



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 08:52 PM EDT

PDB ID : 2E74 / pdb_00002e74
Title : Crystal Structure of the Cytochrome b6f Complex from M.laminosus
Authors : Cramer, W.A.; Yamashita, E.; Zhang, H.
Deposited on : 2007-01-05
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

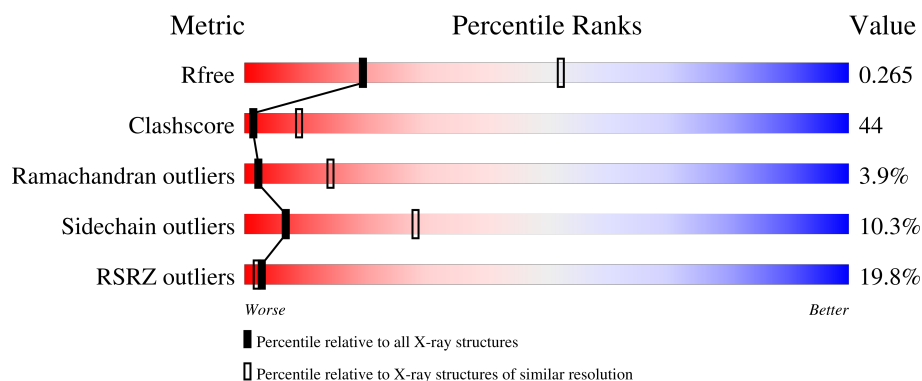
1 Overall quality at a glance

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	6% 56% 34% 9%
2	B	160	40% 48% 11%
3	C	289	30% 42% 47% 11%
4	D	179	48% 37% 49% 6% 7%
5	E	32	6% 38% 53% 9%

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	HEC	A	303	X	-	-	-
11	HEC	C	301	X	-	-	-
12	UMQ	A	1101	X	-	-	-
12	UMQ	A	1102	X	-	-	-
12	UMQ	A	1103	X	-	-	-
12	UMQ	A	1104	X	-	-	-
13	CLA	B	201	X	-	-	-
14	OPC	H	1002	-	-	X	-
15	FES	D	200	-	-	X	-
16	SQD	D	201	X	-	-	-

2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 8025 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
			1711	1140	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
			1249	841	193	209	6			

- Molecule 3 is a protein called Apocytochrome f.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	288	Total	C	N	O	S	0	0	0
			2216	1415	369	424	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	166	Total	C	N	O	S	0	0	0
			1260	805	218	230	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	N	O	S	0	0	0
			248	179	34	34	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	32	Total	C	N	O	S	0	0	0
			242	165	35	40	2			

- | Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 7 | G | 37 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 283 | 188 | 44 | 50 | 1 | | | |

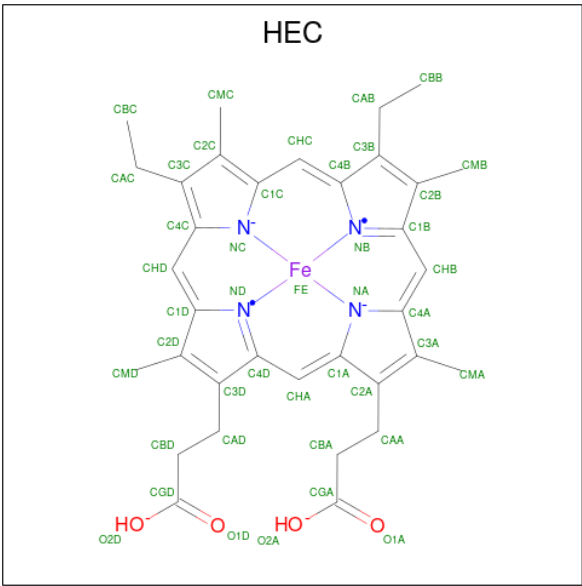
- | Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|----|----|---|---------|---------|-------|
| 8 | H | 29 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 230 | 156 | 36 | 36 | 2 | | | |

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

-
- The diagram shows the chemical structure of the HEM molecule. The central iron atom (Fe) is coordinated by four nitrogen atoms (N) in a porphyrin-like ring. The ring is substituted with two hydroxyl groups (OH) and two carboxylate groups (COO). The atoms are labeled with their respective positions: O1A, O2A, O1D, O2D for the hydroxyl groups; CAA, CBA, CAD, CBD for the carboxylate groups; and CMA, CMB, CMC, CMD for the methyl groups. The nitrogen atoms are labeled NA, ND, NC, and NB. The iron atom is labeled FE. The bonds are shown with thermal ellipsoids at the 50% probability level.

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

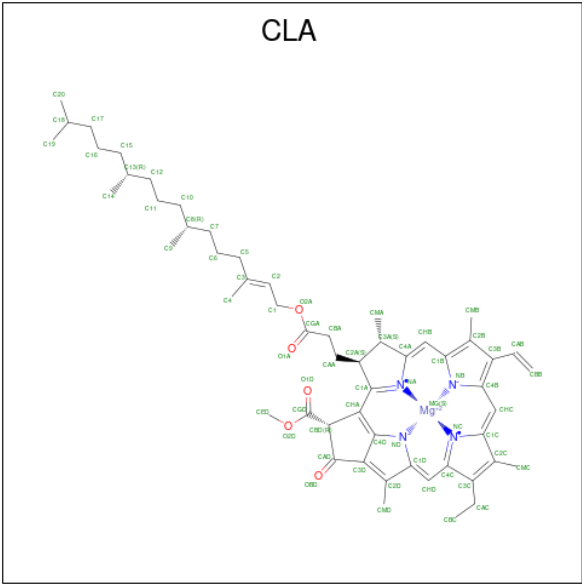
- Molecule 11 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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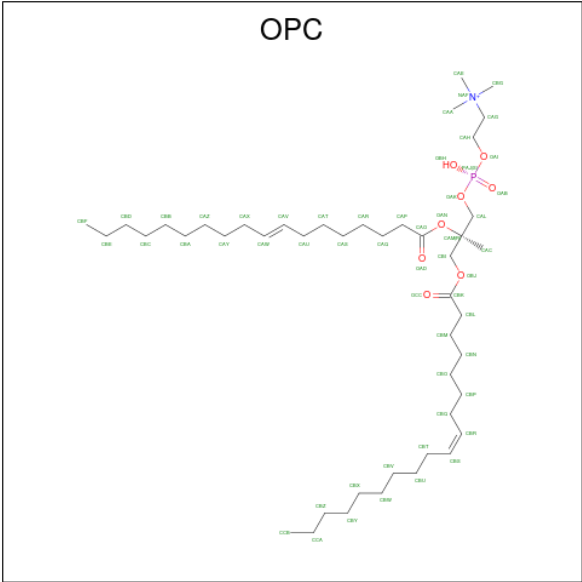
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	A	1	Total	C	O	0	0
			34	23	11		
12	A	1	Total	C	O	0	0
			34	23	11		
12	A	1	Total	C	O	0	0
			34	23	11		

- Molecule 13 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



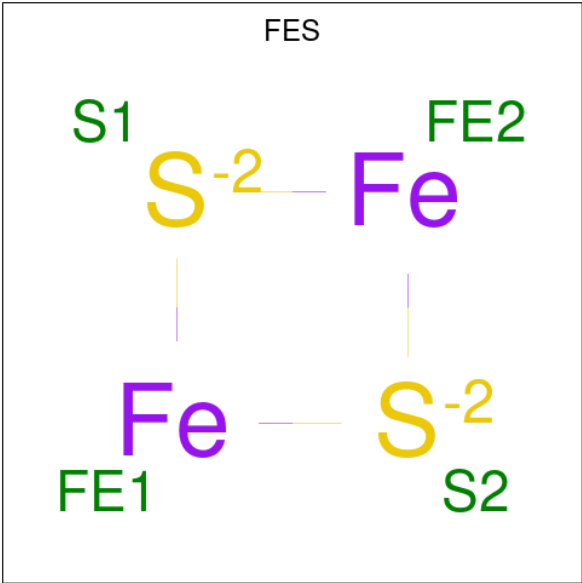
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 14 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
14	B	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
14	H	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

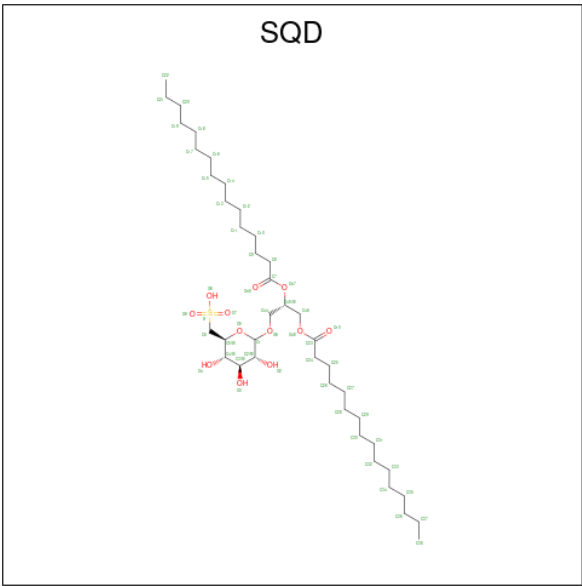
- Molecule 15 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



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

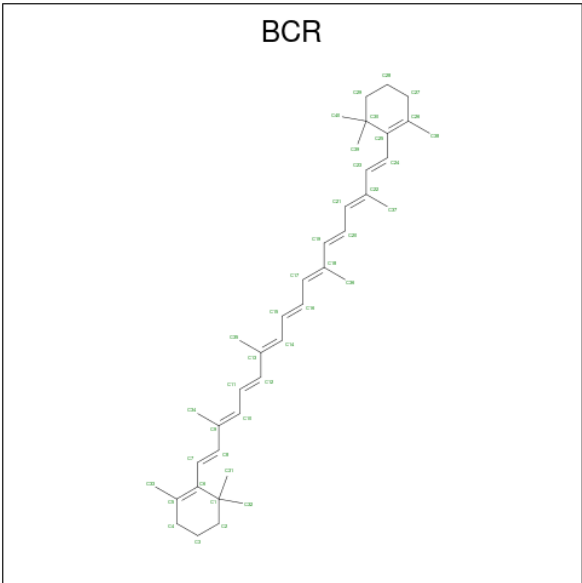
- Molecule 16 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

L]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
16	D	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 17 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



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

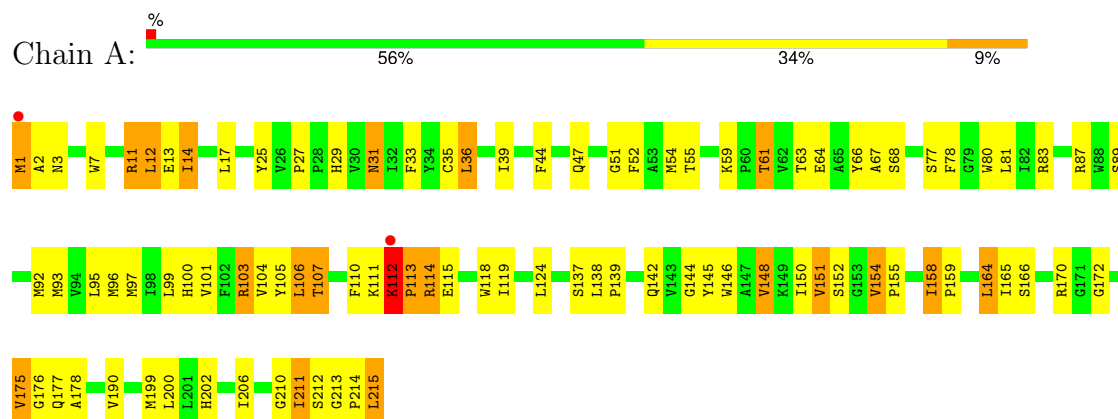
- Molecule 18 is water.

