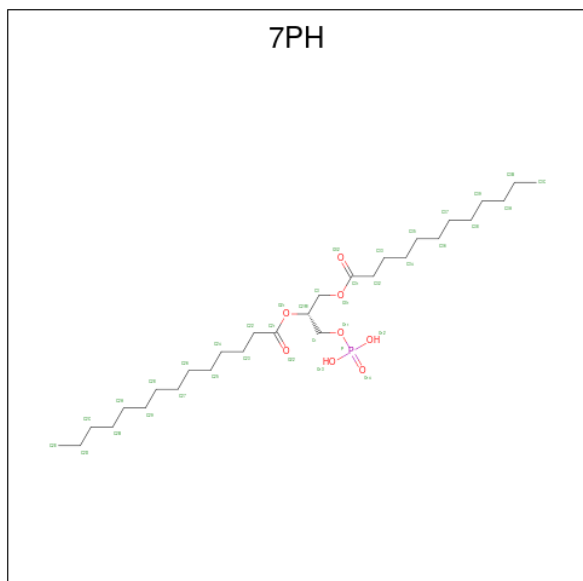
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
15	B	1	Total	C	H	O	0	0
			68	25	38	5		

- Molecule 16 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



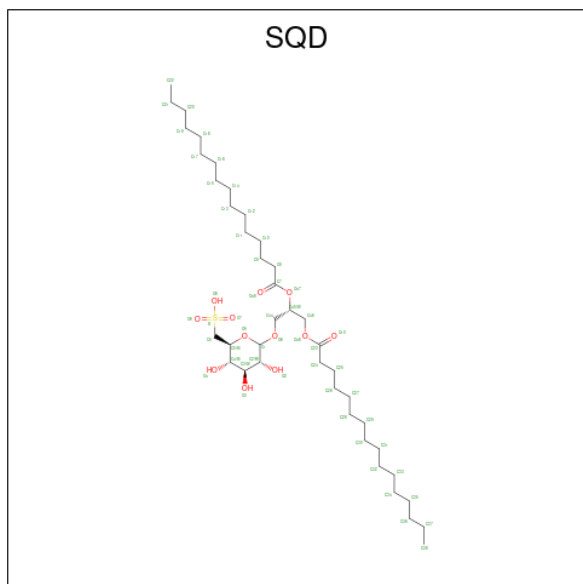
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
16	B	1	Total	C	H	Mg	N	O	0	0
			127	55	62	1	4	5		

- Molecule 17 is (1R)-2-(dodecanoyloxy)-1-[(phosphonoxy)methyl]ethyl tetradecanoate (CCD ID: 7PH) (formula: $C_{29}H_{57}O_8P$).



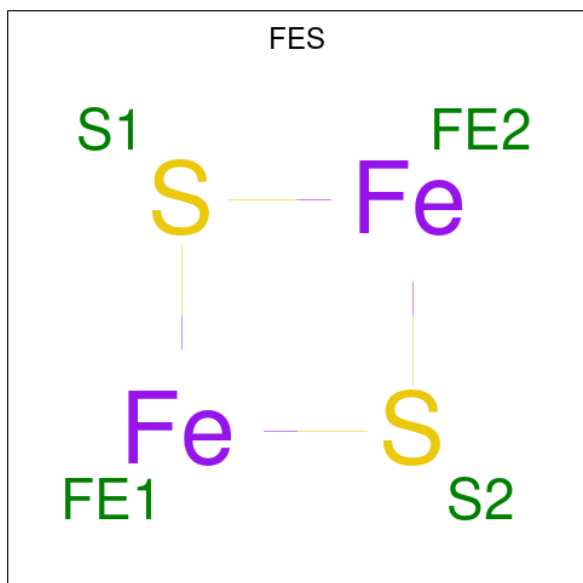
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	C	1	Total	C	H	O	0	0
			81	27	49	5		

- Molecule 18 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



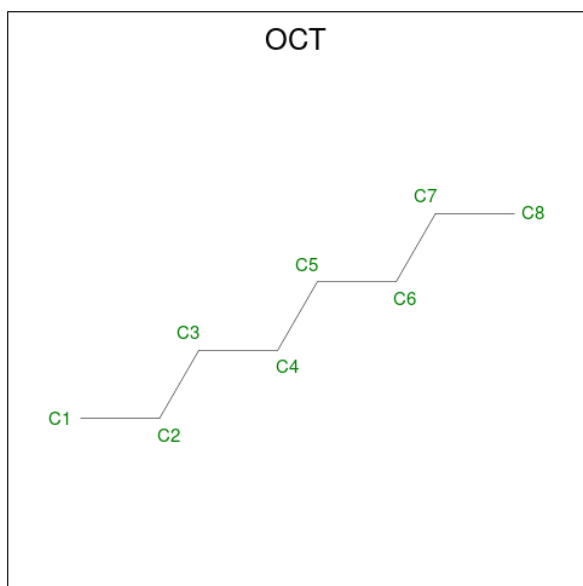
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	D	1	Total	C	H	O	S	1	0
			131	41	78	11	1		

- Molecule 19 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



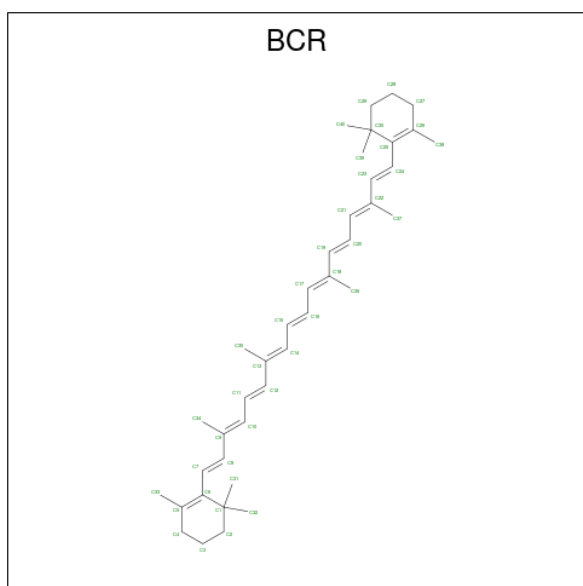
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	D	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 20 is N-OCTANE (CCD ID: OCT) (formula: C_8H_{18}).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
20	F	1	Total	C	H	0	0
			26	8	18		

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



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

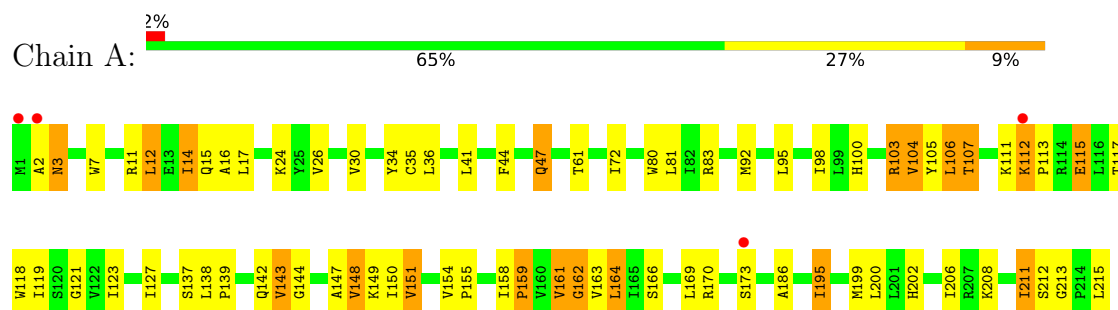
- Molecule 22 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
22	A	12	Total	O	0	0
			12	12		
22	B	6	Total	O	0	0
			6	6		
22	C	4	Total	O	0	0
			4	4		
22	F	1	Total	O	0	0
			1	1		
22	G	1	Total	O	0	0
			1	1		

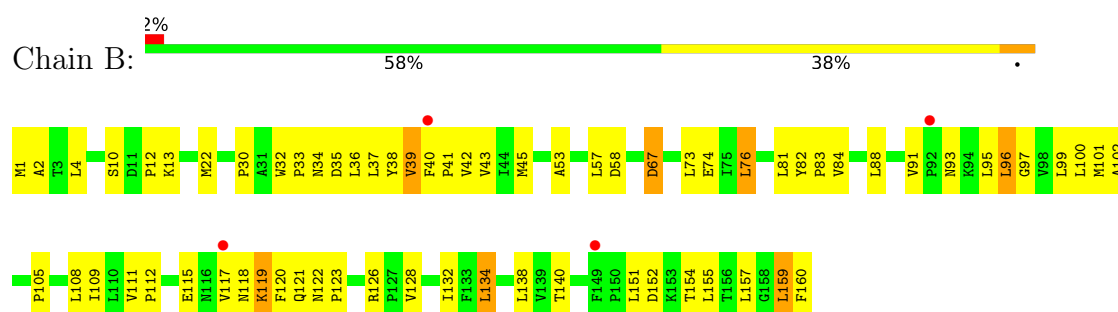
3 Residue-property plots [i](#)

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.

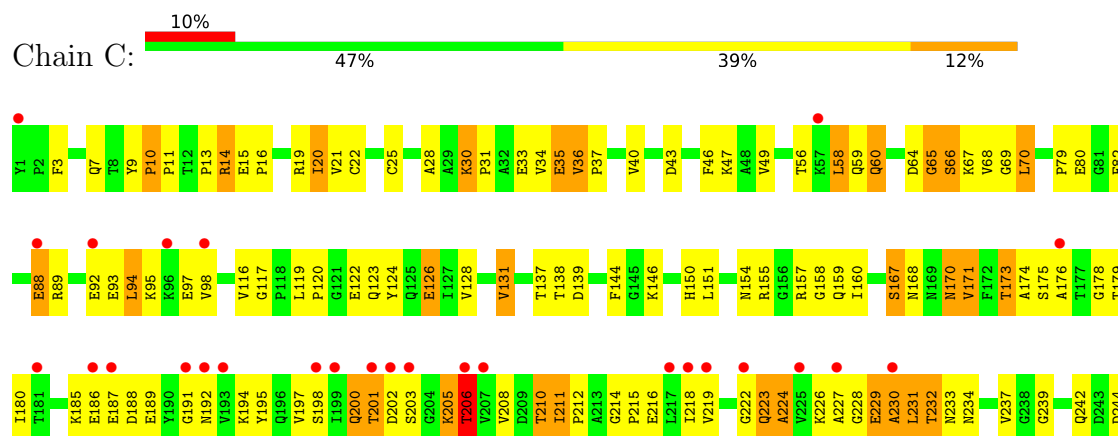
• Molecule 1: Cytochrome b6



• Molecule 2: Cytochrome b6-f complex subunit 4

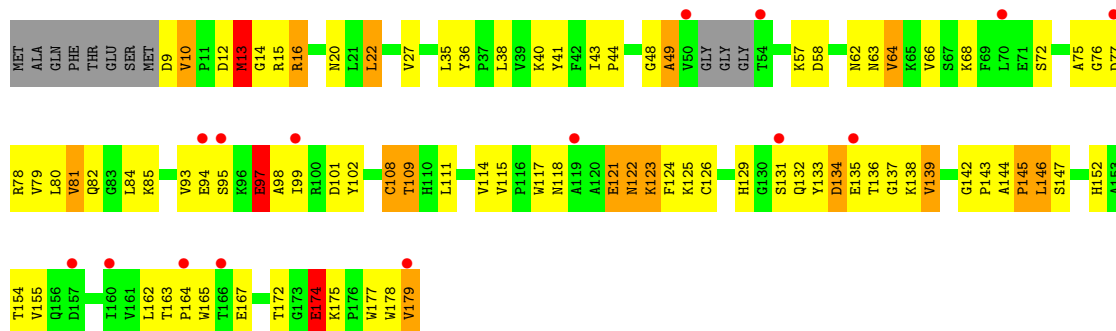
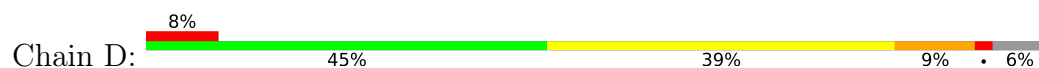


• Molecule 3: Apocytochrome f





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



• Molecule 5: Cytochrome b6-f complex subunit 6



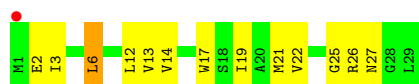
• Molecule 6: Cytochrome b6-f complex subunit 7



• 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	157.20Å 157.20Å 363.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.57 – 3.07 34.57 – 3.07	Depositor EDS
% Data completeness (in resolution range)	99.1 (34.57-3.07) 99.1 (34.57-3.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.69 (at 3.06Å)	Xtriage
Refinement program	REFMAC 5.7.0029, PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.214 , 0.238 0.221 , 0.247	Depositor DCC
R_{free} test set	2544 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	91.8	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 79.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	16526	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.06% 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: MYS, HEM, UMQ, FES, 8K6, BCR, OCT, CD, 7PH, TDS, CLA, OPC, SQD

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	0.39	0/1763	0.82	2/2405 (0.1%)
2	B	0.39	0/1288	0.86	4/1765 (0.2%)
3	C	0.38	0/2264	0.83	2/3082 (0.1%)
4	D	0.35	0/1320	0.81	2/1798 (0.1%)
5	E	0.45	0/253	1.08	1/340 (0.3%)
6	F	0.47	0/238	0.92	0/321
7	G	0.46	0/289	0.97	2/391 (0.5%)
8	H	0.42	0/236	0.93	1/323 (0.3%)
All	All	0.39	0/7651	0.85	14/10425 (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
4	D	0	1

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	23	ILE	CB-CA-C	-6.99	103.02	111.97
2	B	126	ARG	CA-C-N	6.73	128.26	119.84
2	B	126	ARG	C-N-CA	6.73	128.26	119.84
8	H	3	ILE	N-CA-C	-6.47	103.00	111.09
7	G	31	ARG	CA-C-N	6.43	127.88	119.84
7	G	31	ARG	C-N-CA	6.43	127.88	119.84
4	D	76	GLY	N-CA-C	-6.14	106.60	113.79
3	C	10	PRO	N-CA-C	5.93	117.93	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	GLY	CA-C-N	5.81	125.78	120.21
1	A	213	GLY	C-N-CA	5.81	125.78	120.21
3	C	229	GLU	N-CA-C	5.51	116.89	108.52
2	B	67	ASP	CA-C-N	5.43	125.78	119.47
2	B	67	ASP	C-N-CA	5.43	125.78	119.47
4	D	98	ALA	N-CA-C	-5.43	101.37	109.96

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	97	GLU	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	1711	1738	1737	72	0
2	B	1249	1309	1308	66	0
3	C	2216	2235	2233	117	0
4	D	1288	1275	1273	57	0
5	E	248	284	284	16	0
6	F	234	249	248	12	0
7	G	283	289	289	22	0
8	H	230	239	239	12	0
9	A	1	0	0	0	0
10	A	129	90	90	23	0
10	C	43	30	30	10	0
11	A	54	83	83	5	0
11	B	54	83	83	1	0
12	A	15	32	32	5	0
13	A	18	38	38	0	0
14	A	34	43	41	0	0
14	B	34	43	41	1	0
15	A	30	38	38	5	0
15	B	30	38	37	4	0
16	B	65	62	71	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	C	32	49	45	1	0
18	D	53	78	75	3	0
19	D	4	0	0	1	0
20	F	8	18	18	0	0
21	G	40	56	56	7	0
22	A	12	0	0	5	0
22	B	6	0	0	1	0
22	C	4	0	0	0	0
22	F	1	0	0	0	0
22	G	1	0	0	0	0
All	All	8127	8399	8389	370	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 22.