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

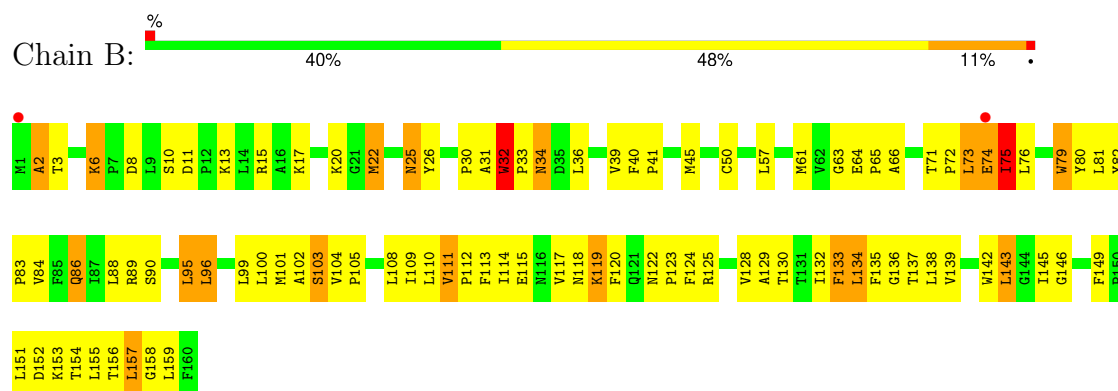
3 Residue-property plots

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

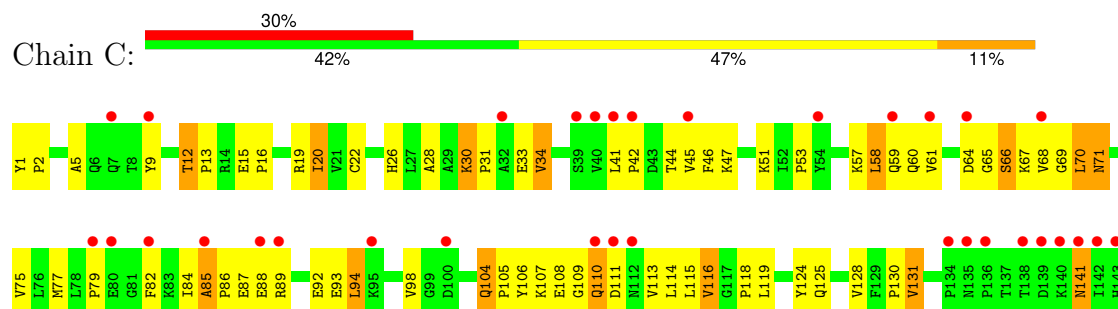
• Molecule 1: Cytochrome b6

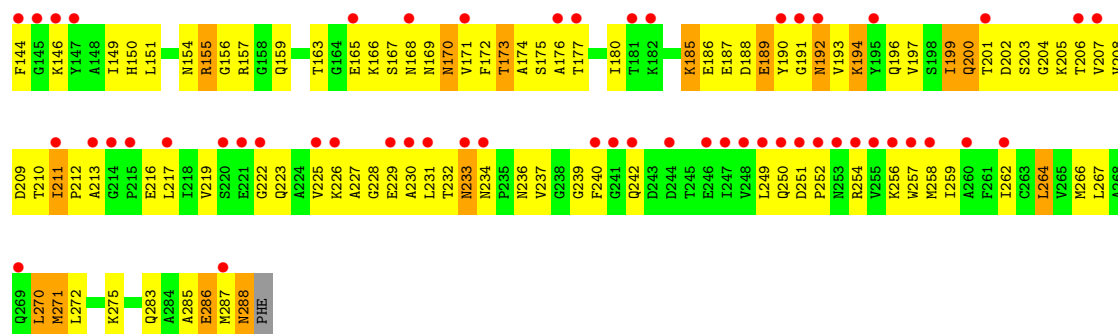


• Molecule 2: Cytochrome b6-f complex subunit 4

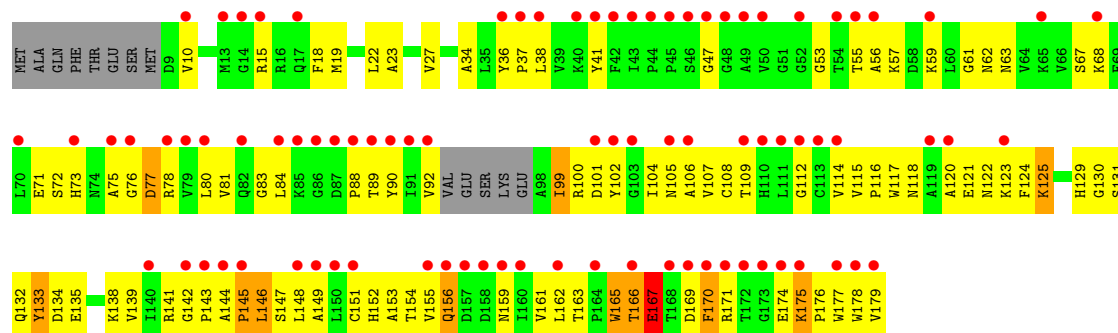


• Molecule 3: Apocytochrome f

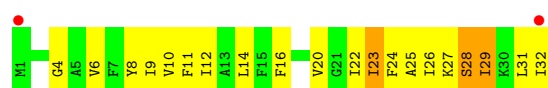




• Molecule 4: Cytochrome b6-f complex iron-sulfur subunit



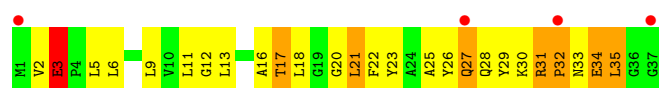
• Molecule 5: Cytochrome b6-f complex subunit 6



• 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	158.34Å 158.34Å 361.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.30 – 3.00 39.30 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.30-3.00) 99.6 (39.30-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.222 , 0.268 0.219 , 0.265	Depositor DCC
R_{free} test set	2740 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	89.0	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 81.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8025	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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: CLA, BCR, HEM, HEC, OPC, CD, FES, UMQ, 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	1.01	3/1763 (0.2%)	1.21	11/2405 (0.5%)
2	B	0.90	0/1288	1.19	4/1765 (0.2%)
3	C	0.71	0/2264	1.05	12/3082 (0.4%)
4	D	0.60	0/1292	0.83	0/1760
5	E	0.73	0/253	1.15	2/340 (0.6%)
6	F	0.79	0/246	1.08	0/331
7	G	0.83	0/289	1.14	2/391 (0.5%)
8	H	0.98	0/236	1.11	1/323 (0.3%)
All	All	0.82	3/7631 (0.0%)	1.09	32/10397 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
8	H	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	175	VAL	CA-CB	-6.17	1.48	1.54
1	A	67	ALA	CA-CB	-5.67	1.44	1.53
1	A	113	PRO	CB-CG	5.15	1.75	1.49

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	111	VAL	CA-C-N	-7.82	111.74	119.64
2	B	111	VAL	C-N-CA	-7.82	111.74	119.64
1	A	158	ILE	CA-C-N	7.81	129.60	119.84
1	A	158	ILE	C-N-CA	7.81	129.60	119.84
7	G	3	GLU	CA-C-N	7.20	126.73	119.24
7	G	3	GLU	C-N-CA	7.20	126.73	119.24
1	A	190	VAL	N-CA-C	6.82	117.33	110.23
3	C	30	LYS	CA-C-N	6.59	126.51	119.85
3	C	30	LYS	C-N-CA	6.59	126.51	119.85
3	C	9	TYR	CA-C-N	6.54	127.12	120.38
3	C	9	TYR	C-N-CA	6.54	127.12	120.38
5	E	23	ILE	CB-CA-C	-6.45	103.75	111.81
1	A	148	VAL	N-CA-C	-6.31	104.34	110.72
1	A	114	ARG	N-CA-C	6.22	120.14	111.56
8	H	14	VAL	CB-CA-C	-5.98	104.06	112.14
1	A	106	LEU	N-CA-C	-5.97	106.64	112.97
1	A	112	LYS	CA-C-N	-5.91	113.54	119.56
1	A	112	LYS	C-N-CA	-5.91	113.54	119.56
3	C	104	GLN	CA-C-N	5.77	125.53	119.76
3	C	104	GLN	C-N-CA	5.77	125.53	119.76
3	C	34	VAL	CB-CA-C	-5.76	102.10	110.63
3	C	12	THR	CA-C-N	5.65	126.72	120.45
3	C	12	THR	C-N-CA	5.65	126.72	120.45
1	A	213	GLY	CA-C-N	5.62	126.10	120.14
1	A	213	GLY	C-N-CA	5.62	126.10	120.14
3	C	85	ALA	CA-C-N	5.40	126.59	119.84
3	C	85	ALA	C-N-CA	5.40	126.59	119.84
1	A	154	VAL	CB-CA-C	-5.32	108.64	113.70
3	C	259	ILE	CB-CA-C	-5.30	105.08	112.02
2	B	75	ILE	N-CA-C	5.24	113.92	106.53
2	B	157	LEU	N-CA-C	-5.23	106.85	113.23
5	E	23	ILE	N-CA-CB	5.22	116.31	110.62

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	32	TRP	Peptide
8	H	27	ASN	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	0	1736	145	1
2	B	1249	0	1308	143	0
3	C	2216	0	2232	203	2
4	D	1260	0	1243	125	0
5	E	248	0	284	30	0
6	F	242	0	260	27	0
7	G	283	0	289	45	1
8	H	230	0	239	21	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	86	0	60	19	0
11	A	43	0	31	6	0
11	C	43	0	31	6	0
12	A	136	0	164	13	0
13	B	65	0	72	4	0
14	B	54	0	83	2	0
14	H	54	0	83	23	0
15	D	4	0	0	2	0
16	D	54	0	57	11	0
17	G	40	0	52	11	0
18	A	2	0	0	0	0
18	B	2	0	0	0	0
18	C	1	0	0	0	0
All	All	8025	0	8224	717	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 44.