All (370) 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	10:A:304:HEM:CAB	2.57	0.92
3:C:25:CYS:SG	10:C:302:HEM:CAC	2.58	0.92
21:G:101:BCR:H321	21:G:101:BCR:HC8	1.53	0.89
10:A:303:HEM:O1A	22:A:403:HOH:O	1.98	0.81
1:A:117:THR:OG1	22:A:404:HOH:O	2.01	0.79
10:A:304:HEM:HBD1	10:A:304:HEM:HHA	1.65	0.79
1:A:35:CYS:SG	10:A:304:HEM:CBB	2.71	0.78
3:C:25:CYS:SG	10:C:302:HEM:CBC	2.72	0.78
3:C:157:ARG:HB2	10:C:302:HEM:HAD2	1.68	0.74
5:E:8:TYR:CZ	5:E:12:ILE:HD11	2.23	0.73
7:G:20:GLY:N	21:G:101:BCR:H363	2.06	0.69
3:C:171:VAL:HG12	3:C:234:ASN:HA	1.74	0.69
1:A:30:VAL:HG22	1:A:34:TYR:CD1	2.29	0.68
3:C:34:VAL:HG21	3:C:151:LEU:HB2	1.74	0.68
1:A:112:LYS:CB	1:A:113:PRO:CD	2.72	0.67
11:B:204:OPC:HAE2	11:B:204:OPC:OAI	1.94	0.67
1:A:35:CYS:HG	10:A:304:HEM:CAB	2.08	0.67
3:C:200:GLN:HA	3:C:205:LYS:HB3	1.76	0.67
3:C:19:ARG:O	3:C:20:ILE:HB	1.93	0.67
1:A:83:ARG:NH1	10:A:302:HEM:O2A	2.28	0.66
3:C:70:LEU:N	3:C:70:LEU:HD23	2.11	0.66
3:C:211:ILE:O	3:C:211:ILE:HG13	1.96	0.66
2:B:82:TYR:HB2	2:B:83:PRO:HD3	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:A:309:TDS:HAQ2	2:B:81:LEU:HD13	1.80	0.64
2:B:119:LYS:O	2:B:119:LYS:HG2	1.96	0.64
2:B:82:TYR:OH	22:B:305:HOH:O	2.14	0.64
2:B:151:LEU:O	2:B:154:THR:HG22	1.98	0.64
11:A:305:OPC:HBV1	7:G:9:LEU:HD21	1.80	0.64
2:B:33:PRO:HB3	2:B:38:TYR:CE1	2.33	0.63
7:G:1:MET:O	7:G:2:VAL:HG13	1.99	0.63
4:D:78:ARG:HD2	4:D:117:TRP:CD1	2.33	0.63
3:C:251:ASP:HB3	3:C:254:ARG:HD3	1.81	0.63
4:D:129:HIS:HB2	19:D:202:FES:S1	2.38	0.63
3:C:65:GLY:O	3:C:66:SER:O	2.16	0.62
3:C:200:GLN:HG2	3:C:201:THR:N	2.14	0.62
10:A:302:HEM:HBB2	10:A:302:HEM:HMB2	1.81	0.62
4:D:134:ASP:OD1	4:D:135:GLU:N	2.32	0.62
2:B:159:LEU:N	2:B:159:LEU:HD23	2.14	0.62
3:C:34:VAL:HG22	3:C:151:LEU:HD22	1.80	0.62
2:B:35:ASP:HA	2:B:39:VAL:HG13	1.83	0.61
10:A:303:HEM:HBC2	10:A:303:HEM:HMC2	1.82	0.60
2:B:151:LEU:O	2:B:154:THR:CG2	2.50	0.60
10:A:304:HEM:HBC2	10:A:304:HEM:HHH	1.83	0.60
3:C:180:ILE:HG22	3:C:222:GLY:O	2.01	0.60
5:E:10:VAL:O	5:E:14:LEU:HB2	2.01	0.60
1:A:112:LYS:CB	1:A:113:PRO:HD3	2.32	0.60
3:C:257:TRP:HB2	17:C:301:7PH:H26A	1.82	0.60
4:D:108:CYS:CB	4:D:115:VAL:CG2	2.80	0.60
1:A:112:LYS:HB3	1:A:113:PRO:HD3	1.83	0.59
1:A:112:LYS:HB2	1:A:113:PRO:CD	2.32	0.59
2:B:30:PRO:HG2	2:B:34:ASN:OD1	2.01	0.59
7:G:31:ARG:N	7:G:32:PRO:CD	2.65	0.59
1:A:211:ILE:HD12	1:A:212:SER:H	1.66	0.59
3:C:60:GLN:HE22	3:C:157:ARG:HG2	1.68	0.59
3:C:230:ALA:O	3:C:232:THR:N	2.35	0.59
3:C:170:ASN:OD1	3:C:170:ASN:N	2.35	0.59
10:A:302:HEM:HMC1	10:A:302:HEM:HBC2	1.85	0.59
4:D:146:LEU:HD12	4:D:177:TRP:CD2	2.38	0.59
2:B:40:PHE:HB2	2:B:41:PRO:HD3	1.84	0.58
1:A:195:ILE:HD13	1:A:199:MET:HE3	1.85	0.58
1:A:80:TRP:CH2	3:C:254:ARG:HG2	2.39	0.58
7:G:1:MET:O	7:G:2:VAL:HG22	2.04	0.57
1:A:100:HIS:ND1	22:A:410:HOH:O	2.26	0.57
3:C:40:VAL:HG11	3:C:46:PHE:CD2	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:262:ILE:HG22	3:C:263:CYS:N	2.19	0.57
4:D:12:ASP:O	4:D:14:GLY:N	2.36	0.57
21:G:101:BCR:H323	8:H:19:ILE:HG13	1.86	0.57
2:B:22:MET:O	2:B:22:MET:HG3	2.05	0.57
10:C:302:HEM:HBC2	10:C:302:HEM:HMC2	1.87	0.57
4:D:63:ASN:O	4:D:64:VAL:C	2.47	0.57
3:C:167:SER:OG	3:C:168:ASN:N	2.36	0.57
5:E:29:ILE:HG22	5:E:29:ILE:O	2.03	0.57
2:B:159:LEU:O	2:B:160:PHE:HB3	2.05	0.56
2:B:33:PRO:CB	2:B:38:TYR:CE1	2.88	0.56
4:D:48:GLY:O	4:D:49:ALA:C	2.48	0.56
5:E:12:ILE:O	5:E:15:PHE:N	2.38	0.56
2:B:40:PHE:CB	2:B:41:PRO:HD3	2.36	0.56
12:A:306:MYS:H101	12:A:306:MYS:H61	1.88	0.56
6:F:7:TYR:O	6:F:11:LEU:HD12	2.04	0.56
3:C:47:LYS:HG3	3:C:128:VAL:HG13	1.87	0.56
3:C:59:GLN:HB2	3:C:67:LYS:CE	2.35	0.56
15:A:309:TDS:HAJ2	2:B:76:LEU:O	2.05	0.56
2:B:96:LEU:HD13	2:B:100:LEU:HD11	1.88	0.56
4:D:139:VAL:HG22	4:D:147:SER:CA	2.36	0.56
2:B:151:LEU:HD13	2:B:151:LEU:C	2.30	0.55
3:C:46:PHE:CZ	3:C:131:VAL:CG2	2.89	0.55
5:E:12:ILE:O	5:E:13:ALA:C	2.49	0.55
4:D:108:CYS:HB2	4:D:115:VAL:CG2	2.37	0.55
3:C:200:GLN:CG	3:C:201:THR:N	2.68	0.55
1:A:112:LYS:O	1:A:115:GLU:OE1	2.25	0.55
3:C:34:VAL:HG21	3:C:151:LEU:CB	2.36	0.55
2:B:119:LYS:O	2:B:119:LYS:CG	2.55	0.55
2:B:40:PHE:HZ	15:B:201:TDS:OBD	1.90	0.54
3:C:22:CYS:HB2	10:C:302:HEM:CAB	2.37	0.54
2:B:91:VAL:HG12	2:B:91:VAL:O	2.07	0.54
1:A:103:ARG:O	1:A:104:VAL:C	2.50	0.54
3:C:237:VAL:HG22	3:C:237:VAL:O	2.06	0.54
2:B:36:LEU:O	2:B:40:PHE:HB2	2.08	0.54
3:C:271:MET:HE2	4:D:22:LEU:HD12	1.90	0.54
4:D:12:ASP:O	4:D:13:MET:C	2.51	0.54
3:C:15:GLU:HB3	3:C:16:PRO:CD	2.38	0.54
4:D:152:HIS:O	4:D:162:LEU:HA	2.08	0.54
4:D:13:MET:HA	4:D:16:ARG:HD3	1.90	0.53
3:C:158:GLY:C	3:C:159:GLN:NE2	2.67	0.53
7:G:16:ALA:O	21:G:101:BCR:H16C	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:46:PHE:CZ	3:C:131:VAL:HG22	2.44	0.53
3:C:270:LEU:C	3:C:270:LEU:HD13	2.33	0.53
1:A:100:HIS:HA	22:A:410:HOH:O	2.09	0.53
3:C:160:ILE:O	10:C:302:HEM:HMD2	2.09	0.53
2:B:32:TRP:NE1	18:D:201:SQD:O3	2.42	0.53
3:C:19:ARG:O	3:C:20:ILE:CB	2.56	0.53
4:D:152:HIS:CE1	4:D:165:TRP:CE3	2.97	0.53
6:F:11:LEU:O	6:F:15:LEU:HD12	2.08	0.53
4:D:134:ASP:OD1	4:D:134:ASP:C	2.52	0.52
2:B:84:VAL:CG1	2:B:101:MET:SD	2.97	0.52
7:G:1:MET:C	7:G:2:VAL:HG22	2.35	0.52
10:A:303:HEM:HBA1	10:A:303:HEM:HHA	1.92	0.52
3:C:150:HIS:ND1	3:C:244:ASP:OD1	2.42	0.52
1:A:195:ILE:CD1	1:A:199:MET:HE3	2.40	0.52
2:B:154:THR:HG23	2:B:155:LEU:N	2.24	0.52
4:D:57:LYS:HB2	4:D:82:GLN:HB2	1.91	0.52
3:C:28:ALA:HB3	3:C:239:GLY:HA2	1.92	0.52
2:B:154:THR:HG23	2:B:155:LEU:HG	1.91	0.52
3:C:282:VAL:HG12	4:D:10:VAL:HG13	1.91	0.52
3:C:79:PRO:HG2	3:C:82:PHE:CD1	2.45	0.52
5:E:18:ILE:O	5:E:22:ILE:HG22	2.10	0.52
1:A:211:ILE:HG23	1:A:212:SER:O	2.10	0.51
5:E:8:TYR:OH	6:F:15:LEU:HD23	2.09	0.51
1:A:92:MET:HE3	11:A:305:OPC:HBZ2	1.91	0.51
1:A:41:LEU:HD23	10:A:304:HEM:CBC	2.40	0.51
1:A:30:VAL:HG22	1:A:34:TYR:CE1	2.46	0.51
10:A:304:HEM:HMB1	10:A:304:HEM:HBB2	1.92	0.51
6:F:6:LEU:O	6:F:10:LEU:HB2	2.11	0.51
2:B:93:ASN:OD1	2:B:96:LEU:HB2	2.11	0.51
10:C:302:HEM:HMB2	10:C:302:HEM:HBB2	1.91	0.51
2:B:160:PHE:CD1	2:B:160:PHE:C	2.88	0.50
8:H:17:TRP:CZ2	8:H:21:MET:HE3	2.46	0.50
1:A:138:LEU:N	1:A:139:PRO:CD	2.73	0.50
3:C:144:PHE:CZ	3:C:251:ASP:HB2	2.46	0.50
4:D:99:ILE:HD11	4:D:155:VAL:HG23	1.94	0.50
1:A:186:ALA:HB2	12:A:306:MYS:H81	1.93	0.50
3:C:211:ILE:O	3:C:211:ILE:CG1	2.59	0.50
6:F:30:GLN:HG3	6:F:31:GLY:N	2.26	0.50
1:A:103:ARG:HA	7:G:21:LEU:HD21	1.94	0.50
1:A:215:LEU:HD22	2:B:121:GLN:CB	2.42	0.50
1:A:111:LYS:HE2	2:B:115:GLU:O	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:34:GLU:O	7:G:35:LEU:HB2	2.11	0.50
1:A:24:LYS:HE2	22:A:407:HOH:O	2.11	0.49
3:C:35:GLU:HG3	3:C:49:VAL:HB	1.93	0.49
3:C:68:VAL:HG22	3:C:69:GLY:N	2.27	0.49
1:A:47:GLN:HG3	10:A:302:HEM:C3B	2.47	0.49
3:C:70:LEU:N	3:C:70:LEU:CD2	2.76	0.49
4:D:109:THR:HG22	4:D:144:ALA:HB1	1.93	0.49
7:G:10:VAL:HG12	7:G:11:LEU:N	2.26	0.49
2:B:96:LEU:HD13	2:B:100:LEU:CD1	2.42	0.49
3:C:117:GLY:HA2	3:C:119:LEU:HD12	1.94	0.49
6:F:13:PHE:CE2	6:F:17:PHE:HE1	2.30	0.49
1:A:144:GLY:O	1:A:148:VAL:HG23	2.13	0.49
3:C:9:TYR:CD1	3:C:21:VAL:HB	2.48	0.49
3:C:194:LYS:O	3:C:195:TYR:C	2.56	0.49
3:C:214:GLY:N	3:C:215:PRO:CD	2.75	0.49
1:A:211:ILE:HD12	1:A:212:SER:N	2.27	0.49
14:B:202:UMQ:H6'1	18:D:201:SQD:H3	1.94	0.49
10:A:303:HEM:HMB1	10:A:303:HEM:HBB2	1.94	0.48
4:D:36:TYR:OH	4:D:40:LYS:HE3	2.12	0.48
5:E:12:ILE:O	5:E:14:LEU:N	2.46	0.48
5:E:24:PHE:CZ	6:F:29:ILE:HD12	2.49	0.48
3:C:60:GLN:OE1	3:C:70:LEU:HB3	2.13	0.48
4:D:80:LEU:C	4:D:81:VAL:CG2	2.86	0.48
4:D:143:PRO:O	4:D:145:PRO:HD3	2.14	0.48
2:B:102:ALA:O	2:B:105:PRO:HG2	2.13	0.48
3:C:19:ARG:O	3:C:242:GLN:OE1	2.32	0.48
4:D:139:VAL:HG22	4:D:146:LEU:C	2.37	0.48
3:C:33:GLU:HG2	3:C:34:VAL:N	2.28	0.48
3:C:206:THR:O	3:C:206:THR:CG2	2.61	0.48
3:C:197:VAL:HG12	3:C:198:SER:N	2.29	0.48
4:D:142:GLY:HA2	4:D:144:ALA:H	1.79	0.48
7:G:34:GLU:O	7:G:35:LEU:CB	2.61	0.48
1:A:154:VAL:HB	1:A:155:PRO:HD3	1.94	0.48
3:C:222:GLY:O	3:C:223:GLN:O	2.31	0.48
3:C:88:GLU:O	3:C:88:GLU:HG2	2.14	0.47
1:A:107:THR:HG23	1:A:107:THR:O	2.13	0.47
2:B:45:MET:HE1	4:D:27:VAL:HG22	1.96	0.47
2:B:123:PRO:HD2	7:G:25:ALA:HB1	1.95	0.47
3:C:200:GLN:HG2	3:C:201:THR:H	1.77	0.47
3:C:286:GLU:N	3:C:286:GLU:OE1	2.48	0.47
16:B:203:CLA:HMB1	16:B:203:CLA:HBB1	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:TYR:CE1	16:B:203:CLA:HBB1	2.49	0.47
3:C:266:MET:SD	8:H:13:VAL:HG12	2.54	0.47
1:A:142:GLN:HE22	2:B:67:ASP:HB3	1.80	0.47
2:B:159:LEU:O	2:B:160:PHE:CB	2.63	0.47
3:C:138:THR:OG1	3:C:139:ASP:N	2.48	0.47
3:C:231:LEU:C	3:C:231:LEU:HD12	2.40	0.47
6:F:25:LEU:O	6:F:29:ILE:HG23	2.15	0.47
3:C:79:PRO:HG2	3:C:82:PHE:CE1	2.50	0.47
4:D:163:THR:HG22	4:D:164:PRO:HD2	1.97	0.46
4:D:121:GLU:O	4:D:122:ASN:C	2.59	0.46
2:B:40:PHE:O	2:B:43:VAL:N	2.49	0.46
3:C:13:PRO:O	3:C:20:ILE:HA	2.15	0.46
4:D:108:CYS:HB3	4:D:115:VAL:CG2	2.44	0.46
3:C:259:ILE:CD1	8:H:6:LEU:HD13	2.46	0.46
7:G:31:ARG:N	7:G:32:PRO:HD3	2.31	0.46
4:D:78:ARG:HD2	4:D:117:TRP:CG	2.50	0.46
4:D:85:LYS:O	4:D:85:LYS:HG2	2.15	0.46
4:D:139:VAL:HG22	4:D:147:SER:HA	1.96	0.46
4:D:142:GLY:HA2	4:D:144:ALA:N	2.31	0.46
1:A:7:TRP:NE1	1:A:11:ARG:HH21	2.13	0.46
3:C:15:GLU:CB	3:C:16:PRO:CD	2.94	0.46
3:C:144:PHE:CE2	3:C:251:ASP:HB2	2.51	0.46
4:D:117:TRP:CH2	4:D:123:LYS:N	2.84	0.46
2:B:84:VAL:HG11	2:B:101:MET:SD	2.54	0.46
3:C:288:ASN:OD1	3:C:288:ASN:C	2.58	0.45
1:A:147:ALA:O	1:A:151:VAL:HG13	2.16	0.45
12:A:306:MYS:H101	12:A:306:MYS:C6	2.47	0.45
1:A:15:GLN:O	1:A:16:ALA:C	2.58	0.45
1:A:35:CYS:SG	10:A:304:HEM:C3B	3.04	0.45
1:A:202:HIS:O	1:A:206:ILE:HG13	2.16	0.45
2:B:128:VAL:O	2:B:132:ILE:HD12	2.16	0.45
21:G:101:BCR:H321	21:G:101:BCR:C8	2.36	0.45
21:G:101:BCR:H323	8:H:19:ILE:CG1	2.46	0.45
1:A:44:PHE:O	1:A:47:GLN:HB2	2.16	0.45
12:A:306:MYS:H61	12:A:306:MYS:C10	2.46	0.45
2:B:154:THR:HG23	2:B:155:LEU:H	1.81	0.45
1:A:111:LYS:NZ	2:B:120:PHE:O	2.41	0.45
2:B:45:MET:HE3	4:D:27:VAL:HG13	1.97	0.45
7:G:2:VAL:HG23	7:G:2:VAL:O	2.16	0.45
1:A:105:TYR:C	1:A:107:THR:H	2.23	0.45
1:A:127:ILE:CG2	1:A:195:ILE:HG13	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:305:OPC:HBQ1	8:H:12:LEU:HD21	1.98	0.45
3:C:46:PHE:CE2	3:C:131:VAL:HG22	2.52	0.45
3:C:173:THR:O	3:C:231:LEU:CD2	2.65	0.45
3:C:259:ILE:HD13	8:H:6:LEU:HD13	1.99	0.45
1:A:161:VAL:O	1:A:163:VAL:N	2.49	0.45
1:A:166:SER:HB3	1:A:170:ARG:NH2	2.32	0.45
4:D:146:LEU:HD23	4:D:146:LEU:N	2.32	0.45
3:C:14:ARG:CZ	3:C:150:HIS:CD2	3.00	0.45
3:C:25:CYS:SG	10:C:302:HEM:C3C	3.10	0.45
3:C:58:LEU:C	3:C:58:LEU:HD12	2.42	0.45
3:C:278:GLN:HG3	5:E:31:LEU:O	2.18	0.45
3:C:60:GLN:NE2	3:C:157:ARG:HG2	2.32	0.44
3:C:93:GLU:O	3:C:97:GLU:HG3	2.17	0.44
3:C:43:ASP:CG	3:C:89:ARG:HH22	2.26	0.44
3:C:49:VAL:HG13	3:C:126:GLU:HG3	1.99	0.44
3:C:201:THR:O	3:C:203:SER:N	2.50	0.44
3:C:274:LEU:HD11	5:E:22:ILE:HG23	1.98	0.44
1:A:24:LYS:HB3	15:B:201:TDS:HAA1	1.98	0.44
3:C:154:ASN:CG	3:C:155:ARG:N	2.75	0.44
4:D:139:VAL:HG22	4:D:147:SER:N	2.32	0.44
3:C:275:LYS:HE2	4:D:20:ASN:OD1	2.18	0.44
1:A:107:THR:O	1:A:107:THR:CG2	2.65	0.44
1:A:215:LEU:HD22	2:B:121:GLN:HB2	1.98	0.44
6:F:27:LEU:HA	6:F:30:GLN:HG2	1.98	0.44
4:D:108:CYS:CB	4:D:115:VAL:HG22	2.47	0.44
12:A:306:MYS:H101	12:A:306:MYS:H41	1.99	0.44
15:B:201:TDS:HAQ2	15:B:201:TDS:HAI3	1.77	0.44
1:A:142:GLN:OE1	1:A:142:GLN:HA	2.18	0.44
2:B:40:PHE:CB	2:B:41:PRO:CD	2.96	0.44
3:C:9:TYR:CE1	3:C:21:VAL:HB	2.53	0.44
8:H:26:ARG:O	8:H:27:ASN:C	2.59	0.44
3:C:94:LEU:O	3:C:95:LYS:C	2.61	0.44
3:C:160:ILE:O	10:C:302:HEM:HH2	2.18	0.44
3:C:245:THR:OG1	3:C:246:GLU:N	2.50	0.44
2:B:109:ILE:O	2:B:112:PRO:HD2	2.17	0.43
2:B:134:LEU:HD12	2:B:134:LEU:HA	1.80	0.43
1:A:105:TYR:CZ	16:B:203:CLA:CBB	3.01	0.43
3:C:15:GLU:OE1	3:C:19:ARG:HB3	2.18	0.43
3:C:34:VAL:CG2	3:C:151:LEU:HB2	2.43	0.43
4:D:93:VAL:HG12	4:D:97:GLU:HB3	2.00	0.43
2:B:111:VAL:N	2:B:112:PRO:CD	2.81	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:94:LEU:O	3:C:98:VAL:HG23	2.17	0.43
3:C:119:LEU:HB3	3:C:120:PRO:HD2	1.99	0.43
7:G:26:TYR:C	7:G:28:GLN:N	2.75	0.43
1:A:34:TYR:CZ	1:A:103:ARG:NH1	2.85	0.43
4:D:134:ASP:OD2	4:D:138:LYS:HB3	2.18	0.43
1:A:158:ILE:HA	1:A:159:PRO:HD3	1.83	0.43
3:C:30:LYS:HB3	3:C:31:PRO:HD2	2.01	0.43
3:C:64:ASP:OD2	3:C:65:GLY:N	2.52	0.43
3:C:119:LEU:HD22	3:C:124:TYR:CE1	2.54	0.43
3:C:144:PHE:CE1	3:C:251:ASP:HB2	2.54	0.43
3:C:273:ILE:HG23	8:H:25:GLY:HA2	2.00	0.43
1:A:137:SER:HB2	1:A:148:VAL:CG2	2.48	0.43
2:B:37:LEU:HD12	15:B:201:TDS:HBB1	2.00	0.43
4:D:75:ALA:HB1	4:D:95:SER:HA	2.01	0.43
4:D:178:TRP:CD1	4:D:179:VAL:HB	2.54	0.43
15:A:309:TDS:HAW1	16:B:203:CLA:H93	2.00	0.43
2:B:30:PRO:O	2:B:34:ASN:HB2	2.18	0.43
4:D:108:CYS:HB3	4:D:115:VAL:HG22	2.00	0.43
4:D:174:GLU:HB2	4:D:175:LYS:H	1.68	0.43
21:G:101:BCR:C32	8:H:19:ILE:HG12	2.48	0.43
2:B:97:GLY:HA2	2:B:100:LEU:HD12	2.02	0.42
4:D:137:GLY:O	4:D:138:LYS:C	2.61	0.42
8:H:22:VAL:O	8:H:26:ARG:HG2	2.19	0.42
3:C:34:VAL:CG2	3:C:151:LEU:CB	2.96	0.42
3:C:34:VAL:CG2	3:C:151:LEU:HD22	2.47	0.42
3:C:160:ILE:O	10:C:302:HEM:HAC	2.19	0.42
5:E:23:ILE:O	5:E:27:LYS:N	2.52	0.42
1:A:83:ARG:NH1	10:A:302:HEM:CGA	2.82	0.42
3:C:28:ALA:HB3	3:C:239:GLY:CA	2.49	0.42
4:D:115:VAL:CG1	4:D:124:PHE:HB3	2.49	0.42
4:D:132:GLN:C	4:D:133:TYR:CD1	2.97	0.42
3:C:36:VAL:HG23	3:C:37:PRO:O	2.19	0.42
3:C:139:ASP:OD1	3:C:139:ASP:C	2.62	0.42
3:C:229:GLU:HG3	3:C:230:ALA:CB	2.49	0.42
3:C:285:ALA:C	3:C:286:GLU:OE1	2.62	0.42
1:A:47:GLN:OE1	1:A:47:GLN:HA	2.20	0.42
1:A:106:LEU:HD12	7:G:21:LEU:HD23	2.02	0.42
1:A:143:VAL:HG12	1:A:144:GLY:N	2.34	0.42
1:A:211:ILE:HG12	10:A:304:HEM:HMA3	2.02	0.42
3:C:229:GLU:O	3:C:231:LEU:N	2.43	0.42
1:A:118:TRP:CD1	2:B:112:PRO:HG3	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:VAL:O	2:B:42:VAL:HB	2.20	0.42
4:D:108:CYS:HB2	4:D:115:VAL:HG21	2.01	0.42
1:A:2:ALA:O	1:A:3:ASN:C	2.63	0.42
1:A:12:LEU:HB2	1:A:14:ILE:CD1	2.49	0.42
2:B:117:VAL:HG23	2:B:118:ASN:N	2.34	0.42
3:C:255:VAL:O	3:C:259:ILE:HG13	2.19	0.42
3:C:265:VAL:O	3:C:269:GLN:HG3	2.20	0.42
10:A:303:HEM:HBB2	10:A:303:HEM:CMB	2.50	0.42
3:C:15:GLU:HB3	3:C:16:PRO:HD2	2.02	0.42
18:D:201:SQD:H162	18:D:201:SQD:H131	1.78	0.42
15:A:309:TDS:HAJ2	2:B:76:LEU:C	2.45	0.42
2:B:10:SER:O	2:B:12:PRO:HD3	2.19	0.42
3:C:194:LYS:HD3	3:C:210:THR:CG2	2.50	0.42
4:D:102:TYR:OH	4:D:136:THR:HG22	2.20	0.42
2:B:95:LEU:HD23	2:B:99:LEU:CD1	2.50	0.41
2:B:117:VAL:HG23	2:B:118:ASN:H	1.85	0.41
4:D:38:LEU:O	4:D:41:TYR:HB3	2.20	0.41
5:E:22:ILE:HG13	5:E:22:ILE:O	2.19	0.41
1:A:161:VAL:O	1:A:164:LEU:N	2.52	0.41
2:B:40:PHE:C	2:B:42:VAL:N	2.77	0.41
3:C:10:PRO:HD2	3:C:11:PRO:HD3	2.02	0.41
1:A:161:VAL:O	1:A:162:GLY:C	2.63	0.41
4:D:43:ILE:HA	4:D:44:PRO:HD3	1.93	0.41
3:C:266:MET:CE	5:E:15:PHE:CD1	3.03	0.41
1:A:112:LYS:HB3	1:A:113:PRO:CD	2.45	0.41
2:B:82:TYR:N	2:B:83:PRO:CD	2.84	0.41
6:F:13:PHE:CE2	6:F:17:PHE:CE1	3.07	0.41
1:A:215:LEU:HD22	2:B:121:GLN:HB3	2.03	0.41
10:A:304:HEM:HAB	2:B:43:VAL:HG21	2.02	0.41
2:B:37:LEU:HD23	2:B:38:TYR:CZ	2.56	0.41
7:G:21:LEU:HD12	7:G:21:LEU:HA	1.89	0.41
7:G:33:ASN:O	7:G:34:GLU:O	2.39	0.41
4:D:115:VAL:HG12	4:D:124:PHE:HB3	2.02	0.41
7:G:35:LEU:HD23	7:G:35:LEU:N	2.35	0.41
1:A:98:ILE:HD11	16:B:203:CLA:HED3	2.02	0.41
11:A:305:OPC:CBV	7:G:9:LEU:HD21	2.50	0.41
1:A:7:TRP:CD1	1:A:11:ARG:HH21	2.39	0.41
1:A:121:GLY:HA3	10:A:303:HEM:C3C	2.56	0.41
10:A:302:HEM:HBB2	10:A:302:HEM:CMB	2.50	0.41
2:B:122:ASN:HA	2:B:123:PRO:HD3	1.91	0.41
3:C:173:THR:O	3:C:231:LEU:HD23	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:176:ALA:HB1	3:C:205:LYS:NZ	2.35	0.41
3:C:178:GLY:O	3:C:224:ALA:HA	2.21	0.41
3:C:229:GLU:HG3	3:C:230:ALA:HB2	2.03	0.41
2:B:1:MET:O	2:B:2:ALA:C	2.62	0.41
3:C:206:THR:O	3:C:206:THR:HG22	2.20	0.41
2:B:58:ASP:OD2	3:C:146:LYS:CE	2.68	0.40
4:D:15:ARG:HB3	5:E:31:LEU:HD23	2.03	0.40
4:D:58:ASP:N	4:D:62:ASN:O	2.53	0.40
4:D:118:ASN:ND2	4:D:121:GLU:OE2	2.54	0.40
4:D:139:VAL:CG2	4:D:146:LEU:C	2.94	0.40
5:E:24:PHE:CZ	6:F:29:ILE:CD1	3.04	0.40
6:F:27:LEU:HD11	8:H:27:ASN:HA	2.03	0.40
1:A:139:PRO:HG3	10:A:302:HEM:O2A	2.22	0.40
7:G:10:VAL:O	7:G:11:LEU:C	2.64	0.40
2:B:53:ALA:O	2:B:57:LEU:HG	2.21	0.40
3:C:19:ARG:O	3:C:242:GLN:CD	2.65	0.40
1:A:92:MET:HB3	11:A:305:OPC:HCB2	2.03	0.40
1:A:150:ILE:HD13	15:A:309:TDS:HAA3	2.03	0.40
7:G:26:TYR:O	7:G:28:GLN:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	213/215 (99%)	190 (89%)	17 (8%)	6 (3%)	4	18
2	B	158/160 (99%)	137 (87%)	21 (13%)	0	100	100
3	C	286/289 (99%)	229 (80%)	36 (13%)	21 (7%)	1	4
4	D	164/179 (92%)	135 (82%)	21 (13%)	8 (5%)	1	9
5	E	30/32 (94%)	26 (87%)	3 (10%)	1 (3%)	3	15

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	29/35 (83%)	26 (90%)	3 (10%)	0	100	100
7	G	35/37 (95%)	22 (63%)	6 (17%)	7 (20%)	0	0
8	H	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
All	All	942/976 (96%)	791 (84%)	108 (12%)	43 (5%)	2	10

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	LYS
1	A	162	GLY
3	C	66	SER
3	C	192	ASN
3	C	201	THR
3	C	202	ASP
3	C	205	LYS
4	D	13	MET
4	D	49	ALA
4	D	64	VAL
7	G	2	VAL
7	G	32	PRO
7	G	34	GLU
3	C	20	ILE
3	C	186	GLU
3	C	223	GLN
3	C	224	ALA
3	C	227	ALA
3	C	228	GLY
3	C	230	ALA
3	C	231	LEU
4	D	122	ASN
4	D	123	LYS
7	G	10	VAL
7	G	27	GLN
1	A	3	ASN
3	C	173	THR
3	C	187	GLU
3	C	191	GLY
3	C	200	GLN
3	C	206	THR
4	D	97	GLU
4	D	145	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	174	ALA
3	C	212	PRO
7	G	33	ASN
7	G	35	LEU
1	A	104	VAL
1	A	159	PRO
1	A	106	LEU
4	D	174	GLU
5	E	13	ALA
3	C	65	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	184/184 (100%)	157 (85%)	27 (15%)	3	12
2	B	137/137 (100%)	121 (88%)	16 (12%)	5	20
3	C	242/243 (100%)	194 (80%)	48 (20%)	1	5
4	D	139/146 (95%)	107 (77%)	32 (23%)	1	3
5	E	25/25 (100%)	23 (92%)	2 (8%)	11	35
6	F	23/27 (85%)	15 (65%)	8 (35%)	0	0
7	G	28/28 (100%)	22 (79%)	6 (21%)	1	4
8	H	24/24 (100%)	21 (88%)	3 (12%)	4	17
All	All	802/814 (98%)	660 (82%)	142 (18%)	2	8

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	14	ILE
1	A	17	LEU
1	A	26	VAL
1	A	36	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	47	GLN
1	A	61	THR
1	A	72	ILE
1	A	81	LEU
1	A	95	LEU
1	A	103	ARG
1	A	107	THR
1	A	115	GLU
1	A	119	ILE
1	A	123	ILE
1	A	143	VAL
1	A	148	VAL
1	A	149	LYS
1	A	151	VAL
1	A	161	VAL
1	A	164	LEU
1	A	169	LEU
1	A	173	SER
1	A	195	ILE
1	A	200	LEU
1	A	208	LYS
1	A	211	ILE
2	B	4	LEU
2	B	13	LYS
2	B	39	VAL
2	B	73	LEU
2	B	74	GLU
2	B	76	LEU
2	B	88	LEU
2	B	96	LEU
2	B	108	LEU
2	B	119	LYS
2	B	134	LEU
2	B	138	LEU
2	B	140	THR
2	B	152	ASP
2	B	157	LEU
2	B	159	LEU
3	C	3	PHE
3	C	7	GLN
3	C	14	ARG
3	C	30	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	35	GLU
3	C	36	VAL
3	C	56	THR
3	C	58	LEU
3	C	60	GLN
3	C	70	LEU
3	C	80	GLU
3	C	88	GLU
3	C	92	GLU
3	C	94	LEU
3	C	116	VAL
3	C	122	GLU
3	C	123	GLN
3	C	126	GLU
3	C	131	VAL
3	C	137	THR
3	C	167	SER
3	C	170	ASN
3	C	171	VAL
3	C	175	SER
3	C	179	THR
3	C	185	LYS
3	C	188	ASP
3	C	189	GLU
3	C	206	THR
3	C	208	VAL
3	C	210	THR
3	C	211	ILE
3	C	216	GLU
3	C	218	ILE
3	C	219	VAL
3	C	226	LYS
3	C	232	THR
3	C	233	ASN
3	C	249	LEU
3	C	254	ARG
3	C	262	ILE
3	C	264	LEU
3	C	267	LEU
3	C	270	LEU
3	C	271	MET
3	C	279	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	282	VAL
3	C	286	GLU
4	D	9	ASP
4	D	10	VAL
4	D	13	MET
4	D	16	ARG
4	D	22	LEU
4	D	35	LEU
4	D	66	VAL
4	D	68	LYS
4	D	72	SER
4	D	77	ASP
4	D	79	VAL
4	D	81	VAL
4	D	84	LEU
4	D	94	GLU
4	D	97	GLU
4	D	101	ASP
4	D	108	CYS
4	D	109	THR
4	D	111	LEU
4	D	114	VAL
4	D	121	GLU
4	D	125	LYS
4	D	126	CYS
4	D	131	SER
4	D	134	ASP
4	D	139	VAL
4	D	146	LEU
4	D	154	THR
4	D	167	GLU
4	D	172	THR
4	D	174	GLU
4	D	179	VAL
5	E	12	ILE
5	E	14	LEU
6	F	6	LEU
6	F	10	LEU
6	F	15	LEU
6	F	22	LEU
6	F	25	LEU
6	F	26	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	29	ILE
6	F	30	GLN
7	G	5	LEU
7	G	6	LEU
7	G	9	LEU
7	G	21	LEU
7	G	30	LYS
7	G	35	LEU
8	H	2	GLU
8	H	6	LEU
8	H	14	VAL

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	15	GLN
3	C	24	ASN
3	C	60	GLN
3	C	200	GLN
3	C	242	GLN
3	C	269	GLN
4	D	17	GLN
8	H	27	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 1 is monoatomic - leaving 18 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
10	HEM	A	304	15,22	50,50,50	1.98	7 (14%)	67,82,82	1.53	7 (10%)
11	OPC	B	204	-	53,53,54	1.07	3 (5%)	59,61,64	1.01	4 (6%)
21	BCR	G	101	-	41,41,41	2.16	20 (48%)	56,56,56	2.22	20 (35%)
11	OPC	A	305	-	53,53,54	1.00	4 (7%)	59,61,64	1.07	3 (5%)
19	FES	D	202	4	0,4,4	-	-	-	-	-
12	MYS	A	306	-	14,14,14	0.37	0	13,13,13	0.78	0
10	HEM	A	302	1	50,50,50	1.81	9 (18%)	67,82,82	1.28	7 (10%)
15	TDS	A	309	-	31,31,31	1.20	2 (6%)	37,40,40	2.15	8 (21%)
15	TDS	B	201	10	31,31,31	1.16	2 (6%)	37,40,40	1.88	9 (24%)
17	7PH	C	301	-	31,31,37	1.00	2 (6%)	33,33,42	1.22	3 (9%)
10	HEM	C	302	3	50,50,50	1.76	8 (16%)	67,82,82	1.35	7 (10%)
18	SQD	D	201	-	51,53,54	3.21	17 (33%)	60,63,65	2.21	13 (21%)
20	OCT	F	101	-	7,7,7	0.29	0	6,6,6	0.65	0
14	UMQ	B	202	-	35,35,35	1.18	3 (8%)	46,46,46	2.61	15 (32%)
10	HEM	A	303	1	50,50,50	1.81	8 (16%)	67,82,82	1.18	2 (2%)
16	CLA	B	203	22	69,73,73	1.17	6 (8%)	82,113,113	1.33	8 (9%)
14	UMQ	A	308	-	35,35,35	1.22	5 (14%)	46,46,46	2.47	17 (36%)
13	8K6	A	307	-	17,17,17	0.25	0	16,16,16	0.58	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	HEM	A	304	15,22	-	6/14/54/54	-
11	OPC	B	204	-	-	18/57/57/60	-
13	8K6	A	307	-	-	5/15/15/15	-
21	BCR	G	101	-	-	18/29/63/63	0/2/2/2
11	OPC	A	305	-	-	31/57/57/60	-
19	FES	D	202	4	-	-	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	MYS	A	306	-	-	3/12/12/12	-
10	HEM	A	302	1	-	4/14/54/54	-
15	TDS	A	309	-	-	7/17/17/17	0/2/2/2
15	TDS	B	201	10	-	12/17/17/17	0/2/2/2
17	7PH	C	301	-	-	13/33/33/39	-
10	HEM	C	302	3	-	7/14/54/54	-
20	OCT	F	101	-	-	0/5/5/5	-
16	CLA	B	203	22	1/1/17/20	20/39/115/115	-
10	HEM	A	303	1	-	5/14/54/54	-
18	SQD	D	201	-	2/2/9/9	27/49/65/69	0/1/1/1
14	UMQ	A	308	-	3/3/10/10	6/20/60/60	0/2/2/2
14	UMQ	B	202	-	2/2/10/10	12/20/60/60	0/2/2/2