All (717) 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)
16:D:201:SQD:C4	16:D:201:SQD:C3	1.85	1.54
1:A:113:PRO:CG	1:A:113:PRO:CB	1.75	1.41
16:D:201:SQD:C4	16:D:201:SQD:C2	2.11	1.27
2:B:151:LEU:O	2:B:154:THR:HG22	1.25	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:LEU:O	2:B:154:THR:CG2	1.86	1.23
2:B:139:VAL:O	2:B:143:LEU:HD12	1.43	1.19
1:A:1:MET:N	1:A:1:MET:HE2	1.59	1.18
7:G:30:LYS:O	7:G:32:PRO:HD3	1.43	1.17
3:C:65:GLY:O	3:C:66:SER:O	1.64	1.14
3:C:70:LEU:N	3:C:70:LEU:HD23	1.63	1.13
3:C:107:LYS:CE	3:C:110:GLN:NE2	2.12	1.12
1:A:1:MET:HE2	1:A:1:MET:H1	0.97	1.12
4:D:78:ARG:HG2	4:D:92:VAL:HG22	1.26	1.12
4:D:166:THR:O	4:D:167:GLU:O	1.63	1.12
2:B:128:VAL:O	2:B:132:ILE:HD12	1.48	1.12
16:D:201:SQD:C4	16:D:201:SQD:H2	1.75	1.08
3:C:70:LEU:HD23	3:C:70:LEU:H	1.07	1.07
1:A:211:ILE:HD12	1:A:212:SER:H	1.19	1.07
4:D:131:SER:CB	4:D:142:GLY:HA3	1.84	1.07
4:D:109:THR:HG21	4:D:146:LEU:HB3	1.38	1.05
2:B:88:LEU:HD12	2:B:101:MET:SD	1.95	1.05
3:C:107:LYS:HE2	3:C:110:GLN:NE2	1.70	1.04
3:C:107:LYS:HE2	3:C:110:GLN:HE22	1.23	1.03
4:D:131:SER:HB3	4:D:142:GLY:HA3	1.39	1.02
2:B:158:GLY:O	2:B:159:LEU:HD23	1.57	1.02
1:A:111:LYS:O	1:A:113:PRO:HD2	1.59	1.02
2:B:128:VAL:O	2:B:132:ILE:CD1	2.09	1.01
10:A:301:HEM:HBB2	10:A:301:HEM:HMB2	1.39	0.98
4:D:133:TYR:CD2	4:D:139:VAL:HG12	1.98	0.98
16:D:201:SQD:H82	16:D:201:SQD:H241	1.45	0.98
3:C:107:LYS:HE3	3:C:110:GLN:NE2	1.78	0.98
7:G:30:LYS:C	7:G:32:PRO:HD3	1.88	0.97
1:A:112:LYS:HB3	1:A:113:PRO:HD3	1.46	0.97
3:C:232:THR:O	3:C:233:ASN:HB3	1.64	0.96
17:G:101:BCR:H333	14:H:1002:OPC:HBZ1	1.47	0.96
4:D:155:VAL:C	4:D:156:GLN:HE21	1.73	0.95
2:B:73:LEU:O	2:B:74:GLU:HB3	1.66	0.94
3:C:107:LYS:HE3	3:C:110:GLN:HE21	1.31	0.94
4:D:129:HIS:HB2	15:D:200:FES:S1	2.07	0.94
2:B:139:VAL:O	2:B:143:LEU:CD1	2.14	0.94
4:D:133:TYR:CE2	4:D:139:VAL:HG12	2.03	0.94
3:C:175:SER:HB2	3:C:209:ASP:OD1	1.67	0.93
1:A:7:TRP:CE2	1:A:11:ARG:NH2	2.35	0.93
3:C:188:ASP:O	3:C:190:TYR:N	2.00	0.93
4:D:131:SER:HA	4:D:142:GLY:HA3	1.49	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:131:SER:CA	4:D:142:GLY:HA3	1.98	0.93
2:B:32:TRP:CD1	2:B:33:PRO:HD3	2.04	0.92
4:D:15:ARG:HB3	5:E:31:LEU:HD23	1.51	0.92
1:A:92:MET:HE3	14:H:1002:OPC:HCB3	1.51	0.91
3:C:206:THR:HG22	3:C:206:THR:O	1.69	0.91
16:D:201:SQD:H2	16:D:201:SQD:H4	1.49	0.91
3:C:262:ILE:HG23	8:H:14:VAL:HG13	1.52	0.91
3:C:199:ILE:HG22	3:C:200:GLN:H	1.36	0.90
3:C:199:ILE:O	3:C:200:GLN:HG3	1.72	0.90
2:B:22:MET:HG2	2:B:22:MET:O	1.72	0.90
5:E:8:TYR:CZ	5:E:12:ILE:HD11	2.07	0.90
2:B:123:PRO:HD2	7:G:25:ALA:HB1	1.54	0.90
16:D:201:SQD:H241	16:D:201:SQD:C8	2.01	0.90
4:D:67:SER:O	4:D:71:GLU:HG3	1.73	0.89
4:D:133:TYR:CE2	4:D:139:VAL:CG1	2.56	0.89
2:B:118:ASN:HD22	2:B:120:PHE:H	1.20	0.89
1:A:47:GLN:NE2	1:A:89:SER:HB3	1.86	0.89
4:D:77:ASP:O	4:D:92:VAL:HA	1.70	0.88
3:C:174:ALA:HB2	3:C:231:LEU:HD23	1.54	0.88
3:C:70:LEU:N	3:C:70:LEU:CD2	2.37	0.87
3:C:231:LEU:HD12	3:C:231:LEU:O	1.73	0.87
3:C:155:ARG:H	3:C:155:ARG:HD2	1.39	0.87
1:A:211:ILE:HD12	1:A:212:SER:N	1.90	0.86
1:A:112:LYS:HB3	1:A:113:PRO:CD	2.06	0.86
3:C:94:LEU:O	3:C:94:LEU:HD23	1.76	0.86
12:A:1101:UMQ:HL3	4:D:37:PRO:HG2	1.58	0.85
1:A:92:MET:CE	14:H:1002:OPC:HBY1	2.05	0.85
1:A:103:ARG:NH1	1:A:104:VAL:HA	1.92	0.85
2:B:73:LEU:O	2:B:74:GLU:CB	2.24	0.85
2:B:109:ILE:O	2:B:112:PRO:HD2	1.77	0.84
16:D:201:SQD:C3	16:D:201:SQD:C5	2.55	0.84
10:A:301:HEM:HBB2	10:A:301:HEM:CMB	2.06	0.84
1:A:211:ILE:CD1	1:A:212:SER:H	1.91	0.83
7:G:2:VAL:CG1	7:G:3:GLU:N	2.42	0.83
4:D:156:GLN:HE21	4:D:156:GLN:N	1.76	0.82
5:E:16:PHE:CD2	6:F:22:LEU:HD21	2.14	0.82
5:E:4:GLY:HA3	14:H:1002:OPC:HAS1	1.60	0.82
4:D:133:TYR:CD2	4:D:139:VAL:CG1	2.63	0.82
1:A:215:LEU:H	1:A:215:LEU:HD23	1.45	0.82
4:D:131:SER:HB3	4:D:143:PRO:HD2	1.62	0.81
1:A:36:LEU:HD23	1:A:99:LEU:C	2.05	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:188:ASP:C	3:C:190:TYR:H	1.87	0.81
3:C:225:VAL:CG1	3:C:229:GLU:HG2	2.10	0.81
7:G:5:LEU:HD11	14:H:1002:OPC:HBN1	1.62	0.81
4:D:135:GLU:N	4:D:135:GLU:OE2	2.14	0.81
7:G:2:VAL:HG12	7:G:3:GLU:N	1.93	0.81
7:G:28:GLN:O	7:G:32:PRO:HB3	1.81	0.80
10:A:302:HEM:CMB	10:A:302:HEM:HBB2	2.12	0.80
3:C:180:ILE:CG2	3:C:222:GLY:H	1.94	0.80
1:A:111:LYS:O	1:A:113:PRO:CD	2.28	0.80
6:F:20:TRP:CZ3	17:G:101:BCR:H19C	2.17	0.80
1:A:112:LYS:O	1:A:115:GLU:OE1	1.99	0.80
3:C:30:LYS:HB3	3:C:31:PRO:HD2	1.64	0.80
10:A:302:HEM:HBB2	10:A:302:HEM:HMB1	1.64	0.79
2:B:84:VAL:HG13	2:B:101:MET:HG2	1.61	0.79
7:G:2:VAL:CG1	7:G:3:GLU:H	1.95	0.79
1:A:215:LEU:HD23	1:A:215:LEU:N	1.98	0.79
1:A:137:SER:HB2	1:A:148:VAL:HG21	1.64	0.79
7:G:30:LYS:O	7:G:32:PRO:CD	2.29	0.79
3:C:34:VAL:HG22	3:C:151:LEU:HD22	1.65	0.79
3:C:216:GLU:O	3:C:217:LEU:HD23	1.82	0.79
16:D:201:SQD:C4	16:D:201:SQD:O3	2.30	0.79
3:C:201:THR:HG22	3:C:202:ASP:N	1.97	0.78
2:B:143:LEU:HD12	2:B:143:LEU:H	1.48	0.78
3:C:199:ILE:O	3:C:200:GLN:CG	2.30	0.78
2:B:32:TRP:HB3	2:B:33:PRO:CD	2.13	0.78
1:A:11:ARG:HB2	1:A:12:LEU:HD22	1.66	0.78
1:A:1:MET:N	1:A:1:MET:CE	2.43	0.78
2:B:99:LEU:O	2:B:103:SER:OG	2.01	0.78
7:G:5:LEU:HD11	14:H:1002:OPC:CBN	2.13	0.78
6:F:20:TRP:HZ3	17:G:101:BCR:H19C	1.48	0.77
3:C:232:THR:O	3:C:233:ASN:CB	2.30	0.77
1:A:29:HIS:CD2	1:A:214:PRO:HA	2.20	0.76
4:D:131:SER:HA	4:D:142:GLY:CA	2.14	0.76
3:C:22:CYS:SG	3:C:240:PHE:CD1	2.76	0.76
3:C:155:ARG:HD2	3:C:155:ARG:N	1.97	0.76
3:C:177:THR:HG23	3:C:226:LYS:HG2	1.68	0.76
2:B:45:MET:HE3	4:D:27:VAL:HG13	1.67	0.76
4:D:155:VAL:C	4:D:156:GLN:NE2	2.43	0.76
1:A:83:ARG:NH2	2:B:61:MET:O	2.16	0.75
2:B:118:ASN:ND2	2:B:120:PHE:H	1.84	0.75
1:A:92:MET:CE	14:H:1002:OPC:CBY	2.64	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:94:LEU:HD23	3:C:94:LEU:C	2.12	0.75
3:C:196:GLN:NE2	3:C:210:THR:OG1	2.18	0.75
6:F:25:LEU:O	6:F:29:ILE:HG22	1.87	0.75
3:C:211:ILE:HD12	3:C:212:PRO:O	1.87	0.74
4:D:138:LYS:HA	4:D:147:SER:OG	1.86	0.74
2:B:31:ALA:O	2:B:32:TRP:O	2.04	0.74
4:D:67:SER:O	4:D:71:GLU:CG	2.36	0.74
1:A:7:TRP:NE1	1:A:11:ARG:NH2	2.36	0.74
2:B:82:TYR:HB2	2:B:83:PRO:HD3	1.70	0.74
1:A:61:THR:HG22	1:A:64:GLU:H	1.51	0.73
6:F:13:PHE:CE2	6:F:17:PHE:HE1	2.06	0.73
4:D:108:CYS:HB2	4:D:133:TYR:OH	1.88	0.73
1:A:202:HIS:O	1:A:206:ILE:HG13	1.88	0.73
3:C:19:ARG:O	3:C:20:ILE:HB	1.89	0.73