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	D	201	SQD	O6-C44	9.87	1.61	1.43
18	D	201	SQD	C2-C3	-9.72	1.34	1.52
10	A	304	HEM	C3D-C2D	7.91	1.53	1.36
18	D	201	SQD	C8-C7	7.87	1.73	1.50
10	A	302	HEM	C3D-C2D	7.83	1.53	1.36
10	A	303	HEM	C3D-C2D	7.80	1.53	1.36
10	C	302	HEM	C3D-C2D	7.66	1.53	1.36
18	D	201	SQD	C4-C5	-6.65	1.38	1.53
18	D	201	SQD	O47-C7	5.89	1.50	1.34
18	D	201	SQD	O5-C1	5.83	1.57	1.42
10	A	302	HEM	FE-ND	5.35	2.11	1.94
10	A	304	HEM	FE-NB	5.24	2.11	1.94
18	D	201	SQD	C3-C4	5.04	1.60	1.52
18	D	201	SQD	O47-C45	4.81	1.57	1.46
18	D	201	SQD	C46-C45	-4.63	1.36	1.50
10	A	304	HEM	FE-ND	4.41	2.08	1.94
10	A	304	HEM	FE-NC	4.40	2.09	1.95
15	B	201	TDS	CAH-CAG	-4.04	1.38	1.47
15	A	309	TDS	CAH-CAG	-4.02	1.38	1.47
10	A	303	HEM	FE-NB	3.94	2.07	1.94
10	C	302	HEM	FE-ND	3.75	2.06	1.94
16	B	203	CLA	C1D-ND	3.58	1.42	1.37
11	A	305	OPC	OAN-CAO	3.52	1.44	1.34
17	C	301	7PH	O21-C2	-3.48	1.38	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	G	101	BCR	C20-C21	3.45	1.53	1.43
10	A	303	HEM	FE-ND	3.43	2.05	1.94
11	B	204	OPC	OAN-CAO	3.35	1.43	1.34
10	A	303	HEM	FE-NC	3.32	2.06	1.95
21	G	101	BCR	C15-C14	3.31	1.53	1.43
21	G	101	BCR	C11-C10	3.29	1.53	1.43
10	C	302	HEM	FE-NB	3.27	2.05	1.94
21	G	101	BCR	C16-C17	3.24	1.53	1.43
21	G	101	BCR	C19-C18	3.22	1.52	1.46
15	A	309	TDS	OAO-CAP	-3.21	1.33	1.36
21	G	101	BCR	C23-C22	3.20	1.52	1.46
21	G	101	BCR	C12-C13	3.17	1.52	1.46
11	B	204	OPC	OBJ-CBK	3.10	1.42	1.33
21	G	101	BCR	C26-C25	3.09	1.39	1.34
10	C	302	HEM	CAC-C3C	3.04	1.55	1.47
15	B	201	TDS	OAO-CAP	-3.02	1.33	1.36
21	G	101	BCR	C32-C1	-2.97	1.48	1.53
10	A	303	HEM	CAC-C3C	2.95	1.55	1.47
18	D	201	SQD	O48-C46	-2.94	1.38	1.45
10	C	302	HEM	CAB-C3B	2.94	1.55	1.47
16	B	203	CLA	C4B-NB	2.92	1.41	1.37
18	D	201	SQD	O5-C5	2.91	1.51	1.44
10	A	303	HEM	CAB-C3B	2.89	1.55	1.47
10	A	304	HEM	CAB-C3B	2.89	1.55	1.47
16	B	203	CLA	C1B-C2B	2.88	1.49	1.43
14	B	202	UMQ	O5'-C5'	-2.86	1.37	1.44
10	A	304	HEM	CAC-C3C	2.85	1.55	1.47
18	D	201	SQD	C2-C1	-2.83	1.43	1.50
17	C	301	7PH	O31-C3	-2.83	1.38	1.45
10	A	302	HEM	CAC-C3C	2.82	1.54	1.47
10	A	302	HEM	CAB-C3B	2.78	1.54	1.47
10	C	302	HEM	FE-NC	2.78	2.04	1.95
10	A	303	HEM	FE-NA	2.72	2.04	1.95
10	C	302	HEM	FE-NA	2.72	2.04	1.95
18	D	201	SQD	C10-C9	2.69	1.65	1.51
18	D	201	SQD	C9-C8	2.68	1.62	1.52
21	G	101	BCR	C8-C9	2.67	1.51	1.46
10	A	302	HEM	FE-NC	2.67	2.04	1.95
10	A	304	HEM	FE-NA	2.66	2.03	1.95
10	A	302	HEM	FE-NB	2.57	2.02	1.94
21	G	101	BCR	C40-C30	-2.55	1.48	1.53
11	A	305	OPC	OBJ-CBI	-2.41	1.39	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	A	308	UMQ	O5'-C5'	-2.41	1.38	1.44
14	B	202	UMQ	O3'-C3'	-2.34	1.37	1.43
14	A	308	UMQ	C4-C5	-2.32	1.48	1.53
14	A	308	UMQ	O2'-C2'	-2.31	1.37	1.43
14	A	308	UMQ	O3'-C3'	-2.30	1.37	1.43
21	G	101	BCR	C24-C23	2.28	1.39	1.33
21	G	101	BCR	C31-C1	-2.27	1.49	1.53
11	A	305	OPC	OBJ-CBK	2.26	1.39	1.33
18	D	201	SQD	C18-C17	2.26	1.63	1.51
21	G	101	BCR	C29-C28	-2.25	1.47	1.52
11	B	204	OPC	CAV-CAW	2.24	1.44	1.31
18	D	201	SQD	C11-C10	2.23	1.62	1.51
21	G	101	BCR	C39-C30	-2.23	1.49	1.53
21	G	101	BCR	C7-C6	2.22	1.52	1.45
21	G	101	BCR	C20-C19	2.22	1.40	1.34
21	G	101	BCR	C24-C25	2.22	1.52	1.45
14	B	202	UMQ	O2'-C2'	-2.21	1.37	1.43
11	A	305	OPC	CAV-CAW	2.20	1.44	1.31
10	A	302	HEM	CMB-C2B	2.18	1.55	1.50
14	A	308	UMQ	C3-C4	-2.16	1.46	1.52
10	A	302	HEM	CMC-C2C	2.15	1.55	1.50
21	G	101	BCR	C5-C6	2.15	1.38	1.34
10	A	302	HEM	C2A-C3A	-2.15	1.33	1.38
16	B	203	CLA	C3B-C4B	2.13	1.48	1.42
18	D	201	SQD	O6-C1	2.12	1.47	1.40
16	B	203	CLA	CHC-C1C	2.12	1.42	1.38
16	B	203	CLA	MG-NB	-2.06	2.01	2.05
21	G	101	BCR	C11-C12	2.05	1.40	1.34
10	C	302	HEM	CMB-C2B	2.03	1.54	1.50
10	A	303	HEM	CMC-C2C	2.02	1.54	1.50

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D	201	SQD	C3-C4-C5	8.65	118.67	109.99
14	A	308	UMQ	O5-C5-C4	7.76	123.68	109.70
15	A	309	TDS	OAK-CAL-CAM	7.74	122.62	114.53
14	B	202	UMQ	O1-C1-C2	7.40	126.31	108.09
16	B	203	CLA	C4A-NA-C1A	6.78	109.77	106.68
10	A	304	HEM	C4D-ND-C1D	6.18	112.53	105.21
15	B	201	TDS	OAK-CAL-CAM	5.70	120.49	114.53
10	C	302	HEM	C4D-ND-C1D	5.67	111.92	105.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	202	UMQ	C1'-C2'-C3'	5.66	121.93	110.01
14	B	202	UMQ	O2-C2-C1	5.65	123.55	110.08
14	B	202	UMQ	O2-C2-C3	5.29	122.84	110.38
10	A	303	HEM	C4D-ND-C1D	5.28	111.46	105.21
14	A	308	UMQ	O1-C1-C2	5.20	120.87	108.09
21	G	101	BCR	C2-C1-C6	5.16	117.93	110.44
14	B	202	UMQ	O5-C5-C4	5.13	118.95	109.70
21	G	101	BCR	C16-C17-C18	-5.10	120.13	127.28
18	D	201	SQD	O4-C4-C3	4.99	120.25	110.05
14	A	308	UMQ	O2'-C2'-C1'	4.96	121.90	110.08
15	B	201	TDS	OAO-CAP-CAQ	4.83	120.38	110.12
21	G	101	BCR	C23-C24-C25	-4.81	114.14	127.00
18	D	201	SQD	O5-C5-C4	4.70	118.17	109.70
14	B	202	UMQ	C3-C4-C5	4.67	118.70	110.23
11	A	305	OPC	OAN-CAO-CAP	4.62	121.47	111.48
10	A	302	HEM	C4D-ND-C1D	4.62	110.68	105.21
14	A	308	UMQ	O2'-C2'-C3'	4.59	121.20	110.38
18	D	201	SQD	O4-C4-C5	4.49	120.38	109.32
10	A	304	HEM	CAD-C3D-C4D	4.49	132.51	124.70
21	G	101	BCR	C15-C14-C13	-4.47	121.02	127.28
14	A	308	UMQ	O5-C5-C6	4.44	117.43	106.44
14	A	308	UMQ	O1-C1-O5	4.30	122.02	110.69
15	A	309	TDS	OAK-CAL-CAD	-4.28	116.71	124.08
18	D	201	SQD	C2-C3-C4	4.21	116.73	110.67
18	D	201	SQD	O47-C7-C8	4.08	120.30	111.48
18	D	201	SQD	O5-C1-C2	4.03	117.08	110.84
14	B	202	UMQ	CA-O1'-C1'	3.99	120.49	113.68
15	A	309	TDS	OAO-CAP-CAQ	3.96	118.52	110.12
18	D	201	SQD	C44-O6-C1	3.96	122.23	113.83
14	A	308	UMQ	CA-O1'-C1'	3.92	120.37	113.68
15	A	309	TDS	OAB-CAE-CAF	3.84	121.28	115.84
21	G	101	BCR	C8-C7-C6	-3.80	116.84	127.00
18	D	201	SQD	O9-S-C6	3.78	112.40	106.76
21	G	101	BCR	C20-C21-C22	-3.76	122.01	127.28
18	D	201	SQD	O9-S-O7	-3.74	101.64	113.82
14	B	202	UMQ	O1-C1-O5	3.62	120.21	110.69
15	A	309	TDS	CAJ-OAK-CAL	3.60	122.79	117.51
21	G	101	BCR	C33-C5-C6	-3.57	120.59	124.48
17	C	301	7PH	O21-C21-C22	3.53	119.12	111.48
14	B	202	UMQ	O2'-C2'-C1'	3.51	118.44	110.08
11	B	204	OPC	OAN-CAO-CAP	3.49	119.04	111.48
14	B	202	UMQ	O2'-C2'-C3'	3.45	118.50	110.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	308	UMQ	O5'-C1'-C2'	-3.42	103.35	110.37
14	B	202	UMQ	O1-C4'-C3'	3.41	115.89	107.23
21	G	101	BCR	C33-C5-C4	3.35	120.73	113.60
15	B	201	TDS	OAO-CAN-CAM	3.26	122.73	116.28
10	C	302	HEM	CAD-C3D-C4D	3.19	130.25	124.70
15	B	201	TDS	OAB-CAE-CAF	3.13	120.28	115.84
21	G	101	BCR	C29-C30-C25	3.12	114.97	110.44
15	B	201	TDS	OAK-CAL-CAD	-3.07	118.79	124.08
21	G	101	BCR	C11-C10-C9	-3.05	123.00	127.28
10	A	304	HEM	CHD-C1D-ND	3.05	127.70	124.42
16	B	203	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
21	G	101	BCR	C4-C5-C6	-2.98	118.68	122.70
14	A	308	UMQ	C1'-C2'-C3'	2.96	116.24	110.01
21	G	101	BCR	C38-C26-C25	-2.95	121.27	124.48
11	B	204	OPC	OBJ-CBK-CBL	2.92	120.75	111.83
14	A	308	UMQ	O5'-C5'-C4'	2.89	115.70	109.72
10	A	304	HEM	CAD-C3D-C2D	-2.88	122.47	127.87
15	A	309	TDS	OAO-CAN-CAM	2.87	121.97	116.28
14	A	308	UMQ	C1-O5-C5	-2.86	108.13	113.72
21	G	101	BCR	C7-C8-C9	-2.82	122.06	126.23
14	B	202	UMQ	C3'-C4'-C5'	-2.81	104.71	110.93
14	A	308	UMQ	C1'-O5'-C5'	-2.80	108.25	113.72
18	D	201	SQD	C1-C2-C3	2.76	119.58	111.34
14	A	308	UMQ	O5-C1-C2	2.74	116.01	110.37
21	G	101	BCR	C38-C26-C27	2.73	119.41	113.60
11	B	204	OPC	OAN-CAO-OAD	-2.68	117.45	123.70
18	D	201	SQD	O48-C23-C24	2.67	119.99	111.83
15	A	309	TDS	OAB-CAE-CAD	-2.59	119.61	124.08
10	A	302	HEM	CBA-CAA-C2A	-2.59	105.38	112.53
10	A	302	HEM	CHD-C4C-NC	2.55	127.23	124.45
14	A	308	UMQ	C3-C4-C5	2.54	114.83	110.23
16	B	203	CLA	C3B-C4B-NB	-2.52	108.28	110.53
14	B	202	UMQ	C1-O5-C5	-2.52	108.80	113.72
21	G	101	BCR	C27-C26-C25	-2.50	119.33	122.70
15	B	201	TDS	OAB-CAE-CAD	-2.49	119.78	124.08
21	G	101	BCR	C34-C9-C10	-2.49	118.78	122.82
21	G	101	BCR	C1-C6-C5	-2.47	119.26	122.64
10	A	304	HEM	CHC-C1C-NC	2.46	127.13	124.45
10	C	302	HEM	C2A-C1A-NA	-2.45	107.43	110.15
11	A	305	OPC	OBJ-CBK-CBL	2.43	119.25	111.83
14	B	202	UMQ	C1'-O5'-C5'	-2.41	109.00	113.72
16	B	203	CLA	CAA-C2A-C1A	-2.40	104.10	111.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	203	CLA	C9-C8-C10	2.40	119.83	111.27
16	B	203	CLA	CHB-C4A-NA	2.39	127.85	124.40
14	B	202	UMQ	C6-C5-C4	-2.38	107.17	113.02
10	A	302	HEM	C2A-C1A-NA	-2.36	107.53	110.15
14	A	308	UMQ	O1'-C1'-C2'	2.33	111.82	108.27
10	A	304	HEM	C2A-C1A-NA	-2.28	107.63	110.15
21	G	101	BCR	C10-C11-C12	-2.27	116.62	123.20
21	G	101	BCR	C20-C19-C18	-2.26	120.17	126.36
16	B	203	CLA	O2D-CGD-CBD	2.25	115.17	111.23
11	B	204	OPC	CBI-CAM-CAL	2.25	117.03	111.78
10	A	304	HEM	CAC-C3C-C4C	2.25	130.19	124.82
18	D	201	SQD	O7-S-C6	2.24	110.10	106.76
17	C	301	7PH	O21-C21-O22	-2.23	118.50	123.70
17	C	301	7PH	O31-C31-C32	2.22	118.61	111.83
16	B	203	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
10	C	302	HEM	CHD-C1D-ND	2.17	126.75	124.42
14	A	308	UMQ	C3'-C4'-C5'	2.15	115.70	110.93
15	B	201	TDS	CAF-CAN-CAM	-2.13	118.55	121.44
10	A	302	HEM	CHA-C1A-NA	2.13	127.72	123.86
15	A	309	TDS	CAE-CAF-CAN	2.12	120.65	116.87
11	A	305	OPC	CBI-CAM-CAL	-2.12	106.85	111.78
10	A	302	HEM	CHC-C4B-NB	2.09	126.67	124.42
10	C	302	HEM	C1B-NB-C4B	2.07	107.66	105.21
10	C	302	HEM	C3B-C2B-C1B	2.06	107.96	106.41
21	G	101	BCR	C16-C15-C14	-2.06	119.30	123.52
14	A	308	UMQ	C6-C5-C4	2.05	118.05	113.02
10	A	303	HEM	C3B-C2B-C1B	2.05	107.95	106.41
15	B	201	TDS	CAE-CAF-CAN	2.04	120.50	116.87
15	B	201	TDS	CAI-CAH-CAG	2.04	120.43	116.68
10	A	302	HEM	CAD-C3D-C4D	2.03	128.24	124.70
10	C	302	HEM	CAD-C3D-C2D	-2.03	124.07	127.87

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
14	A	308	UMQ	C2'
14	A	308	UMQ	C5
14	A	308	UMQ	C1
14	B	202	UMQ	C2'
14	B	202	UMQ	C2
16	B	203	CLA	ND
18	D	201	SQD	C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
18	D	201	SQD	C4

All (194) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	304	HEM	C2D-C3D-CAD-CBD
10	A	304	HEM	C4D-C3D-CAD-CBD
11	A	305	OPC	CAL-OAK-PAJ-OBH
11	A	305	OPC	CAL-OAK-PAJ-OAB
11	A	305	OPC	CAL-OAK-PAJ-OAI
11	A	305	OPC	CAH-OAI-PAJ-OBH
11	B	204	OPC	CAH-OAI-PAJ-OAK
11	B	204	OPC	CAH-OAI-PAJ-OBH
11	B	204	OPC	NAF-CAG-CAH-OAI
14	A	308	UMQ	CB-CA-O1'-C1'
16	B	203	CLA	C1A-C2A-CAA-CBA
16	B	203	CLA	C3A-C2A-CAA-CBA
17	C	301	7PH	O11-C1-C2-C3
17	C	301	7PH	O11-C1-C2-O21
17	C	301	7PH	O22-C21-O21-C2
17	C	301	7PH	C22-C21-O21-C2
18	D	201	SQD	C2-C1-O6-C44
18	D	201	SQD	O5-C1-O6-C44
18	D	201	SQD	O47-C45-C46-O48
18	D	201	SQD	O5-C5-C6-S
18	D	201	SQD	C5-C6-S-O7
18	D	201	SQD	C5-C6-S-O8
18	D	201	SQD	C5-C6-S-O9
21	G	101	BCR	C1-C6-C7-C8
21	G	101	BCR	C5-C6-C7-C8
21	G	101	BCR	C11-C12-C13-C14
21	G	101	BCR	C17-C18-C19-C20
21	G	101	BCR	C36-C18-C19-C20
21	G	101	BCR	C20-C21-C22-C23
14	B	202	UMQ	C3'-C4'-O1-C1
14	B	202	UMQ	C2-C1-O1-C4'
14	A	308	UMQ	C4'-C5'-C6'-O6'
14	A	308	UMQ	O5'-C5'-C6'-O6'
15	B	201	TDS	CAM-CAL-OAK-CAJ
15	A	309	TDS	CAD-CAL-OAK-CAJ
11	A	305	OPC	CBL-CBK-OBJ-CBI
16	B	203	CLA	CBD-CGD-O2D-CED

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	D	201	SQD	C13-C14-C15-C16
15	B	201	TDS	CAF-CAE-OAB-CAA
16	B	203	CLA	C11-C10-C8-C9
14	B	202	UMQ	O5-C5-C6-O6
15	B	201	TDS	CAD-CAE-OAB-CAA
21	G	101	BCR	C7-C8-C9-C34
21	G	101	BCR	C11-C12-C13-C35
21	G	101	BCR	C21-C22-C23-C24
15	A	309	TDS	CAM-CAL-OAK-CAJ
18	D	201	SQD	C23-C24-C25-C26
14	A	308	UMQ	C4-C5-C6-O6
16	B	203	CLA	C6-C7-C8-C10
11	A	305	OPC	CAO-CAP-CAQ-CAR
15	B	201	TDS	CAD-CAL-OAK-CAJ
21	G	101	BCR	C18-C19-C20-C21
16	B	203	CLA	C10-C11-C12-C13
11	A	305	OPC	OCC-CBK-OBJ-CBI
11	A	305	OPC	CAH-CAG-NAF-CAE
11	A	305	OPC	CAH-CAG-NAF-CBG
11	A	305	OPC	CAH-CAG-NAF-CAA
11	B	204	OPC	CAP-CAO-OAN-CAM
10	A	303	HEM	C1A-C2A-CAA-CBA
21	G	101	BCR	C37-C22-C23-C24
16	B	203	CLA	C16-C17-C18-C20
21	G	101	BCR	C12-C13-C14-C15
14	A	308	UMQ	CF-CG-CH-CI
17	C	301	7PH	C36-C37-C38-C39
18	D	201	SQD	C11-C12-C13-C14
18	D	201	SQD	C14-C15-C16-C17
11	A	305	OPC	CBN-CBO-CBP-CBQ
18	D	201	SQD	C24-C25-C26-C27
14	B	202	UMQ	CD-CF-CG-CH
16	B	203	CLA	C16-C17-C18-C19
11	B	204	OPC	CBT-CBU-CBV-CBW
11	A	305	OPC	CBV-CBW-CBX-CBY
12	A	306	MYS	C4-C5-C6-C7
15	B	201	TDS	CAU-CAV-CAW-CAX
18	D	201	SQD	C10-C11-C12-C13
14	A	308	UMQ	CG-CH-CI-CJ
16	B	203	CLA	O1D-CGD-O2D-CED
15	A	309	TDS	CAR-CAS-CAT-CAU
17	C	301	7PH	C29-C2A-C2B-C2C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
18	D	201	SQD	C27-C28-C29-C30
18	D	201	SQD	C16-C17-C18-C19
18	D	201	SQD	C34-C35-C36-C37
16	B	203	CLA	C15-C16-C17-C18
11	B	204	OPC	CAY-CAZ-CBA-CBB
15	A	309	TDS	CAT-CAU-CAV-CAW
16	B	203	CLA	C4-C3-C5-C6
14	B	202	UMQ	CF-CG-CH-CI
18	D	201	SQD	C31-C32-C33-C34
17	C	301	7PH	C32-C31-O31-C3
11	B	204	OPC	CAQ-CAR-CAS-CAT
11	A	305	OPC	CAZ-CBA-CBB-CBC
11	A	305	OPC	CAY-CAZ-CBA-CBB
15	B	201	TDS	CAQ-CAR-CAS-CAT
18	D	201	SQD	C29-C30-C31-C32
14	B	202	UMQ	CG-CH-CI-CJ
18	D	201	SQD	C7-C8-C9-C10
14	B	202	UMQ	CC-CD-CF-CG
11	A	305	OPC	CBS-CBT-CBU-CBV
14	B	202	UMQ	O5'-C5'-C6'-O6'
16	B	203	CLA	C2-C3-C5-C6
11	A	305	OPC	CAP-CAQ-CAR-CAS
17	C	301	7PH	C21-C22-C23-C24
11	B	204	OPC	CAP-CAQ-CAR-CAS
13	A	307	8K6	C5-C6-C7-C8
11	B	204	OPC	CAS-CAT-CAU-CAV
11	B	204	OPC	CBM-CBN-CBO-CBP
11	A	305	OPC	CBK-CBL-CBM-CBN
11	B	204	OPC	CBN-CBO-CBP-CBQ
10	C	302	HEM	C4D-C3D-CAD-CBD
18	D	201	SQD	C44-C45-C46-O48
15	B	201	TDS	CAY-CAZ-CBA-CBB
21	G	101	BCR	C11-C10-C9-C34
16	B	203	CLA	O2A-C1-C2-C3
12	A	306	MYS	C6-C7-C8-C9
13	A	307	8K6	C14-C15-C16-C17
11	B	204	OPC	CAR-CAS-CAT-CAU
11	B	204	OPC	CBU-CBV-CBW-CBX
16	B	203	CLA	CBA-CGA-O2A-C1
10	A	302	HEM	C3D-CAD-CBD-CGD
11	A	305	OPC	CBC-CBD-CBE-CBF
18	D	201	SQD	C9-C10-C11-C12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
21	G	101	BCR	C19-C20-C21-C22
18	D	201	SQD	O10-C23-O48-C46
14	B	202	UMQ	CI-CJ-CK-CL
17	C	301	7PH	C1-C2-C3-O31
15	B	201	TDS	CAW-CAX-CAY-CAZ
10	C	302	HEM	C2D-C3D-CAD-CBD
11	A	305	OPC	CBX-CBY-CBZ-CCA
16	B	203	CLA	O1A-CGA-O2A-C1
18	D	201	SQD	C18-C19-C20-C21
18	D	201	SQD	C28-C29-C30-C31
11	A	305	OPC	CAW-CAX-CAY-CAZ
11	B	204	OPC	CAW-CAX-CAY-CAZ
16	B	203	CLA	C5-C6-C7-C8
11	A	305	OPC	CBW-CBX-CBY-CBZ
13	A	307	8K6	C1-C2-C3-C4
21	G	101	BCR	C16-C17-C18-C19
10	A	304	HEM	C4C-C3C-CAC-CBC
15	B	201	TDS	CAX-CAY-CAZ-CBA
11	A	305	OPC	NAF-CAG-CAH-OAI
18	D	201	SQD	C35-C36-C37-C38
13	A	307	8K6	C12-C13-C14-C15
11	B	204	OPC	OAN-CAO-CAP-CAQ
16	B	203	CLA	C12-C13-C15-C16
14	B	202	UMQ	CB-CC-CD-CF
14	B	202	UMQ	O5-C1-O1-C4'
17	C	301	7PH	O21-C2-C3-O31
11	A	305	OPC	CBM-CBN-CBO-CBP
11	A	305	OPC	CAH-OAI-PAJ-OAK
11	A	305	OPC	CAH-OAI-PAJ-OAB
11	B	204	OPC	CAL-OAK-PAJ-OAB
11	B	204	OPC	CAH-OAI-PAJ-OAB
21	G	101	BCR	C9-C10-C11-C12
11	A	305	OPC	CBT-CBU-CBV-CBW
14	B	202	UMQ	C4'-C5'-C6'-O6'
10	A	303	HEM	C2D-C3D-CAD-CBD
10	A	303	HEM	C3A-C2A-CAA-CBA
11	A	305	OPC	CAQ-CAR-CAS-CAT
15	A	309	TDS	CAU-CAV-CAW-CAX
15	A	309	TDS	CAX-CAY-CAZ-CBA
11	B	204	OPC	CBB-CBC-CBD-CBE
15	B	201	TDS	CAV-CAW-CAX-CAY
10	C	302	HEM	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
13	A	307	8K6	C13-C14-C15-C16
10	C	302	HEM	CAD-CBD-CGD-O2D
21	G	101	BCR	C11-C10-C9-C8
15	A	309	TDS	CAV-CAW-CAX-CAY
16	B	203	CLA	C8-C10-C11-C12
11	A	305	OPC	CAM-CAL-OAK-PAJ
12	A	306	MYS	C5-C6-C7-C8
17	C	301	7PH	C35-C36-C37-C38
10	A	303	HEM	C4D-C3D-CAD-CBD
10	A	302	HEM	CAA-CBA-CGA-O2A
18	D	201	SQD	O47-C7-C8-C9
10	A	302	HEM	CAA-CBA-CGA-O1A
11	A	305	OPC	OAN-CAO-CAP-CAQ
16	B	203	CLA	C14-C13-C15-C16
17	C	301	7PH	C31-C32-C33-C34
21	G	101	BCR	C10-C11-C12-C13
15	B	201	TDS	OAO-CAP-CAQ-CAR
10	C	302	HEM	C3D-CAD-CBD-CGD
15	B	201	TDS	CAH-CAP-CAQ-CAR
10	A	304	HEM	C3D-CAD-CBD-CGD
17	C	301	7PH	C27-C28-C29-C2A
11	A	305	OPC	CBL-CBM-CBN-CBO
18	D	201	SQD	C25-C26-C27-C28
10	C	302	HEM	CAA-CBA-CGA-O2A
10	A	302	HEM	CAD-CBD-CGD-O1D
10	A	303	HEM	CAD-CBD-CGD-O2D
10	A	304	HEM	CAD-CBD-CGD-O2D
16	B	203	CLA	C2-C1-O2A-CGA
10	C	302	HEM	CAA-CBA-CGA-O1A
11	A	305	OPC	CBP-CBQ-CBR-CBS
10	A	304	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

15 monomers are involved in 69 short contacts:

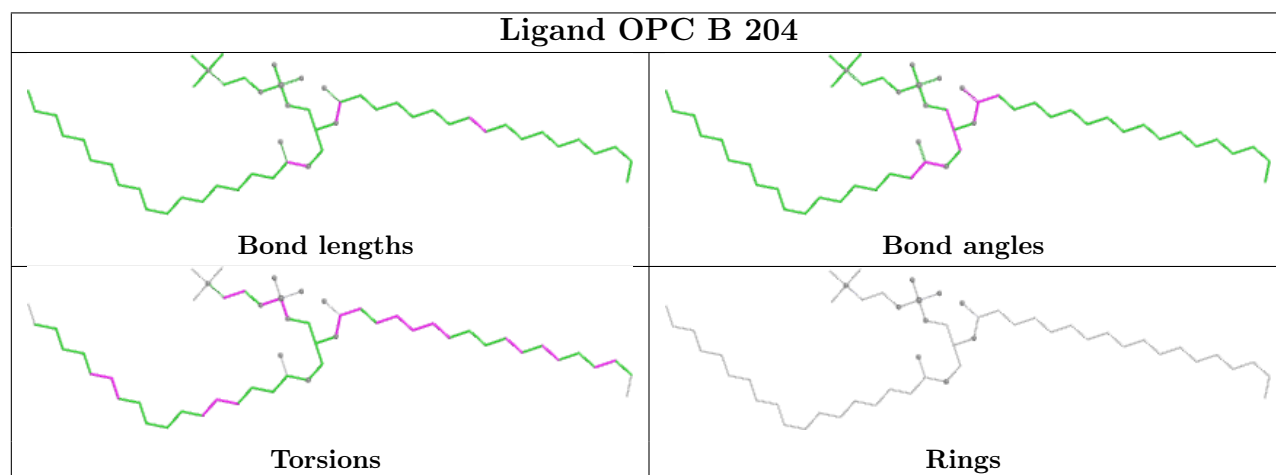
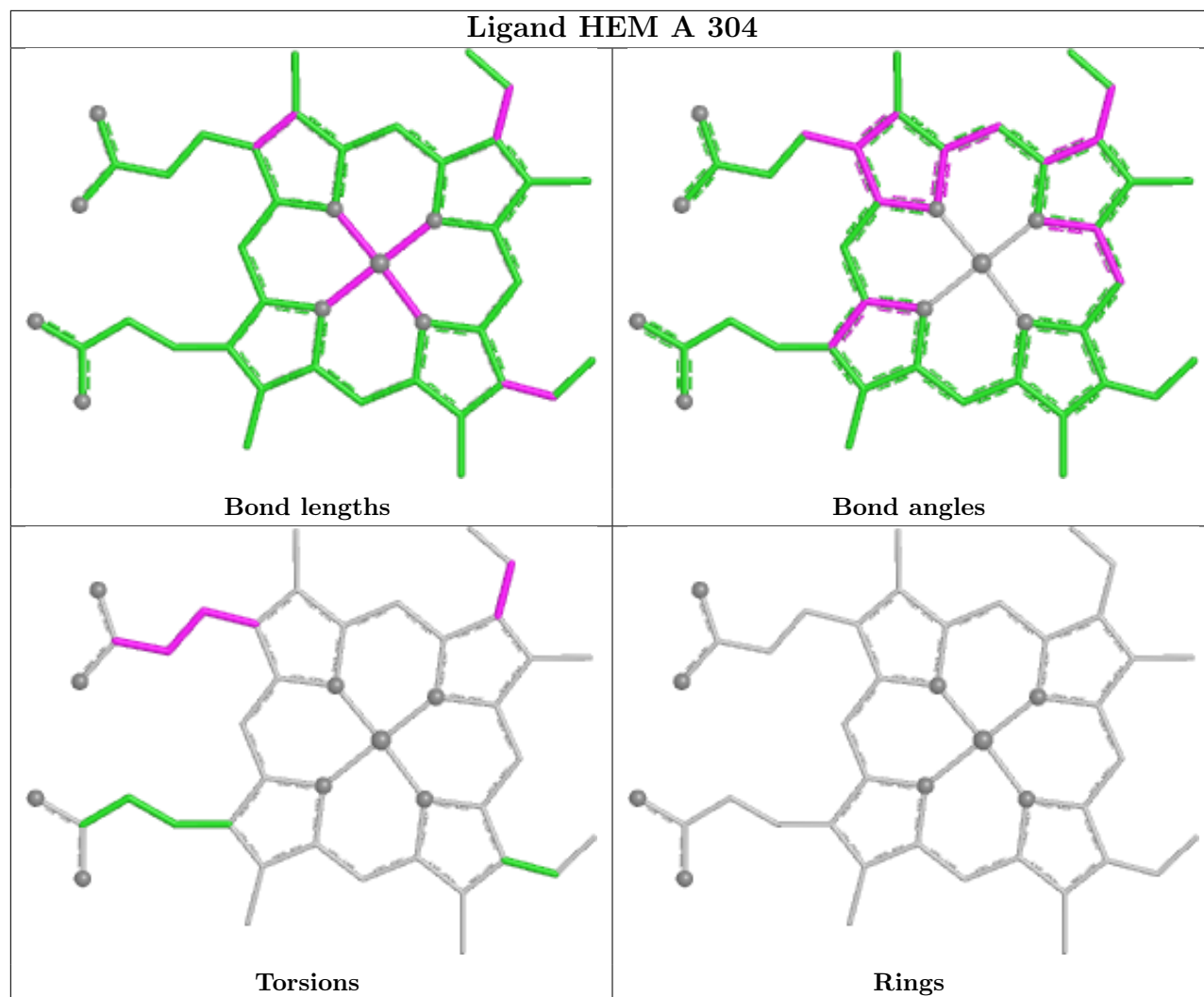
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	304	HEM	10	0
11	B	204	OPC	1	0
21	G	101	BCR	7	0
11	A	305	OPC	5	0
19	D	202	FES	1	0
12	A	306	MYS	5	0

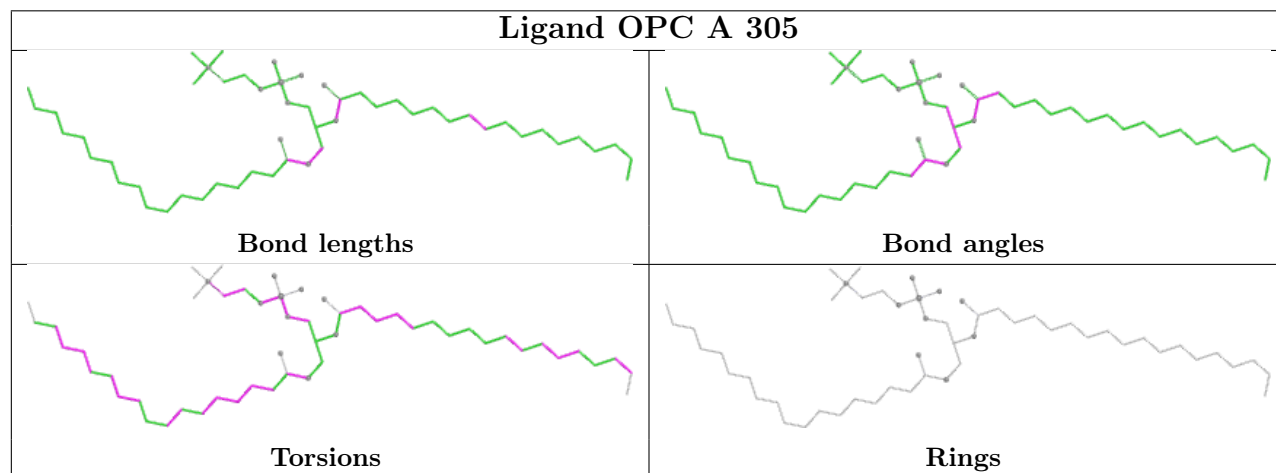
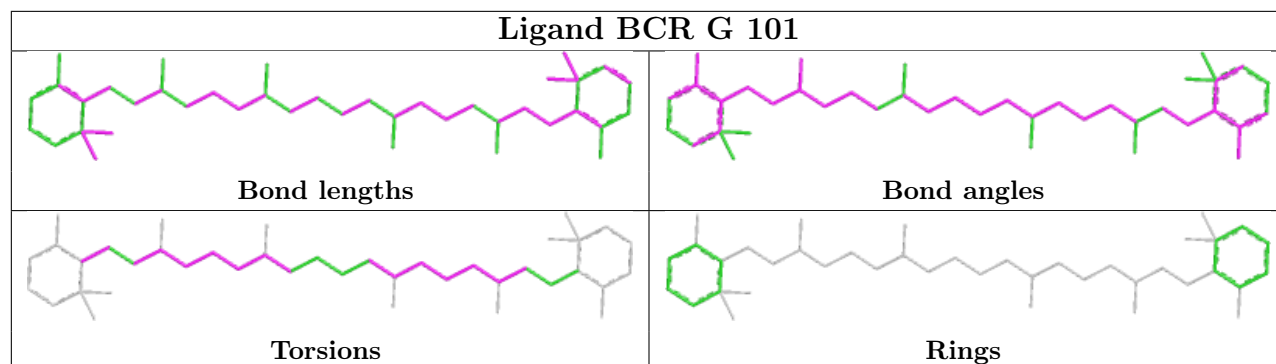
Continued on next page...