1:A:47:GLN:HE22	1:A:89:SER:HB3	1.51	0.72
1:A:103:ARG:HH11	1:A:104:VAL:HA	1.51	0.72
2:B:34:ASN:HD21	3:C:283:GLN:HE22	1.35	0.72
7:G:29:TYR:O	7:G:29:TYR:CD2	2.43	0.72
3:C:68:VAL:HG22	3:C:69:GLY:H	1.53	0.72
2:B:119:LYS:CG	2:B:119:LYS:O	2.37	0.72
3:C:199:ILE:O	3:C:200:GLN:CB	2.37	0.72
3:C:206:THR:O	3:C:206:THR:CG2	2.37	0.72
1:A:54:MET:CE	10:A:301:HEM:HBD1	2.20	0.71
3:C:98:VAL:HG21	3:C:130:PRO:HG3	1.73	0.71
3:C:185:LYS:O	3:C:185:LYS:HD3	1.90	0.71
3:C:176:ALA:HA	3:C:227:ALA:HB2	1.73	0.70
17:G:101:BCR:C32	8:H:19:ILE:HG12	2.21	0.70
2:B:32:TRP:CG	2:B:33:PRO:HD3	2.26	0.70
2:B:135:PHE:O	2:B:139:VAL:HG23	1.91	0.70
2:B:154:THR:HG23	2:B:155:LEU:H	1.56	0.70
3:C:286:GLU:N	3:C:286:GLU:OE1	2.24	0.70
4:D:92:VAL:HB	4:D:100:ARG:HD2	1.73	0.70
1:A:92:MET:HE2	14:H:1002:OPC:CBY	2.21	0.70
2:B:32:TRP:CB	2:B:33:PRO:CD	2.69	0.70
3:C:177:THR:HG23	3:C:226:LYS:HA	1.74	0.70
1:A:92:MET:HE1	14:H:1002:OPC:HBY1	1.74	0.70
7:G:34:GLU:O	7:G:35:LEU:HB2	1.88	0.70
3:C:58:LEU:HD13	3:C:59:GLN:N	2.07	0.70
3:C:94:LEU:CD2	3:C:98:VAL:HG23	2.22	0.69
2:B:118:ASN:ND2	2:B:120:PHE:CD1	2.60	0.69
3:C:94:LEU:HD23	3:C:98:VAL:HG23	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:MET:CE	14:H:1002:OPC:HCB3	2.22	0.69
3:C:141:ASN:C	3:C:141:ASN:HD22	2.00	0.69
5:E:22:ILE:O	5:E:26:ILE:HB	1.92	0.69
1:A:104:VAL:O	1:A:107:THR:HG22	1.92	0.69
3:C:28:ALA:HB3	3:C:239:GLY:HA2	1.72	0.69
6:F:13:PHE:CE2	6:F:17:PHE:CE1	2.80	0.69
3:C:5:ALA:HB2	11:C:301:HEC:HBB2	1.75	0.69
4:D:131:SER:HB3	4:D:142:GLY:CA	2.20	0.68
3:C:94:LEU:C	3:C:94:LEU:CD2	2.66	0.68
1:A:80:TRP:HE1	12:A:1101:UMQ:H6'1	1.57	0.68
11:A:303:HEC:HBD1	11:A:303:HEC:HHA	1.75	0.68
7:G:2:VAL:HG13	7:G:3:GLU:H	1.59	0.68
3:C:163:THR:OG1	3:C:165:GLU:HG2	1.94	0.68
4:D:109:THR:HG21	4:D:146:LEU:CB	2.21	0.68
3:C:13:PRO:O	3:C:20:ILE:HA	1.93	0.68
4:D:15:ARG:HB3	5:E:31:LEU:CD2	2.23	0.68
3:C:189:GLU:N	3:C:189:GLU:OE1	2.26	0.68
3:C:288:ASN:HD22	3:C:288:ASN:H	1.40	0.68
6:F:7:TYR:O	6:F:11:LEU:HD12	1.94	0.68
1:A:111:LYS:C	1:A:113:PRO:HD2	2.19	0.67
3:C:286:GLU:OE1	3:C:286:GLU:CA	2.41	0.67
3:C:79:PRO:HG2	3:C:82:PHE:CD1	2.29	0.67
3:C:176:ALA:C	3:C:227:ALA:HB2	2.19	0.67
2:B:32:TRP:HB3	2:B:33:PRO:HD3	1.76	0.67
1:A:114:ARG:NH1	1:A:210:GLY:O	2.27	0.67
3:C:46:PHE:CE2	3:C:131:VAL:HG22	2.30	0.67
4:D:57:LYS:HB3	4:D:61:GLY:HA2	1.76	0.67
1:A:155:PRO:HB2	1:A:166:SER:OG	1.94	0.67
3:C:219:VAL:HG21	3:C:231:LEU:HB2	1.77	0.66
4:D:118:ASN:C	4:D:118:ASN:HD22	2.03	0.66
3:C:180:ILE:HG23	3:C:222:GLY:H	1.61	0.66
4:D:99:ILE:HG13	4:D:100:ARG:H	1.60	0.66
4:D:99:ILE:HG23	4:D:100:ARG:N	2.09	0.66
3:C:60:GLN:HE22	3:C:156:GLY:HA2	1.60	0.66
3:C:194:LYS:HB2	3:C:194:LYS:NZ	2.11	0.66
3:C:270:LEU:HA	8:H:21:MET:HE2	1.77	0.66
3:C:167:SER:OG	3:C:168:ASN:N	2.27	0.66
3:C:177:THR:N	3:C:227:ALA:HB2	2.10	0.66
5:E:6:VAL:O	5:E:10:VAL:HG23	1.95	0.66
5:E:23:ILE:O	5:E:27:LYS:N	2.29	0.66
1:A:92:MET:HE2	14:H:1002:OPC:HBY2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:SER:HB2	1:A:148:VAL:CG2	2.26	0.65
4:D:122:ASN:HB3	4:D:135:GLU:OE1	1.95	0.65
6:F:18:VAL:O	6:F:22:LEU:HB2	1.96	0.65
1:A:54:MET:HE3	10:A:301:HEM:HBD1	1.76	0.65
3:C:201:THR:CG2	3:C:202:ASP:H	2.09	0.65
3:C:177:THR:CG2	3:C:226:LYS:HG2	2.26	0.65
4:D:63:ASN:HB3	4:D:159:ASN:HD21	1.61	0.65
4:D:63:ASN:HB3	4:D:159:ASN:ND2	2.11	0.65
4:D:109:THR:HG22	4:D:109:THR:O	1.95	0.65
3:C:201:THR:CG2	3:C:202:ASP:N	2.59	0.65
4:D:107:VAL:HG12	4:D:112:GLY:HA2	1.77	0.65
1:A:36:LEU:HB3	1:A:100:HIS:HB2	1.78	0.65
3:C:59:GLN:OE1	3:C:67:LYS:O	2.15	0.65
1:A:83:ARG:HD2	10:A:301:HEM:O1D	1.97	0.65
5:E:16:PHE:HD2	6:F:22:LEU:HD21	1.61	0.65
2:B:142:TRP:CZ2	2:B:155:LEU:O	2.50	0.64
3:C:201:THR:HG22	3:C:202:ASP:H	1.59	0.64
3:C:211:ILE:HD12	3:C:211:ILE:C	2.23	0.64
1:A:7:TRP:NE1	1:A:11:ARG:HH21	1.93	0.64
3:C:229:GLU:HA	3:C:229:GLU:OE1	1.97	0.64
7:G:20:GLY:N	17:G:101:BCR:H363	2.13	0.64
1:A:31:ASN:C	1:A:31:ASN:HD22	2.05	0.64
3:C:251:ASP:HB3	3:C:254:ARG:HD3	1.79	0.64
2:B:45:MET:CE	4:D:27:VAL:HG13	2.27	0.64
2:B:151:LEU:O	2:B:154:THR:HG21	1.96	0.64
1:A:92:MET:HE3	14:H:1002:OPC:CCB	2.24	0.63
2:B:22:MET:O	2:B:22:MET:CG	2.41	0.63
3:C:64:ASP:HB2	3:C:192:ASN:HD22	1.62	0.63
3:C:94:LEU:CD2	3:C:98:VAL:CG2	2.75	0.63
13:B:201:CLA:HAC1	14:B:202:OPC:HBW1	1.80	0.63
2:B:8:ASP:OD1	2:B:10:SER:HB3	1.98	0.63
2:B:119:LYS:O	2:B:119:LYS:HG3	1.97	0.63
3:C:68:VAL:HG22	3:C:69:GLY:N	2.13	0.63
3:C:194:LYS:HB2	3:C:194:LYS:HZ2	1.64	0.63
4:D:116:PRO:HD2	4:D:125:LYS:O	1.98	0.63
1:A:170:ARG:HG3	1:A:172:GLY:O	1.99	0.63
1:A:110:PHE:HD1	2:B:112:PRO:HB3	1.63	0.62
4:D:169:ASP:OD1	4:D:176:PRO:HB3	1.98	0.62
4:D:130:GLY:O	4:D:141:ARG:NH2	2.31	0.62
12:A:1104:UMQ:HC1	2:B:32:TRP:CZ2	2.34	0.62
1:A:36:LEU:HD23	1:A:100:HIS:N	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:TRP:HZ2	2:B:155:LEU:O	1.84	0.61
3:C:275:LYS:HD3	4:D:19:MET:HB3	1.82	0.61
4:D:156:GLN:HE21	4:D:156:GLN:CA	2.13	0.61
1:A:63:THR:HG22	1:A:64:GLU:HG3	1.82	0.61
3:C:119:LEU:HD22	3:C:124:TYR:CE1	2.36	0.61
1:A:142:GLN:HG3	2:B:72:PRO:HG3	1.82	0.61
3:C:65:GLY:C	3:C:66:SER:O	2.44	0.61
3:C:175:SER:HB2	3:C:209:ASP:CG	2.25	0.61
1:A:93:MET:SD	10:A:301:HEM:HBB1	2.41	0.61
3:C:171:VAL:HG12	3:C:233:ASN:O	2.01	0.61
3:C:176:ALA:HA	3:C:227:ALA:CB	2.30	0.61
1:A:1:MET:HE2	1:A:1:MET:H3	1.63	0.61
2:B:75:ILE:O	2:B:75:ILE:HG12	2.00	0.61
2:B:88:LEU:CD1	2:B:101:MET:SD	2.83	0.61
4:D:131:SER:HB3	4:D:143:PRO:CD	2.31	0.61
1:A:100:HIS:HE1	10:A:302:HEM:C1A	2.19	0.61
2:B:32:TRP:CB	2:B:33:PRO:HD3	2.31	0.60
2:B:156:THR:O	2:B:157:LEU:HB2	2.01	0.60
2:B:3:THR:HG23	3:C:287:MET:HE1	1.82	0.60
2:B:114:ILE:O	2:B:117:VAL:HG23	2.01	0.60
1:A:103:ARG:HH12	1:A:104:VAL:HG22	1.66	0.60
10:A:302:HEM:HMB1	10:A:302:HEM:CBB	2.30	0.60
2:B:45:MET:HE1	4:D:27:VAL:HG22	1.82	0.60
4:D:156:GLN:N	4:D:156:GLN:NE2	2.49	0.60
3:C:71:ASN:N	11:C:301:HEC:O2A	2.16	0.60
3:C:15:GLU:HB3	3:C:16:PRO:CD	2.31	0.60
3:C:57:LYS:HE2	3:C:57:LYS:HA	1.82	0.60
5:E:26:ILE:HG22	5:E:32:ILE:HD12	1.83	0.60
4:D:89:THR:HG23	4:D:104:ILE:C	2.27	0.60
7:G:33:ASN:O	7:G:34:GLU:O	2.20	0.60
1:A:137:SER:CB	1:A:148:VAL:HG21	2.30	0.60
2:B:57:LEU:HD13	8:H:8:TRP:HA	1.83	0.60
12:A:1104:UMQ:H21	12:A:1104:UMQ:H62	1.83	0.59
4:D:78:ARG:CG	4:D:92:VAL:HG22	2.15	0.59
2:B:118:ASN:ND2	2:B:120:PHE:HD1	2.00	0.59
4:D:145:PRO:O	4:D:146:LEU:HB2	2.02	0.59
16:D:201:SQD:H241	16:D:201:SQD:H81	1.83	0.59
1:A:154:VAL:HB	1:A:155:PRO:HD3	1.85	0.59
2:B:110:LEU:O	2:B:111:VAL:C	2.43	0.59
7:G:5:LEU:CD1	14:H:1002:OPC:HBN1	2.31	0.59
5:E:29:ILE:HG22	5:E:29:ILE:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:152:ASP:OD2	2:B:153:LYS:HG2	2.03	0.59
1:A:111:LYS:NZ	2:B:120:PHE:O	2.35	0.59
1:A:114:ARG:NH2	1:A:212:SER:HA	2.17	0.59
2:B:79:TRP:CG	2:B:80:TYR:N	2.70	0.59
2:B:139:VAL:HG12	2:B:143:LEU:HD11	1.83	0.59
5:E:25:ALA:O	5:E:29:ILE:HG13	2.02	0.59
1:A:137:SER:CB	1:A:148:VAL:CG2	2.80	0.59
2:B:123:PRO:CD	7:G:25:ALA:HB1	2.31	0.59
3:C:176:ALA:CA	3:C:227:ALA:HB2	2.32	0.59
2:B:2:ALA:O	2:B:3:THR:OG1	2.16	0.59
3:C:199:ILE:O	3:C:200:GLN:HB2	2.03	0.59
4:D:121:GLU:O	4:D:122:ASN:HB2	2.02	0.59
3:C:64:ASP:HB2	3:C:192:ASN:ND2	2.17	0.59
1:A:1:MET:H1	1:A:1:MET:CE	1.92	0.58
1:A:158:ILE:HG23	1:A:159:PRO:HD2	1.83	0.58
4:D:108:CYS:HB3	4:D:115:VAL:CG2	2.34	0.58
4:D:166:THR:C	4:D:167:GLU:O	2.45	0.58
12:A:1101:UMQ:HD2	3:C:257:TRP:HB2	1.85	0.58
2:B:95:LEU:HD22	2:B:99:LEU:CD1	2.33	0.58
4:D:118:ASN:ND2	4:D:120:ALA:H	2.02	0.58
4:D:176:PRO:HD2	4:D:179:VAL:HG22	1.86	0.58
3:C:204:GLY:O	3:C:205:LYS:HB2	2.03	0.58
4:D:105:ASN:HB2	4:D:149:ALA:HB3	1.86	0.58
7:G:31:ARG:O	7:G:31:ARG:HG2	2.02	0.58
4:D:36:TYR:HB3	4:D:37:PRO:HD3	1.86	0.57
1:A:103:ARG:O	1:A:107:THR:HB	2.03	0.57
4:D:133:TYR:CD1	4:D:133:TYR:N	2.71	0.57
1:A:103:ARG:HH11	1:A:104:VAL:CA	2.17	0.57
3:C:285:ALA:C	3:C:286:GLU:OE1	2.47	0.57
11:A:303:HEC:HBD1	11:A:303:HEC:CHA	2.33	0.57
3:C:42:PRO:HG3	3:C:144:PHE:HE2	1.68	0.57
3:C:5:ALA:HB2	11:C:301:HEC:CBB	2.34	0.57
3:C:199:ILE:C	3:C:200:GLN:HG3	2.29	0.57
3:C:71:ASN:N	3:C:71:ASN:HD22	2.03	0.57
5:E:8:TYR:OH	6:F:15:LEU:HD22	2.03	0.57
7:G:3:GLU:C	7:G:3:GLU:OE1	2.47	0.57
1:A:12:LEU:O	1:A:13:GLU:HB2	2.03	0.57
2:B:151:LEU:O	2:B:154:THR:CB	2.53	0.57
6:F:11:LEU:HD21	14:H:1002:OPC:HAV	1.86	0.57
1:A:115:GLU:O	1:A:119:ILE:HG13	2.04	0.56
2:B:84:VAL:HG13	2:B:101:MET:CG	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ARG:O	1:A:103:ARG:HD2	2.06	0.56
2:B:82:TYR:HB2	2:B:83:PRO:CD	2.35	0.56
5:E:28:SER:O	5:E:29:ILE:HG12	2.05	0.56
12:A:1104:UMQ:H21	12:A:1104:UMQ:C6	2.35	0.56
14:H:1002:OPC:HAY1	14:H:1002:OPC:HBC1	1.86	0.56
1:A:39:ILE:HD11	17:G:101:BCR:H312	1.87	0.56
1:A:61:THR:HG22	1:A:64:GLU:N	2.21	0.56
1:A:106:LEU:HD12	7:G:21:LEU:HD23	1.86	0.56
4:D:118:ASN:HD22	4:D:120:ALA:H	1.52	0.56
1:A:29:HIS:CD2	1:A:214:PRO:CA	2.89	0.56
3:C:71:ASN:N	3:C:71:ASN:ND2	2.53	0.56
1:A:115:GLU:OE1	1:A:115:GLU:N	2.39	0.56
6:F:25:LEU:O	6:F:29:ILE:CG2	2.52	0.56
2:B:134:LEU:HD11	7:G:22:PHE:CZ	2.40	0.56
3:C:187:GLU:HG3	3:C:187:GLU:O	2.06	0.56
4:D:133:TYR:CD2	4:D:148:LEU:HG	2.41	0.56
3:C:199:ILE:HG22	3:C:200:GLN:N	2.13	0.55
4:D:138:LYS:HA	4:D:147:SER:CB	2.36	0.55
1:A:103:ARG:HD2	1:A:103:ARG:C	2.30	0.55
2:B:71:THR:HG22	2:B:72:PRO:O	2.06	0.55
1:A:44:PHE:HB2	1:A:93:MET:HE3	1.88	0.55
2:B:128:VAL:O	2:B:132:ILE:HD13	2.02	0.55
3:C:216:GLU:HG3	3:C:217:LEU:H	1.71	0.55
1:A:47:GLN:NE2	1:A:89:SER:CB	2.65	0.55
2:B:32:TRP:O	2:B:33:PRO:C	2.49	0.55
1:A:1:MET:O	1:A:2:ALA:HB3	2.06	0.55
2:B:11:ASP:OD1	2:B:13:LYS:HB2	2.07	0.55
2:B:57:LEU:CD1	8:H:8:TRP:HA	2.36	0.54
6:F:13:PHE:CD2	6:F:17:PHE:HE1	2.25	0.54
3:C:79:PRO:HG2	3:C:82:PHE:CE1	2.41	0.54
3:C:41:LEU:HD22	3:C:252:PRO:HG3	1.88	0.54
3:C:286:GLU:OE1	3:C:286:GLU:HA	2.06	0.54
3:C:173:THR:HB	3:C:228:GLY:HA2	1.88	0.54
3:C:266:MET:HE1	5:E:11:PHE:CE2	2.43	0.54
5:E:24:PHE:O	5:E:25:ALA:C	2.50	0.54
1:A:100:HIS:CE1	10:A:302:HEM:C1A	2.95	0.54
3:C:174:ALA:CB	3:C:231:LEU:HD23	2.34	0.54
3:C:258:MET:O	3:C:262:ILE:HD13	2.07	0.54
4:D:56:ALA:HB1	4:D:81:VAL:HG11	1.90	0.54
5:E:10:VAL:O	5:E:14:LEU:HB2	2.08	0.54
6:F:29:ILE:HD12	6:F:29:ILE:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:169:ASN:O	3:C:236:ASN:HB2	2.08	0.53
3:C:15:GLU:HB3	3:C:16:PRO:HD2	1.90	0.53
4:D:109:THR:O	4:D:109:THR:CG2	2.55	0.53
4:D:55:THR:HG22	4:D:56:ALA:N	2.22	0.53
3:C:197:VAL:O	3:C:208:VAL:HG13	2.08	0.53
3:C:288:ASN:H	3:C:288:ASN:ND2	2.06	0.53
1:A:170:ARG:CG	1:A:172:GLY:O	2.57	0.53
2:B:6:LYS:HB2	2:B:6:LYS:NZ	2.24	0.53
6:F:3:GLU:O	6:F:7:TYR:HB2	2.09	0.53
7:G:29:TYR:O	7:G:29:TYR:CG	2.61	0.53
3:C:172:PHE:O	3:C:232:THR:OG1	2.27	0.53
2:B:34:ASN:N	2:B:34:ASN:HD22	2.07	0.53
3:C:34:VAL:CG2	3:C:151:LEU:HD22	2.35	0.53
16:D:201:SQD:C8	16:D:201:SQD:C24	2.83	0.53
3:C:172:PHE:H	3:C:232:THR:CB	2.20	0.53
3:C:262:ILE:HG23	8:H:14:VAL:CG1	2.34	0.53
2:B:32:TRP:CG	2:B:33:PRO:CD	2.90	0.53
1:A:138:LEU:N	1:A:139:PRO:CD	2.71	0.52
2:B:124:PHE:CE1	7:G:26:TYR:HB2	2.45	0.52
8:H:15:PHE:CG	14:H:1002:OPC:HBT1	2.44	0.52
1:A:144:GLY:O	1:A:148:VAL:HG23	2.10	0.52
3:C:262:ILE:HG22	3:C:266:MET:HE2	1.92	0.52
3:C:22:CYS:HB2	11:C:301:HEC:CAB	2.40	0.52
6:F:20:TRP:CD1	6:F:20:TRP:C	2.87	0.52
11:A:303:HEC:CMB	11:A:303:HEC:HBB2	2.40	0.52
3:C:172:PHE:N	3:C:232:THR:OG1	2.39	0.52
1:A:215:LEU:HB2	2:B:122:ASN:HB2	1.90	0.52
2:B:17:LYS:HE3	2:B:26:TYR:OH	2.10	0.52
2:B:32:TRP:HD1	2:B:33:PRO:HD3	1.70	0.52
3:C:107:LYS:CE	3:C:110:GLN:HE22	1.93	0.52
7:G:34:GLU:O	7:G:35:LEU:CB	2.59	0.51
2:B:86:GLN:HG2	2:B:143:LEU:HB3	1.93	0.51
4:D:75:ALA:O	4:D:76:GLY:C	2.53	0.51
7:G:11:LEU:O	7:G:12:GLY:C	2.50	0.51
2:B:129:ALA:O	2:B:130:THR:C	2.52	0.51
3:C:194:LYS:NZ	3:C:194:LYS:CB	2.74	0.51
4:D:115:VAL:HG13	4:D:125:LYS:C	2.35	0.51
1:A:110:PHE:H	1:A:110:PHE:HD2	1.57	0.51
3:C:94:LEU:HD21	3:C:98:VAL:CG2	2.40	0.51
4:D:169:ASP:C	4:D:171:ARG:H	2.19	0.51
1:A:150:ILE:HG22	1:A:151:VAL:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33:GLU:HB3	3:C:51:LYS:HB2	1.93	0.51
3:C:191:GLY:O	3:C:192:ASN:O	2.29	0.51
4:D:77:ASP:OD2	4:D:77:ASP:N	2.44	0.51
4:D:105:ASN:CB	4:D:149:ALA:HB3	2.40	0.51
8:H:23:VAL:O	8:H:24:TRP:C	2.50	0.51
1:A:35:CYS:SG	11:A:303:HEC:HMB3	2.51	0.51
1:A:215:LEU:N	1:A:215:LEU:CD2	2.73	0.51
3:C:84:ILE:HG12	3:C:114:LEU:HD11	1.93	0.50
4:D:90:TYR:CD1	4:D:106:ALA:HB2	2.46	0.50
1:A:111:LYS:HE2	2:B:115:GLU:O	2.10	0.50
2:B:152:ASP:C	2:B:154:THR:H	2.17	0.50
3:C:271:MET:HB3	4:D:23:ALA:HA	1.93	0.50
4:D:141:ARG:HE	4:D:142:GLY:H	1.59	0.50
2:B:82:TYR:CB	2:B:83:PRO:HD3	2.41	0.50
3:C:231:LEU:O	3:C:231:LEU:CD1	2.53	0.50
12:A:1104:UMQ:C6	12:A:1104:UMQ:C2	2.88	0.50