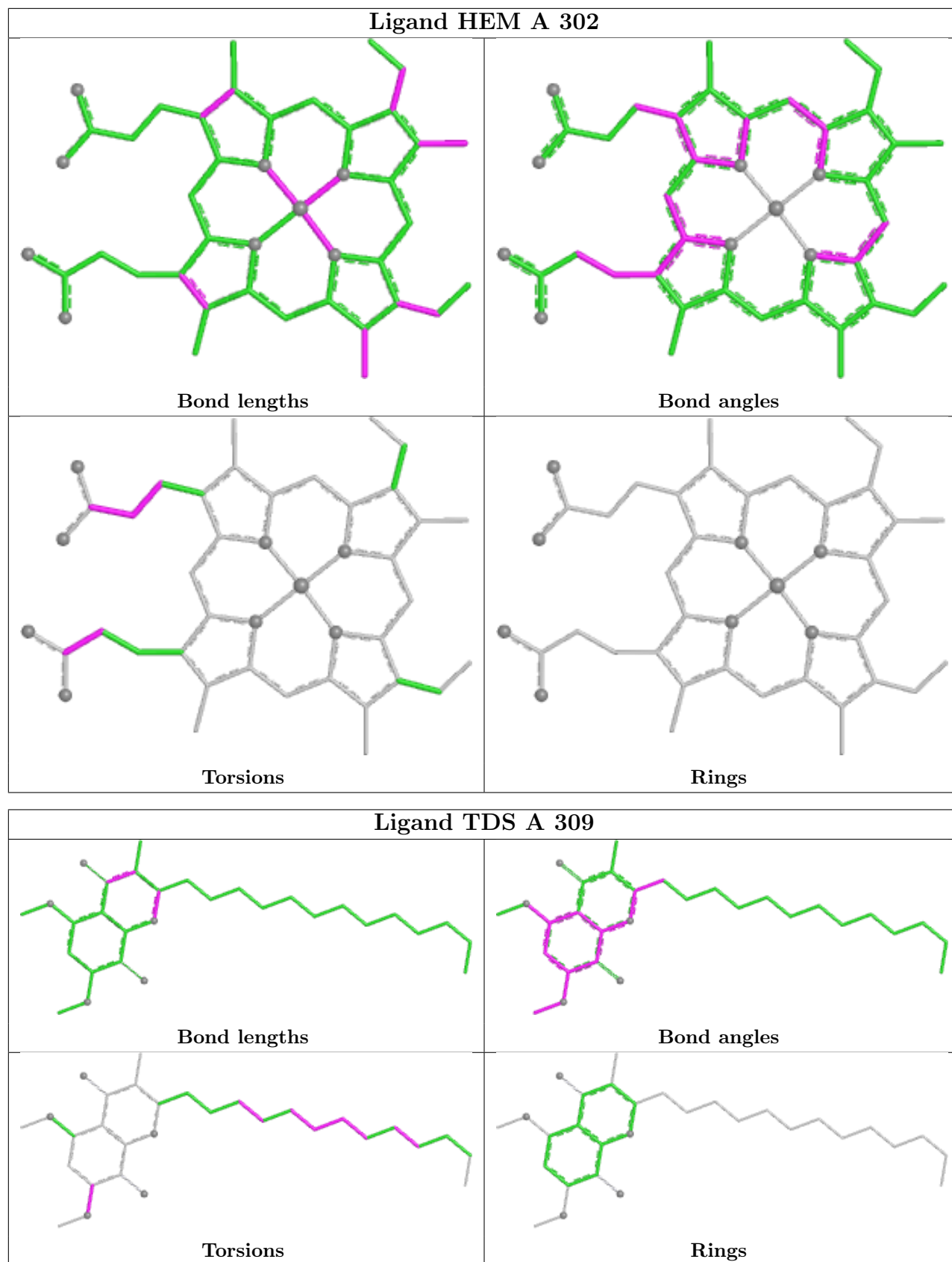
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	302	HEM	7	0
15	A	309	TDS	5	0
15	B	201	TDS	4	0
17	C	301	7PH	1	0
10	C	302	HEM	10	0
18	D	201	SQD	3	0
14	B	202	UMQ	1	0
10	A	303	HEM	6	0
16	B	203	CLA	5	0

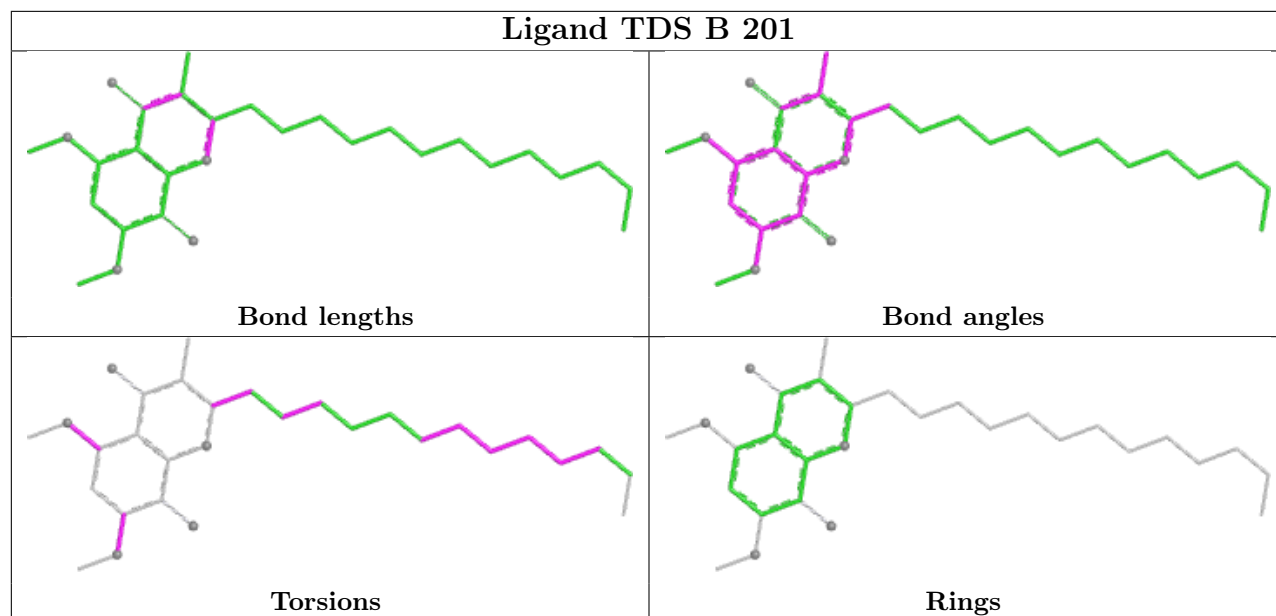
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



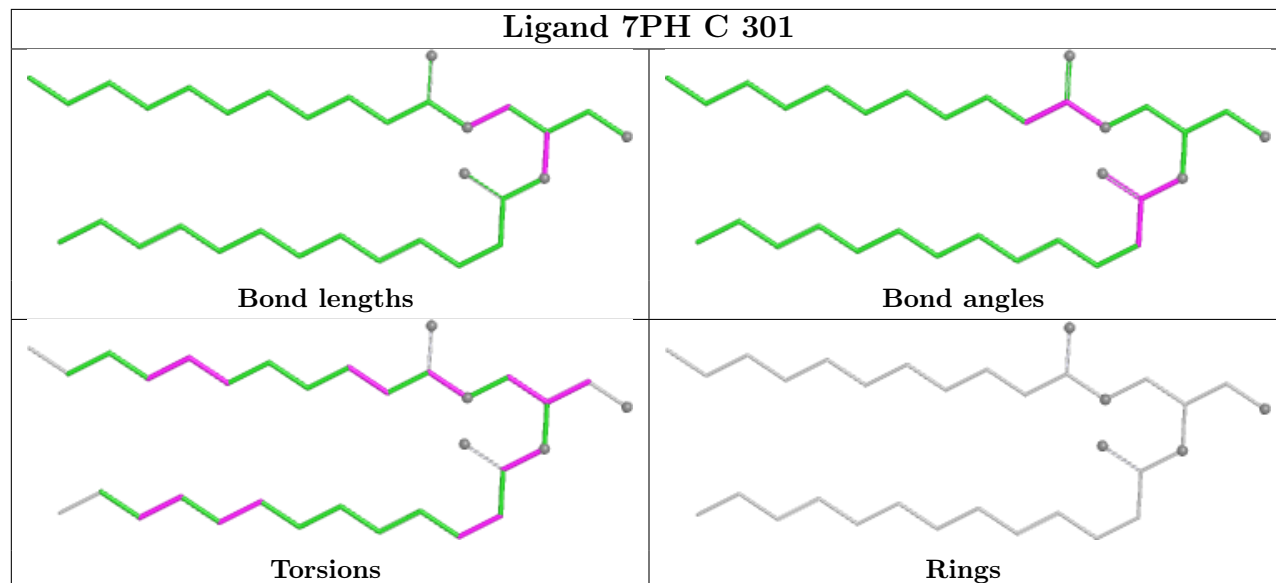


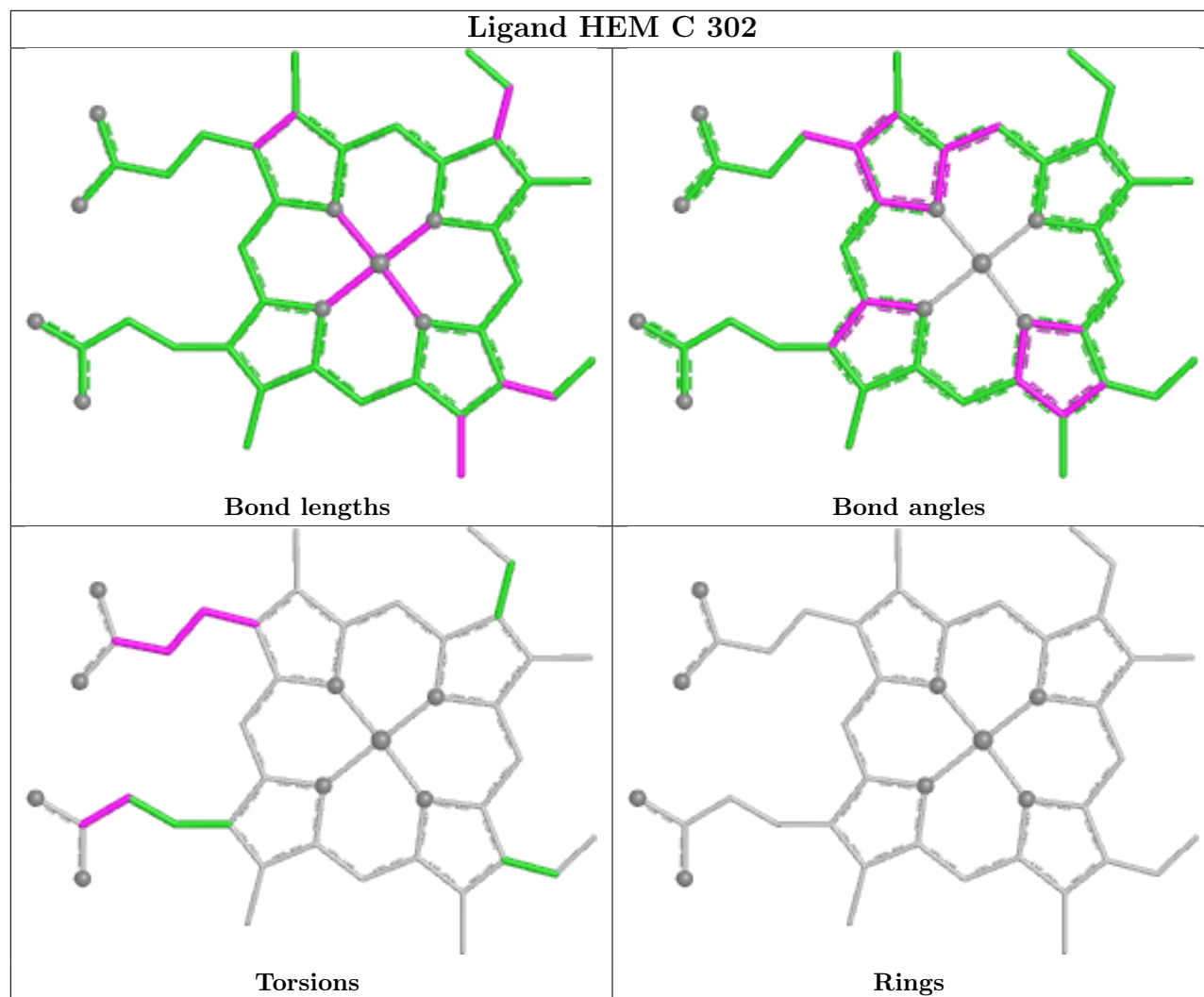


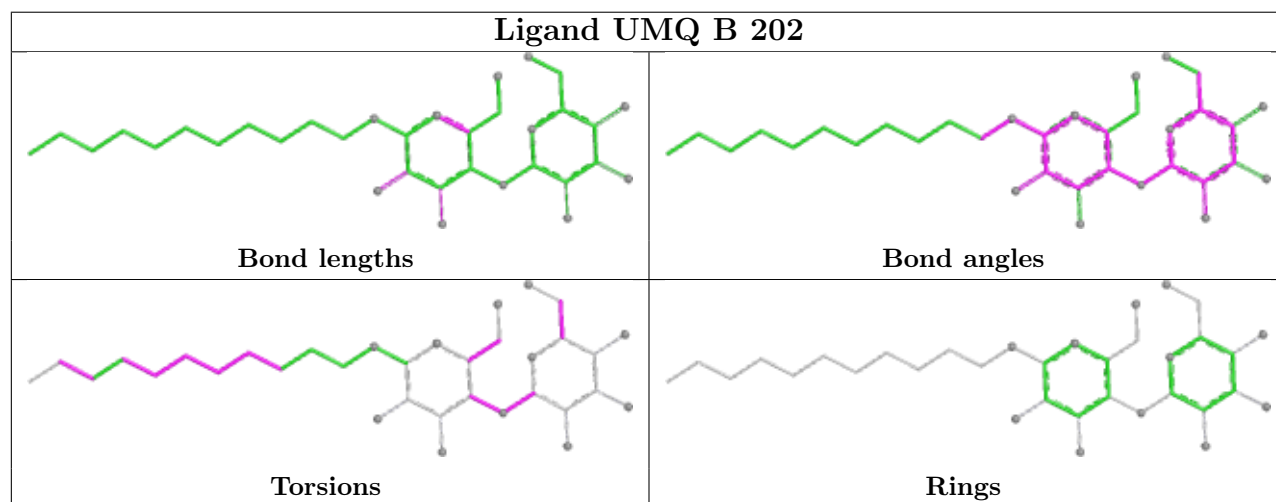
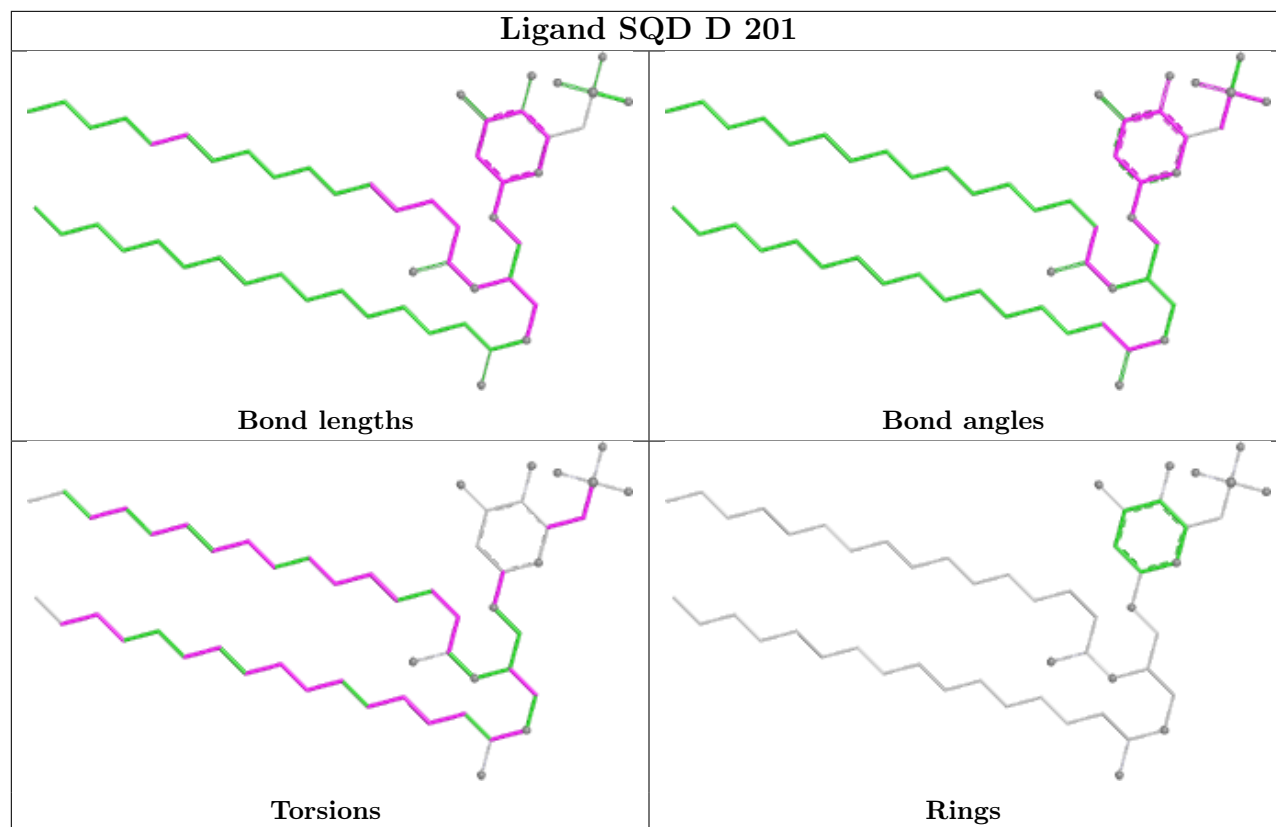
Ligand TDS B 201