16:D:201:SQD:H81	16:D:201:SQD:C24	2.41	0.50
10:A:301:HEM:HMB2	10:A:301:HEM:CBB	2.29	0.50
2:B:118:ASN:HD22	2:B:120:PHE:N	1.98	0.50
3:C:225:VAL:HG11	3:C:229:GLU:HG2	1.93	0.50
1:A:211:ILE:CD1	1:A:212:SER:N	2.63	0.50
2:B:74:GLU:O	2:B:74:GLU:HG3	2.11	0.50
3:C:60:GLN:CD	3:C:70:LEU:HB3	2.37	0.50
3:C:211:ILE:HD12	3:C:211:ILE:O	2.11	0.50
3:C:193:VAL:O	3:C:213:ALA:HB2	2.12	0.49
3:C:109:GLY:O	3:C:111:ASP:N	2.44	0.49
3:C:30:LYS:HB3	3:C:31:PRO:CD	2.39	0.49
1:A:170:ARG:HD2	1:A:172:GLY:O	2.12	0.49
3:C:13:PRO:HB3	3:C:106:TYR:CE1	2.47	0.49
4:D:133:TYR:CD2	4:D:139:VAL:HG13	2.48	0.49
2:B:11:ASP:O	2:B:15:ARG:HG3	2.13	0.49
2:B:132:ILE:HD12	2:B:132:ILE:H	1.76	0.49
17:G:101:BCR:H323	8:H:19:ILE:CG1	2.43	0.49
8:H:8:TRP:CE3	14:H:1002:OPC:HBL1	2.47	0.49
7:G:17:THR:O	7:G:18:LEU:C	2.55	0.49
2:B:79:TRP:CD1	2:B:79:TRP:C	2.89	0.49
4:D:38:LEU:O	4:D:41:TYR:HB3	2.12	0.49
4:D:56:ALA:HB1	4:D:81:VAL:CG1	2.43	0.49
8:H:15:PHE:CD1	14:H:1002:OPC:HBW1	2.48	0.49
1:A:47:GLN:NE2	1:A:47:GLN:HA	2.27	0.49
3:C:157:ARG:HE	11:C:301:HEC:CGD	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:203:SER:O	3:C:205:LYS:HG3	2.13	0.48
4:D:55:THR:CG2	4:D:56:ALA:N	2.76	0.48
2:B:50:CYS:HB3	14:H:1002:OPC:HBX1	1.94	0.48
3:C:288:ASN:HD22	3:C:288:ASN:N	2.02	0.48
4:D:81:VAL:O	4:D:88:PRO:HA	2.14	0.48
2:B:61:MET:HG3	3:C:146:LYS:HB3	1.94	0.48
4:D:77:ASP:OD1	4:D:92:VAL:O	2.30	0.48
4:D:156:GLN:HB2	4:D:161:VAL:CG2	2.43	0.48
4:D:174:GLU:O	4:D:175:LYS:C	2.57	0.48
1:A:105:TYR:C	1:A:107:THR:H	2.21	0.48
1:A:106:LEU:HD21	2:B:133:PHE:CE1	2.48	0.48
1:A:114:ARG:CZ	1:A:212:SER:HA	2.43	0.48
2:B:45:MET:HE1	4:D:27:VAL:HA	1.96	0.48
2:B:104:VAL:HB	2:B:105:PRO:HD3	1.94	0.48
5:E:16:PHE:HZ	6:F:25:LEU:HD22	1.78	0.48
6:F:25:LEU:HD23	6:F:29:ILE:HG22	1.94	0.48
5:E:24:PHE:O	5:E:28:SER:N	2.44	0.48
5:E:27:LYS:C	5:E:29:ILE:H	2.22	0.48
3:C:225:VAL:CG1	3:C:229:GLU:CG	2.87	0.48
5:E:16:PHE:HE1	5:E:20:VAL:HG21	1.79	0.48
2:B:128:VAL:HG12	2:B:132:ILE:CD1	2.44	0.48
1:A:27:PRO:HB2	1:A:29:HIS:ND1	2.29	0.48
1:A:52:PHE:N	10:A:301:HEM:CBC	2.76	0.48
3:C:19:ARG:O	3:C:20:ILE:CB	2.53	0.48
3:C:28:ALA:HB2	3:C:236:ASN:ND2	2.28	0.48
1:A:39:ILE:HG22	1:A:96:MET:HG3	1.94	0.48
3:C:75:VAL:HG13	3:C:75:VAL:O	2.14	0.48
8:H:10:ALA:O	8:H:14:VAL:HG22	2.13	0.48
2:B:95:LEU:O	2:B:95:LEU:HD23	2.14	0.47
3:C:270:LEU:HA	8:H:21:MET:CE	2.41	0.47
1:A:150:ILE:O	1:A:151:VAL:C	2.55	0.47
3:C:77:MET:HB2	3:C:150:HIS:HB2	1.95	0.47
3:C:92:GLU:O	3:C:93:GLU:C	2.57	0.47
8:H:17:TRP:O	8:H:21:MET:HB2	2.14	0.47
2:B:82:TYR:CB	2:B:83:PRO:CD	2.91	0.47
5:E:16:PHE:CD1	5:E:16:PHE:C	2.93	0.47
6:F:8:ALA:HB2	7:G:5:LEU:HD12	1.96	0.47
2:B:32:TRP:CG	2:B:33:PRO:N	2.82	0.47
3:C:116:VAL:HG12	3:C:116:VAL:O	2.15	0.47
6:F:6:LEU:O	6:F:10:LEU:HD23	2.14	0.47
2:B:134:LEU:HD11	7:G:22:PHE:HZ	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:60:GLN:NE2	3:C:70:LEU:HB3	2.29	0.47
1:A:77:SER:O	1:A:78:PHE:HB2	2.15	0.47
2:B:138:LEU:O	2:B:139:VAL:C	2.58	0.47
3:C:1:TYR:CD2	3:C:118:PRO:HG3	2.49	0.47
3:C:104:GLN:HA	3:C:105:PRO:HD3	1.71	0.47
7:G:28:GLN:C	7:G:30:LYS:H	2.22	0.47
1:A:112:LYS:CB	1:A:113:PRO:CD	2.82	0.47
1:A:158:ILE:HA	1:A:159:PRO:HD3	1.63	0.47
3:C:171:VAL:HG13	3:C:234:ASN:HD22	1.79	0.47
3:C:231:LEU:HD12	3:C:231:LEU:C	2.40	0.47
4:D:118:ASN:HD21	4:D:120:ALA:HB3	1.79	0.47
4:D:131:SER:CB	4:D:143:PRO:HD2	2.39	0.47
6:F:30:GLN:HG3	6:F:31:GLY:N	2.28	0.47
17:G:101:BCR:H323	8:H:19:ILE:HG12	1.95	0.47
1:A:105:TYR:CD1	13:B:201:CLA:HMB1	2.50	0.47
3:C:42:PRO:HG3	3:C:144:PHE:CE2	2.50	0.47
1:A:17:LEU:C	1:A:17:LEU:HD13	2.39	0.47
2:B:11:ASP:OD1	2:B:13:LYS:N	2.46	0.47
2:B:137:THR:HG21	7:G:18:LEU:HD11	1.96	0.47
2:B:154:THR:HG23	2:B:155:LEU:N	2.27	0.47
3:C:199:ILE:CG2	3:C:200:GLN:H	2.12	0.47
4:D:57:LYS:HG3	4:D:62:ASN:O	2.15	0.47
4:D:165:TRP:CH2	4:D:170:PHE:HD1	2.33	0.47
1:A:1:MET:CE	1:A:1:MET:H3	2.22	0.46
2:B:34:ASN:HD22	2:B:34:ASN:H	1.62	0.46
2:B:119:LYS:O	2:B:119:LYS:HG2	2.14	0.46
3:C:199:ILE:HD12	3:C:207:VAL:HG23	1.97	0.46
5:E:24:PHE:CZ	6:F:29:ILE:HD11	2.50	0.46
3:C:1:TYR:HD2	3:C:118:PRO:HG3	1.81	0.46
1:A:97:MET:O	1:A:100:HIS:HB3	2.15	0.46
2:B:32:TRP:CD1	2:B:33:PRO:CD	2.89	0.46
3:C:45:VAL:HG21	3:C:89:ARG:O	2.16	0.46
6:F:26:LEU:HD13	6:F:26:LEU:HA	1.77	0.46
10:A:302:HEM:HHA	10:A:302:HEM:HBA1	1.98	0.46
2:B:122:ASN:HA	2:B:123:PRO:HD3	1.88	0.46
3:C:68:VAL:CG2	3:C:69:GLY:H	2.26	0.46
1:A:17:LEU:HD13	1:A:17:LEU:O	2.15	0.46
1:A:106:LEU:HD21	2:B:133:PHE:CD1	2.51	0.46
4:D:152:HIS:O	4:D:162:LEU:HA	2.16	0.46
4:D:141:ARG:CG	4:D:142:GLY:H	2.28	0.46
1:A:11:ARG:H	1:A:11:ARG:HG2	1.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:HIS:CB	7:G:28:GLN:HE22	2.29	0.46
1:A:112:LYS:O	1:A:113:PRO:C	2.57	0.46
6:F:24:VAL:O	6:F:27:LEU:N	2.49	0.46
1:A:112:LYS:O	1:A:115:GLU:CD	2.59	0.46
1:A:211:ILE:HG23	1:A:212:SER:O	2.16	0.46
2:B:89:ARG:HG3	2:B:90:SER:N	2.31	0.46
3:C:53:PRO:HA	3:C:125:GLN:OE1	2.15	0.46
3:C:47:LYS:HG3	3:C:128:VAL:HG13	1.98	0.46
5:E:8:TYR:CZ	5:E:12:ILE:CD1	2.91	0.46
1:A:66:TYR:OH	2:B:63:GLY:O	2.28	0.45
2:B:95:LEU:HD22	2:B:99:LEU:HD11	1.96	0.45
7:G:26:TYR:O	7:G:28:GLN:N	2.48	0.45
14:H:1002:OPC:HBP1	14:H:1002:OPC:HBM1	1.61	0.45
1:A:93:MET:SD	10:A:301:HEM:CBB	3.04	0.45
4:D:139:VAL:HG13	4:D:147:SER:HA	1.98	0.45
4:D:169:ASP:OD1	4:D:176:PRO:CB	2.63	0.45
5:E:8:TYR:CE2	5:E:12:ILE:HD11	2.50	0.45
3:C:22:CYS:SG	3:C:240:PHE:CE1	3.08	0.45
3:C:34:VAL:CG2	3:C:151:LEU:CB	2.95	0.45
1:A:211:ILE:CD1	10:A:302:HEM:O2D	2.65	0.45
4:D:101:ASP:O	4:D:153:ALA:N	2.49	0.45
2:B:6:LYS:HG2	7:G:35:LEU:HD22	1.97	0.45
5:E:8:TYR:CE2	5:E:12:ILE:CD1	2.99	0.45
11:A:303:HEC:HBB2	11:A:303:HEC:HMB3	1.99	0.45
3:C:60:GLN:HE22	3:C:156:GLY:CA	2.28	0.45
1:A:92:MET:HB3	14:H:1002:OPC:CCB	2.47	0.45
1:A:199:MET:HE2	10:A:302:HEM:HBB2	1.98	0.45
4:D:118:ASN:C	4:D:118:ASN:ND2	2.73	0.45
7:G:26:TYR:C	7:G:28:GLN:N	2.75	0.45
2:B:6:LYS:HB2	2:B:6:LYS:HZ3	1.81	0.45
3:C:34:VAL:HG21	3:C:151:LEU:HB2	1.99	0.45
4:D:102:TYR:HA	4:D:151:CYS:O	2.16	0.45
2:B:96:LEU:O	2:B:100:LEU:HD12	2.16	0.45
2:B:124:PHE:HE1	7:G:26:TYR:HB2	1.82	0.44
1:A:80:TRP:CZ2	3:C:254:ARG:HG2	2.52	0.44
2:B:128:VAL:HG12	2:B:132:ILE:HD13	1.98	0.44
3:C:171:VAL:HG12	3:C:233:ASN:C	2.41	0.44
4:D:124:PHE:CE1	4:D:134:ASP:O	2.70	0.44
3:C:119:LEU:HD22	3:C:124:TYR:CD1	2.53	0.44