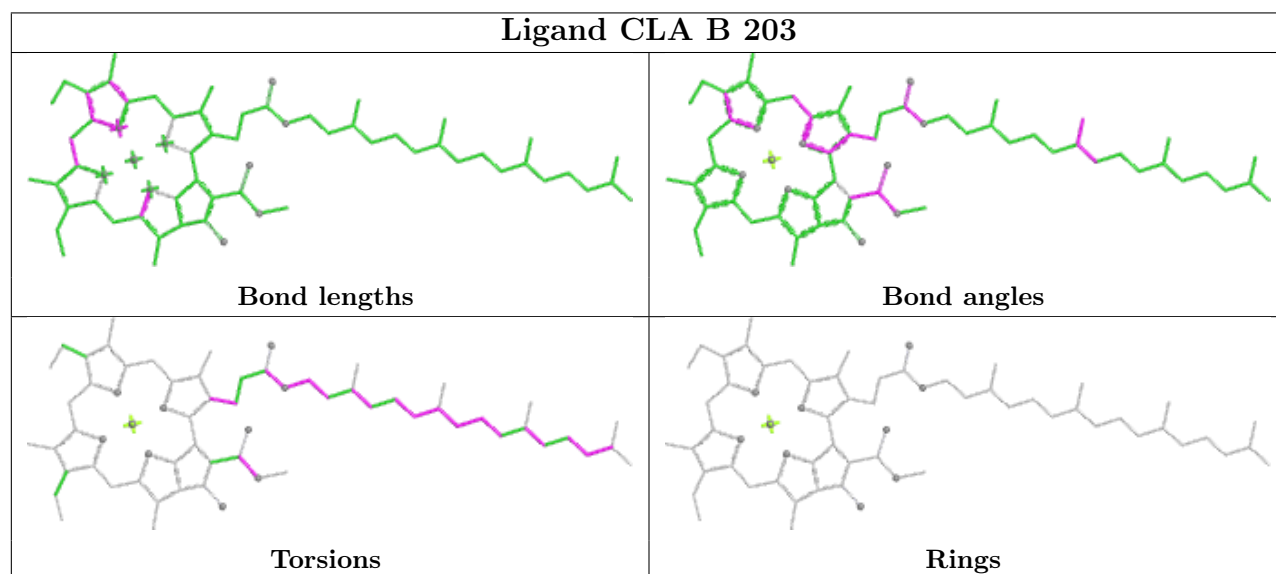
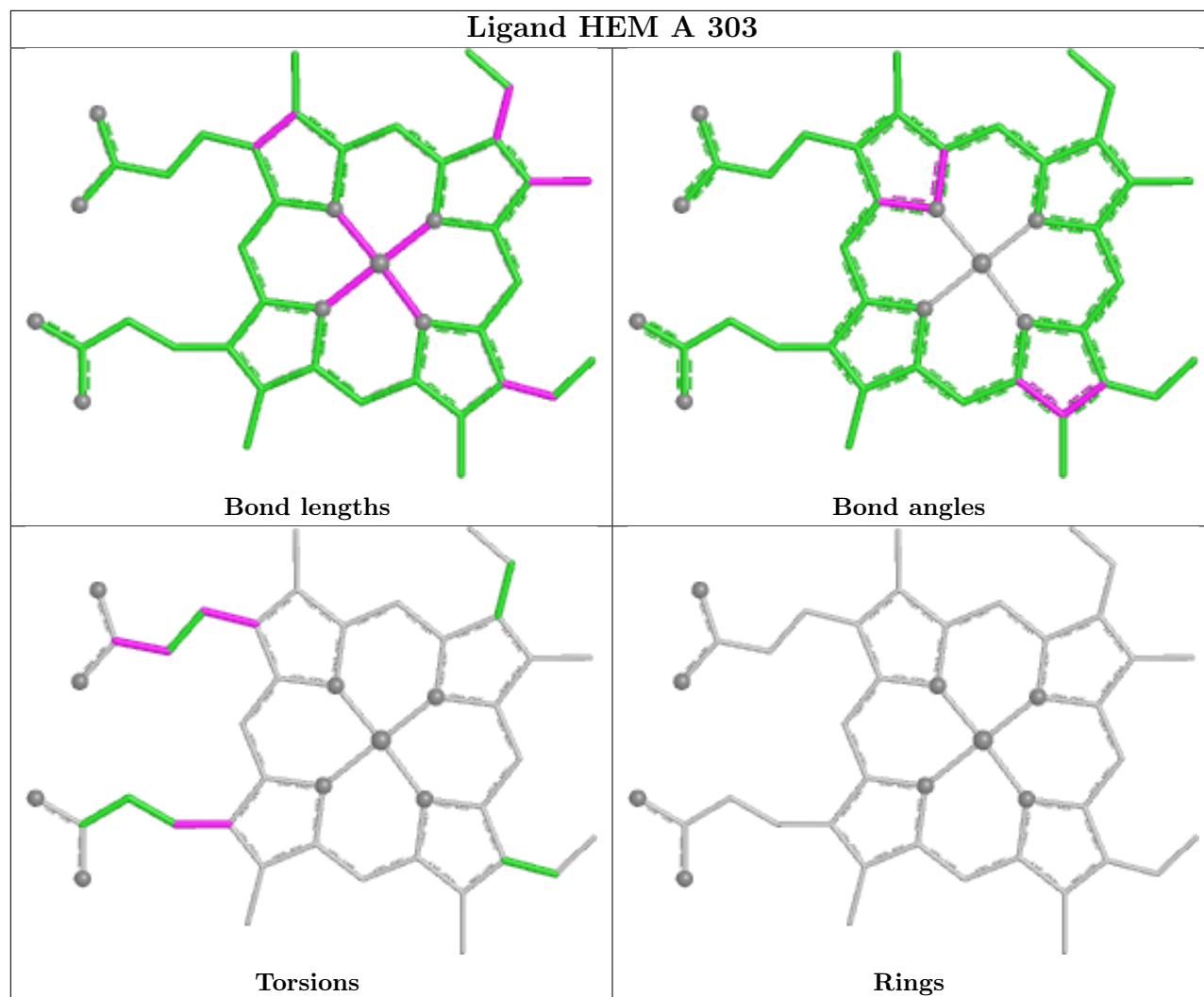


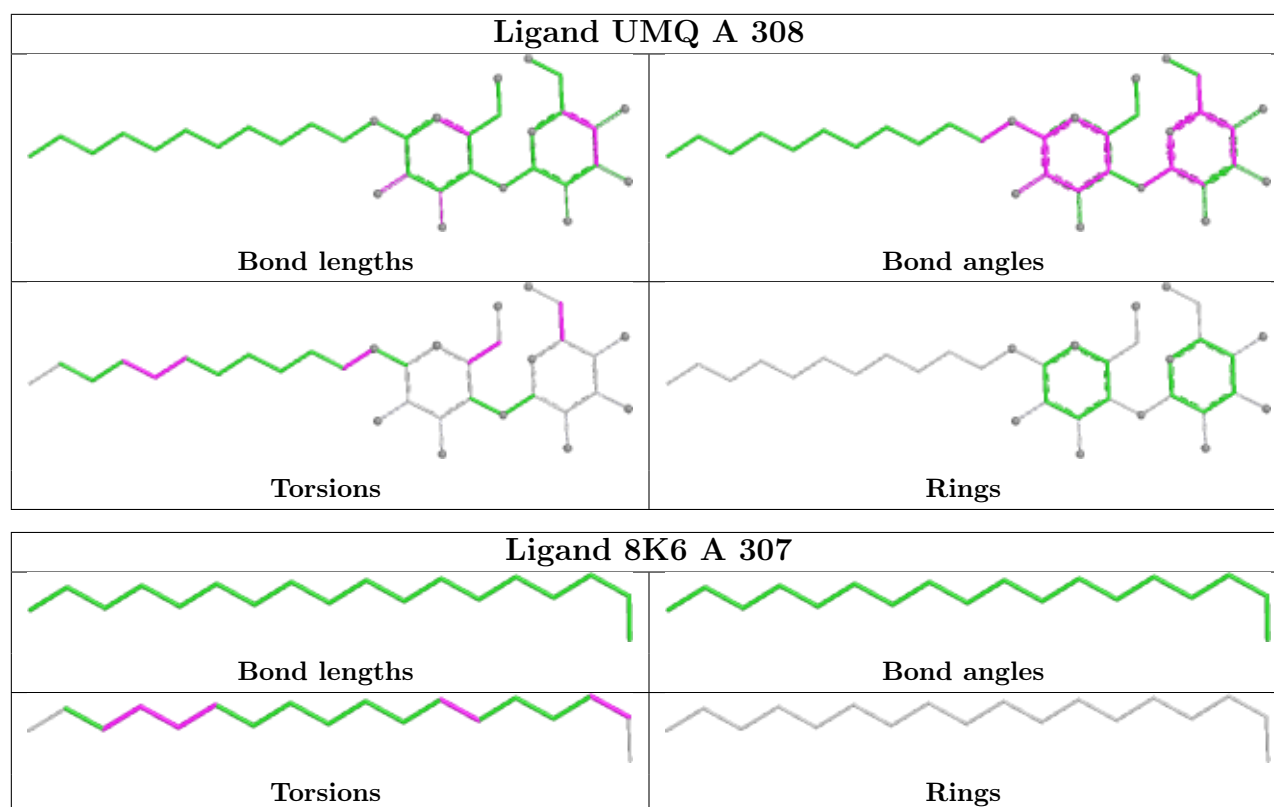
Ligand 7PH C 301











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%)	-0.29	4 (1%) 66 44	51, 75, 117, 241	0
2	B	160/160 (100%)	0.11	4 (2%) 58 36	65, 99, 147, 207	0
3	C	288/289 (99%)	0.58	29 (10%) 12 6	71, 110, 246, 277	1 (0%)
4	D	168/179 (93%)	0.87	15 (8%) 15 8	67, 151, 227, 256	0
5	E	32/32 (100%)	0.40	2 (6%) 26 13	92, 115, 152, 173	0
6	F	31/35 (88%)	0.61	4 (12%) 7 4	82, 104, 159, 177	0
7	G	37/37 (100%)	0.46	3 (8%) 18 10	75, 96, 197, 223	0
8	H	29/29 (100%)	-0.01	1 (3%) 48 27	81, 94, 122, 160	0
All	All	960/976 (98%)	0.33	62 (6%) 25 13	51, 102, 218, 277	1 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	5.7
4	D	70	LEU	4.9
3	C	218	ILE	4.1
3	C	192	ASN	3.6
1	A	1	MET	3.6
6	F	3	GLU	3.5
7	G	1	MET	3.5
4	D	179	VAL	3.4
6	F	32	ALA	3.4
3	C	207	VAL	3.3
4	D	99	ILE	3.3
3	C	193	VAL	3.3
3	C	225	VAL	3.3
4	D	50	VAL	3.3
3	C	202	ASP	3.3
4	D	94	GLU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	201	THR	3.2
2	B	117	VAL	3.1
4	D	95	SER	3.1
3	C	187	GLU	3.1
6	F	4	GLU	3.0
3	C	1	TYR	3.0
5	E	28	SER	3.0
3	C	181	THR	2.8
3	C	217	LEU	2.8
4	D	135	GLU	2.8
2	B	40	PHE	2.7
4	D	77	ASP	2.7
3	C	98	VAL	2.7
3	C	198	SER	2.7
1	A	112	LYS	2.6
3	C	57	LYS	2.6
2	B	149	PHE	2.5
4	D	166	THR	2.5
3	C	206	THR	2.5
3	C	191	GLY	2.5
3	C	88	GLU	2.4
3	C	199	ILE	2.4
3	C	227	ALA	2.4
5	E	29	ILE	2.3
3	C	96	LYS	2.3
3	C	219	VAL	2.3
4	D	131	SER	2.3
3	C	246	GLU	2.3
2	B	92	PRO	2.3
7	G	32	PRO	2.2
7	G	29	TYR	2.2
3	C	186	GLU	2.2
3	C	287	MET	2.2
6	F	7	TYR	2.2
3	C	92	GLU	2.2
8	H	1	MET	2.2
3	C	176	ALA	2.2
3	C	203	SER	2.1
4	D	160	ILE	2.1
4	D	54	THR	2.1
3	C	230	ALA	2.1
4	D	164	PRO	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	119	ALA	2.1
1	A	173	SER	2.0
4	D	157	ASP	2.0
3	C	222	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

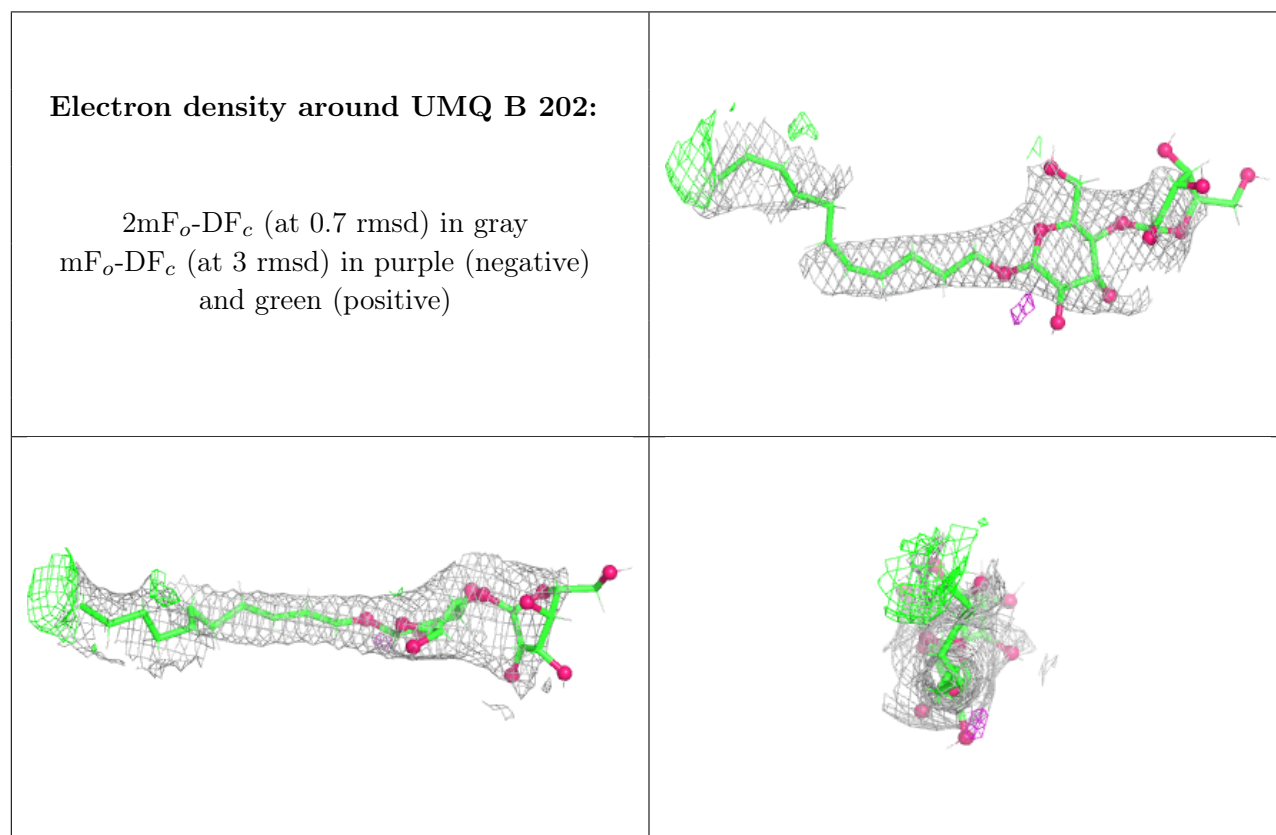
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

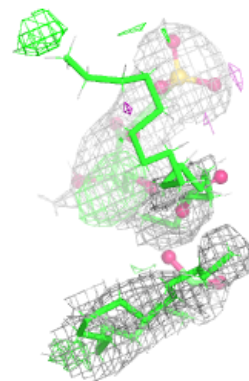
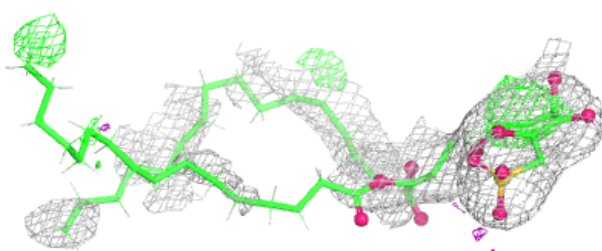
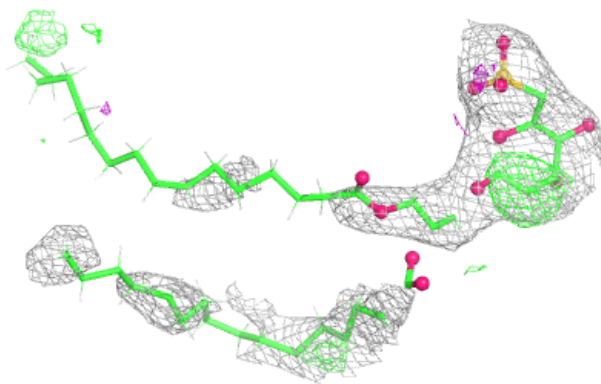
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	OCT	F	101	8/8	0.68	0.24	98,124,131,132	0
14	UMQ	B	202	34/34	0.73	0.18	104,171,232,247	0
18	SQD	D	201	53/54	0.83	0.21	0,163,195,201	1
14	UMQ	A	308	34/34	0.85	0.14	108,160,202,212	0
17	7PH	C	301	32/38	0.85	0.22	73,108,165,198	0
12	MYS	A	306	15/15	0.86	0.22	72,101,126,129	0
15	TDS	A	309	30/30	0.88	0.17	90,119,165,167	0
13	8K6	A	307	18/18	0.88	0.25	83,115,138,142	0
21	BCR	G	101	40/40	0.88	0.22	61,105,223,230	0
11	OPC	B	204	54/55	0.89	0.19	91,133,171,184	0
11	OPC	A	305	54/55	0.90	0.19	77,127,224,237	0
15	TDS	B	201	30/30	0.93	0.13	73,115,141,159	0
16	CLA	B	203	65/65	0.95	0.13	73,104,147,157	0
10	HEM	C	302	43/43	0.97	0.14	71,95,139,149	0
10	HEM	A	304	43/43	0.97	0.10	61,90,109,123	0
10	HEM	A	303	43/43	0.98	0.10	49,68,84,87	0
10	HEM	A	302	43/43	0.98	0.10	44,66,93,112	0
19	FES	D	202	4/4	0.99	0.04	80,95,101,103	0
9	CD	A	301	1/1	1.00	0.01	97,97,97,97	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.

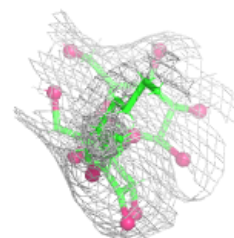
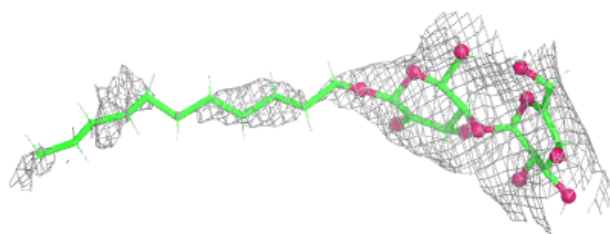
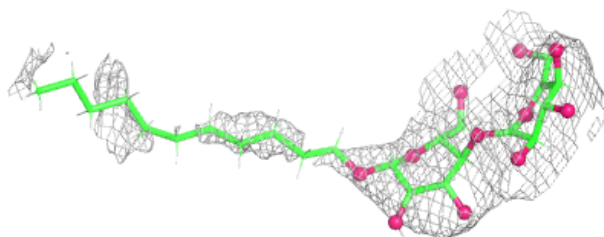


Electron density around SQD D 201:

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

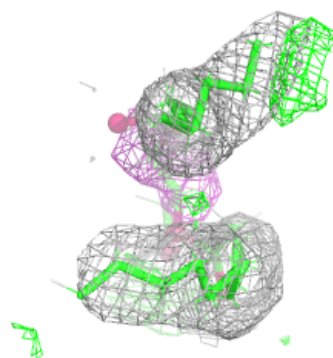
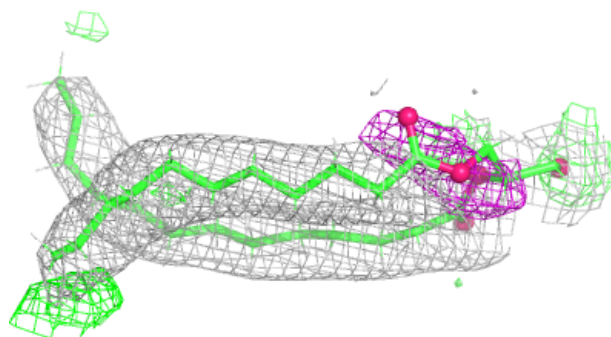
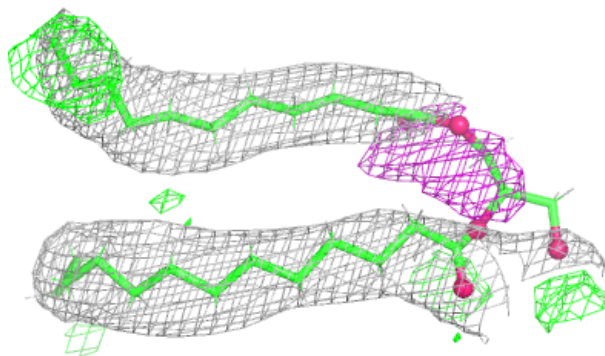
**Electron density around UMQ A 308:**

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

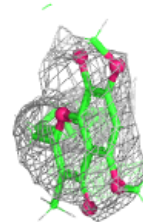
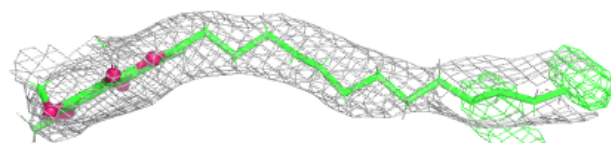
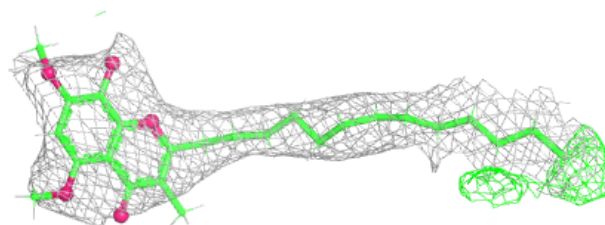


Electron density around 7PH C 301:

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

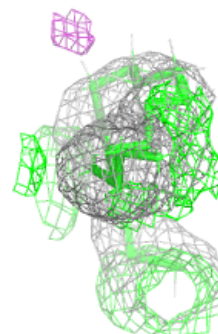
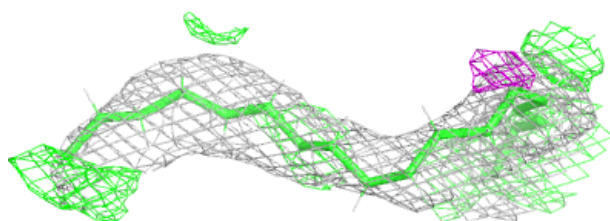
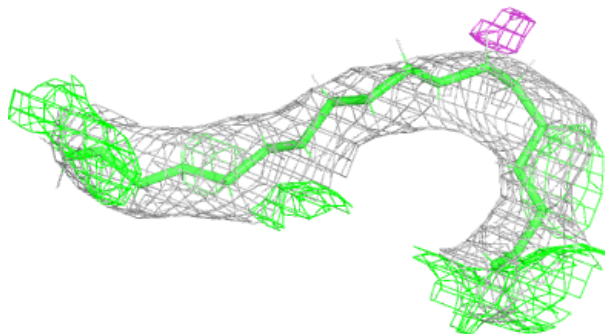
**Electron density around TDS A 309:**

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

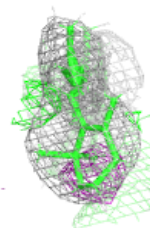
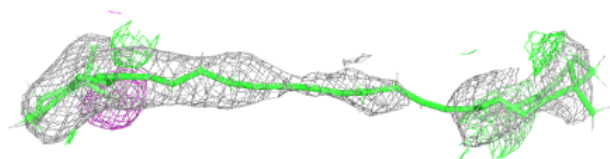
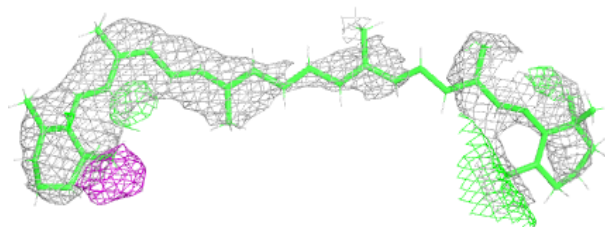


Electron density around 8K6 A 307:

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

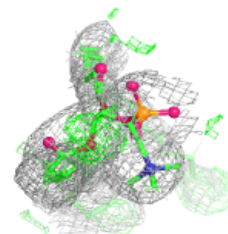
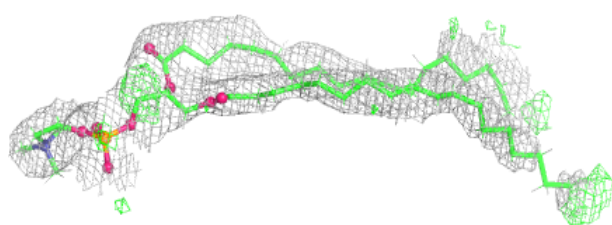
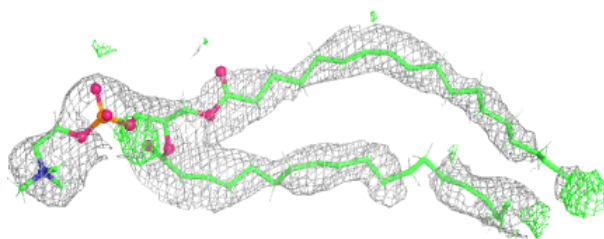
**Electron density around BCR G 101:**

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

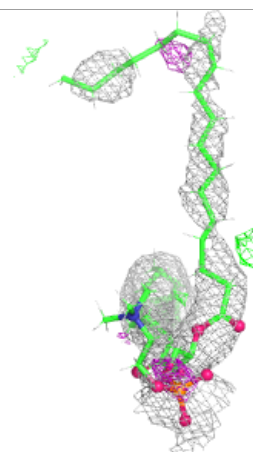
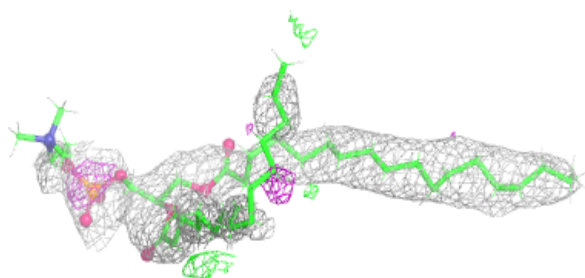
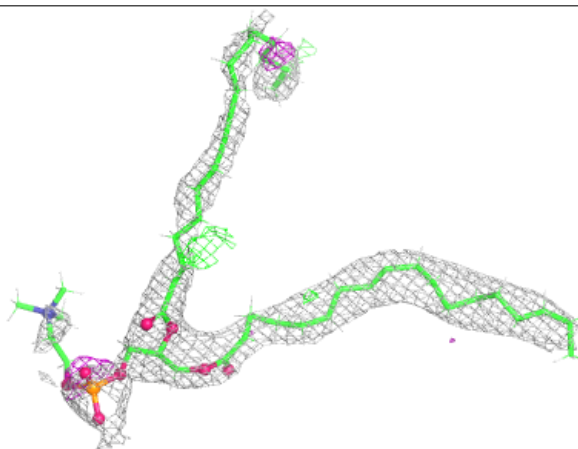


Electron density around OPC B 204:

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

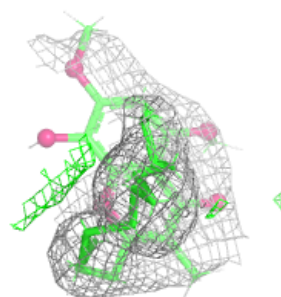
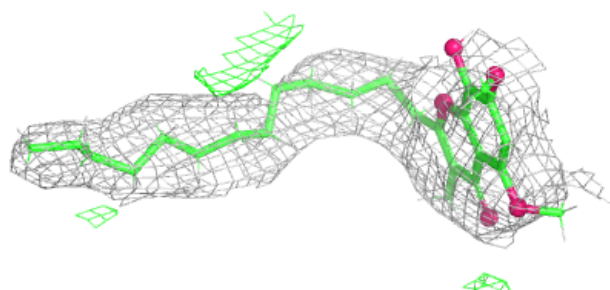
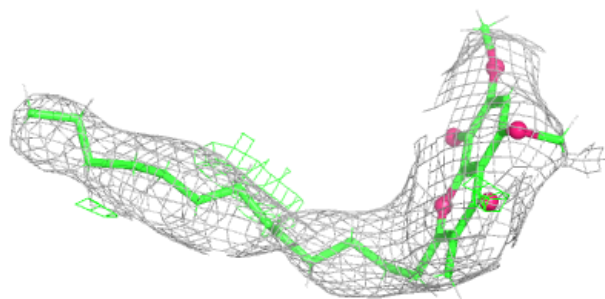
**Electron density around OPC A 305:**

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

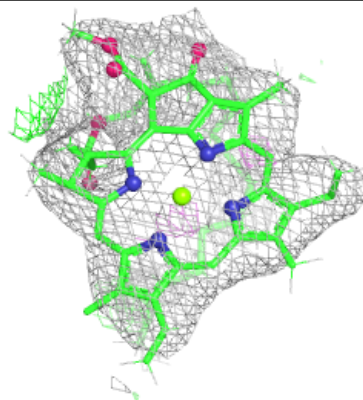
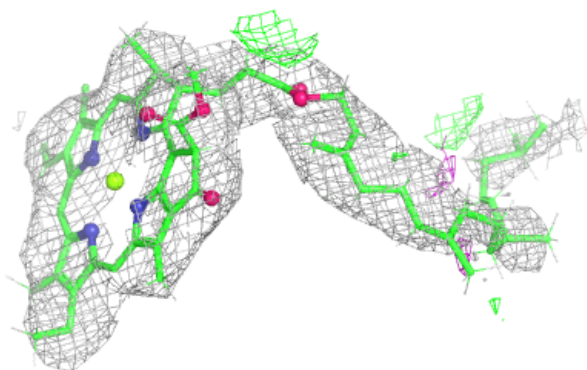
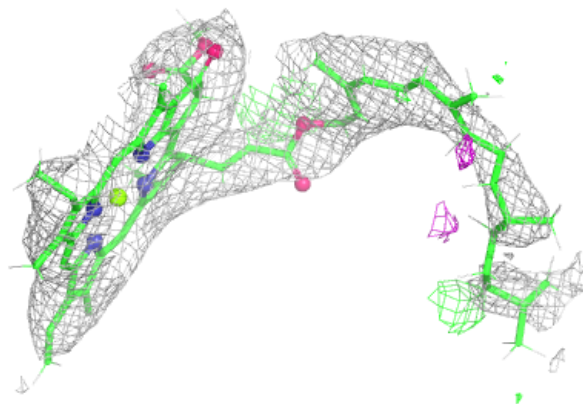


Electron density around TDS B 201:

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

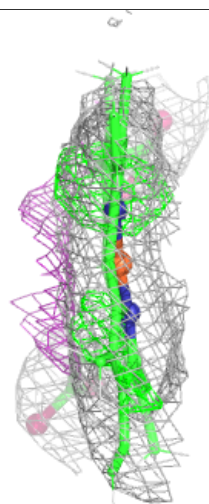
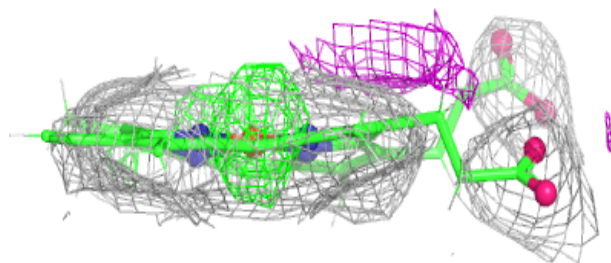
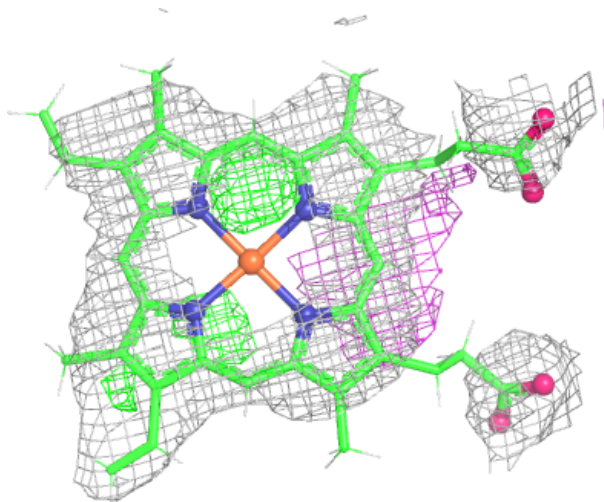
**Electron density around CLA B 203:**

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



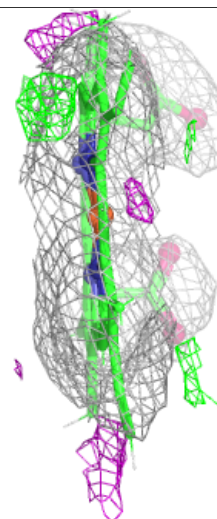
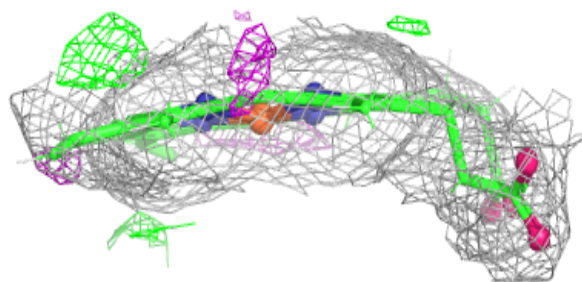
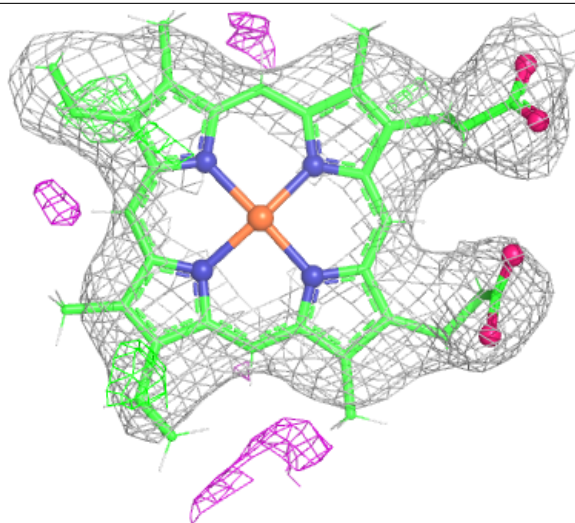
Electron density around HEM C 302:

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



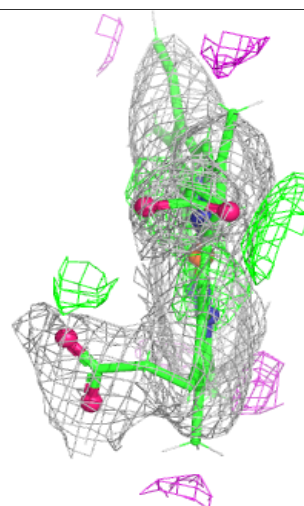
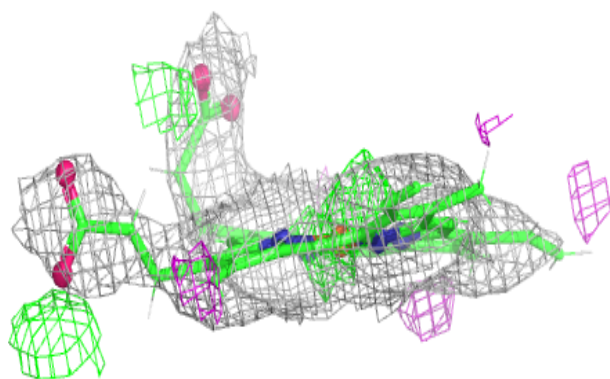
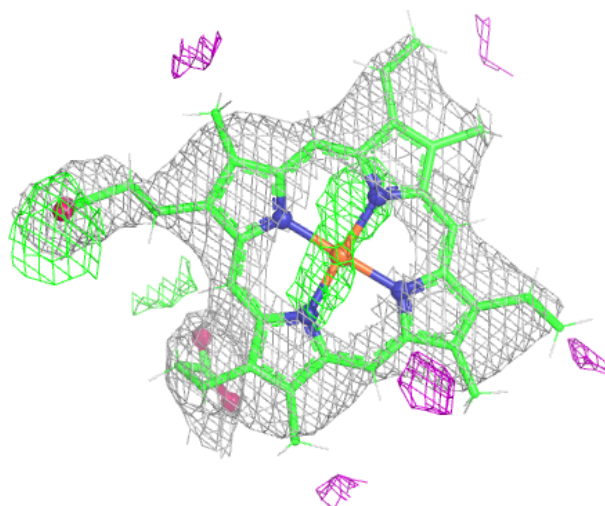
Electron density around HEM A 304:

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



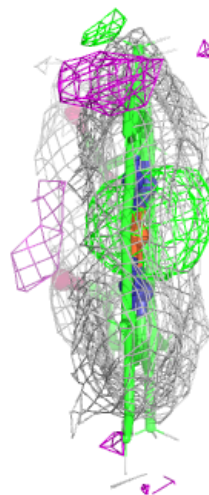
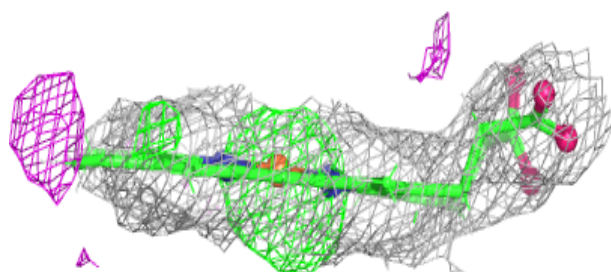
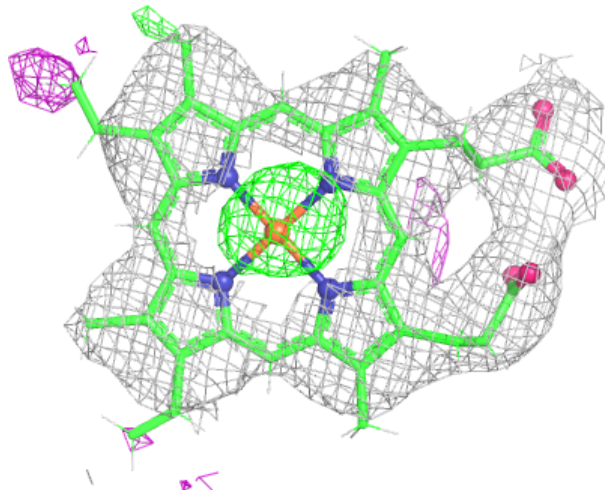
Electron density around HEM A 303:

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.