7:G:13:LEU:HD23	7:G:13:LEU:HA	1.89	0.44
3:C:2:PRO:HD3	11:C:301:HEC:CHB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:285:ALA:HB2	4:D:10:VAL:HG21	1.98	0.44
2:B:109:ILE:O	2:B:112:PRO:CD	2.59	0.44
3:C:141:ASN:C	3:C:141:ASN:ND2	2.72	0.44
1:A:111:LYS:O	1:A:113:PRO:N	2.50	0.44
12:A:1102:UMQ:O3'	12:A:1102:UMQ:H11	2.13	0.44
3:C:79:PRO:HD3	3:C:149:ILE:HG12	1.98	0.44
6:F:20:TRP:HZ3	17:G:101:BCR:C19	2.22	0.44
1:A:110:PHE:HB3	1:A:118:TRP:CE3	2.53	0.44
1:A:177:GLN:O	1:A:178:ALA:C	2.59	0.44
2:B:32:TRP:O	2:B:34:ASN:N	2.51	0.44
1:A:151:VAL:CG2	1:A:152:SER:N	2.81	0.44
2:B:110:LEU:O	2:B:113:PHE:N	2.51	0.44
4:D:152:HIS:CE1	4:D:165:TRP:CD1	3.06	0.44
1:A:112:LYS:C	1:A:115:GLU:OE1	2.60	0.43
4:D:152:HIS:CE1	4:D:165:TRP:NE1	2.86	0.43
7:G:26:TYR:O	7:G:27:GLN:C	2.61	0.43
2:B:31:ALA:C	2:B:32:TRP:O	2.61	0.43
3:C:65:GLY:O	3:C:66:SER:C	2.47	0.43
4:D:80:LEU:HD23	4:D:80:LEU:HA	1.84	0.43
1:A:101:VAL:CG2	10:A:302:HEM:HMC3	2.47	0.43
2:B:36:LEU:HD23	2:B:36:LEU:HA	1.70	0.43
2:B:65:PRO:O	2:B:66:ALA:C	2.60	0.43
2:B:81:LEU:HD23	2:B:81:LEU:HA	1.80	0.43
3:C:144:PHE:CZ	3:C:251:ASP:HB2	2.52	0.43
3:C:225:VAL:HG11	3:C:229:GLU:CG	2.49	0.43
5:E:20:VAL:HA	5:E:23:ILE:HG13	2.00	0.43
3:C:26:HIS:CE1	3:C:154:ASN:OD1	2.72	0.43
5:E:14:LEU:C	5:E:14:LEU:HD23	2.44	0.43
4:D:129:HIS:CB	15:D:200:FES:S1	2.94	0.43
4:D:178:TRP:O	4:D:179:VAL:C	2.62	0.43
7:G:9:LEU:HD22	14:H:1002:OPC:HBV1	2.01	0.43
2:B:154:THR:O	2:B:157:LEU:HD12	2.18	0.43
3:C:34:VAL:CG2	3:C:151:LEU:HB2	2.49	0.43
4:D:117:TRP:CZ3	4:D:122:ASN:O	2.72	0.43
1:A:164:LEU:O	1:A:165:ILE:C	2.60	0.43
3:C:42:PRO:HD3	3:C:250:GLN:O	2.19	0.43
6:F:24:VAL:O	6:F:27:LEU:HB2	2.18	0.43
2:B:156:THR:O	2:B:157:LEU:CB	2.64	0.42
3:C:225:VAL:HG12	3:C:229:GLU:HG2	1.98	0.42
4:D:57:LYS:HB3	4:D:61:GLY:CA	2.48	0.42
4:D:177:TRP:CE2	4:D:178:TRP:HE3	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:22:LEU:O	6:F:26:LEU:HD22	2.19	0.42
1:A:145:TYR:CD1	1:A:145:TYR:C	2.97	0.42
12:A:1102:UMQ:H11	12:A:1102:UMQ:H3'1	1.72	0.42
4:D:90:TYR:OH	4:D:116:PRO:HA	2.19	0.42
1:A:137:SER:HB3	1:A:148:VAL:CG2	2.50	0.42
4:D:101:ASP:O	4:D:153:ALA:HB3	2.19	0.42
1:A:14:ILE:HG23	12:A:1103:UMQ:HD1	2.01	0.42
2:B:102:ALA:O	2:B:105:PRO:HD2	2.20	0.42
7:G:22:PHE:O	7:G:23:TYR:C	2.60	0.42
17:G:101:BCR:H361	17:G:101:BCR:H20C	1.61	0.42
3:C:19:ARG:O	3:C:242:GLN:OE1	2.38	0.42
3:C:44:THR:HG21	8:H:1:MET:SD	2.59	0.42
4:D:53:GLY:HA3	4:D:163:THR:HA	2.02	0.42
4:D:123:LYS:HE2	4:D:132:GLN:NE2	2.35	0.42
2:B:133:PHE:O	2:B:136:GLY:N	2.53	0.42
3:C:157:ARG:H	3:C:157:ARG:HG2	1.58	0.42
4:D:174:GLU:O	4:D:175:LYS:O	2.37	0.42
8:H:14:VAL:O	8:H:18:SER:HB2	2.19	0.42
1:A:139:PRO:HG3	10:A:301:HEM:O2A	2.19	0.42
3:C:266:MET:SD	8:H:13:VAL:HG12	2.60	0.42
2:B:41:PRO:HB2	3:C:272:LEU:HD13	2.02	0.42
2:B:71:THR:O	2:B:72:PRO:C	2.60	0.42
4:D:83:GLY:O	4:D:84:LEU:C	2.62	0.42
4:D:124:PHE:CD1	4:D:134:ASP:O	2.73	0.42
7:G:16:ALA:O	17:G:101:BCR:H16C	2.19	0.42
1:A:51:GLY:O	1:A:55:THR:HG23	2.20	0.42
1:A:215:LEU:HB2	2:B:122:ASN:H	1.85	0.42
3:C:159:GLN:HB3	3:C:170:ASN:HD22	1.85	0.42
1:A:35:CYS:O	1:A:36:LEU:C	2.63	0.42
2:B:25:ASN:HD22	2:B:25:ASN:C	2.27	0.42
2:B:101:MET:O	2:B:104:VAL:HG23	2.19	0.42
2:B:158:GLY:O	2:B:159:LEU:CD2	2.48	0.42
3:C:144:PHE:CE2	3:C:251:ASP:HB2	2.55	0.42
4:D:144:ALA:HA	4:D:145:PRO:HD3	1.93	0.42
1:A:25:TYR:CD2	2:B:30:PRO:HA	2.54	0.41
1:A:31:ASN:HD22	1:A:33:PHE:H	1.68	0.41
1:A:146:TRP:CD1	2:B:72:PRO:CD	3.03	0.41
2:B:89:ARG:NH2	2:B:146:GLY:O	2.53	0.41
4:D:78:ARG:HD2	4:D:117:TRP:CE2	2.55	0.41
4:D:141:ARG:HG2	4:D:142:GLY:H	1.85	0.41
1:A:103:ARG:NH1	1:A:104:VAL:HG22	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:TRP:CG	2:B:72:PRO:HD2	2.55	0.41
12:A:1101:UMQ:HK1	4:D:34:ALA:HA	2.02	0.41
2:B:61:MET:HE2	2:B:61:MET:HB3	1.89	0.41
13:B:201:CLA:HHD	14:B:202:OPC:HBW2	2.02	0.41
3:C:58:LEU:CD1	3:C:237:VAL:HG21	2.50	0.41
4:D:34:ALA:O	4:D:37:PRO:HD2	2.20	0.41
1:A:59:LYS:HG3	1:A:68:SER:HB3	2.02	0.41
2:B:124:PHE:HE1	7:G:26:TYR:CA	2.33	0.41
8:H:3:ILE:HG23	8:H:4:ASP:N	2.34	0.41
8:H:12:LEU:H	8:H:12:LEU:HG	1.64	0.41
1:A:31:ASN:HD21	1:A:33:PHE:HB2	1.84	0.41
12:A:1101:UMQ:HB1	3:C:254:ARG:HA	2.01	0.41
2:B:75:ILE:C	2:B:76:LEU:HD12	2.46	0.41
3:C:180:ILE:HG23	3:C:180:ILE:O	2.20	0.41
2:B:86:GLN:NE2	2:B:86:GLN:HA	2.35	0.41
3:C:28:ALA:HB3	3:C:239:GLY:CA	2.44	0.41
3:C:264:LEU:HA	3:C:264:LEU:HD23	1.86	0.41
4:D:106:ALA:O	4:D:114:VAL:HA	2.19	0.41
4:D:115:VAL:HG11	4:D:124:PHE:HB3	2.02	0.41
1:A:78:PHE:HE2	12:A:1101:UMQ:HC2	1.86	0.41
3:C:211:ILE:HA	3:C:212:PRO:HD3	1.94	0.41
3:C:257:TRP:O	3:C:258:MET:C	2.62	0.41
1:A:7:TRP:CD1	1:A:11:ARG:NH2	2.89	0.41
1:A:124:LEU:HD23	1:A:124:LEU:HA	1.87	0.41
4:D:18:PHE:CZ	4:D:22:LEU:HD21	2.55	0.41
7:G:18:LEU:HD23	7:G:18:LEU:HA	1.81	0.41
1:A:36:LEU:N	1:A:36:LEU:CD1	2.84	0.41
2:B:17:LYS:HB3	2:B:22:MET:O	2.21	0.41
4:D:165:TRP:HZ3	4:D:169:ASP:HA	1.86	0.41
2:B:57:LEU:HD13	8:H:8:TRP:CD2	2.56	0.41
3:C:75:VAL:HG23	3:C:115:LEU:HD23	2.02	0.41
3:C:114:LEU:HA	3:C:114:LEU:HD23	1.73	0.41
4:D:156:GLN:NE2	4:D:156:GLN:CA	2.83	0.41
7:G:21:LEU:HD12	7:G:21:LEU:HA	1.84	0.41
1:A:175:VAL:CG1	1:A:176:GLY:N	2.84	0.41
3:C:77:MET:HG2	3:C:113:VAL:HG13	2.03	0.41
3:C:172:PHE:O	3:C:173:THR:O	2.39	0.41
3:C:266:MET:HE1	5:E:11:PHE:HE2	1.83	0.41
4:D:105:ASN:O	4:D:148:LEU:HD22	2.21	0.41
4:D:177:TRP:NE1	4:D:178:TRP:CE3	2.89	0.41
4:D:56:ALA:C	4:D:57:LYS:HD2	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:H:1002:OPC:HBC1	14:H:1002:OPC:CAY	2.51	0.40
11:A:303:HEC:NB	2:B:40:PHE:CZ	2.90	0.40
4:D:68:LYS:HE3	4:D:68:LYS:HB2	1.77	0.40
1:A:31:ASN:ND2	1:A:33:PHE:HD2	2.20	0.40
3:C:271:MET:HG3	4:D:22:LEU:HB3	2.03	0.40
7:G:26:TYR:C	7:G:28:GLN:H	2.29	0.40
2:B:32:TRP:HB3	2:B:33:PRO:HD2	2.01	0.40
2:B:123:PRO:HD2	7:G:25:ALA:CB	2.37	0.40
2:B:145:ILE:HG22	2:B:149:PHE:HE1	1.86	0.40
13:B:201:CLA:C4	13:B:201:CLA:O2A	2.69	0.40
3:C:85:ALA:HA	3:C:86:PRO:HD2	1.91	0.40
3:C:180:ILE:HD11	3:C:197:VAL:HG13	2.04	0.40
1:A:112:LYS:O	1:A:114:ARG:N	2.55	0.40
3:C:12:THR:OG1	3:C:13:PRO:HD2	2.22	0.40
3:C:180:ILE:HG22	3:C:223:GLN:H	1.87	0.40
5:E:22:ILE:O	5:E:26:ILE:CB	2.64	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:108:GLU:OE1	7:G:33:ASN:CB[8_565]	1.89	0.31
1:A:112:LYS:CE	3:C:87:GLU:OE1[8_665]	2.14	0.06

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%)	185 (87%)	26 (12%)	2 (1%)	14	48
2	B	158/160 (99%)	126 (80%)	25 (16%)	7 (4%)	2	12
3	C	286/289 (99%)	244 (85%)	31 (11%)	11 (4%)	2	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	162/179 (90%)	124 (76%)	28 (17%)	10 (6%)	1	6
5	E	30/32 (94%)	23 (77%)	6 (20%)	1 (3%)	3	17
6	F	30/35 (86%)	25 (83%)	5 (17%)	0	100	100
7	G	35/37 (95%)	16 (46%)	14 (40%)	5 (14%)	0	1
8	H	27/29 (93%)	24 (89%)	2 (7%)	1 (4%)	2	15
All	All	941/976 (96%)	767 (82%)	137 (15%)	37 (4%)	2	14

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	LYS
2	B	32	TRP
2	B	74	GLU
2	B	125	ARG
3	C	66	SER
3	C	173	THR
3	C	189	GLU
3	C	192	ASN
3	C	200	GLN
3	C	230	ALA
4	D	77	ASP
4	D	167	GLU
7	G	34	GLU
1	A	3	ASN
2	B	22	MET
3	C	110	GLN
4	D	47	GLY
4	D	73	HIS
7	G	31	ARG
3	C	186	GLU
7	G	27	GLN
2	B	133	PHE
3	C	20	ILE
3	C	233	ASN
4	D	146	LEU
7	G	35	LEU
2	B	86	GLN
4	D	166	THR
4	D	170	PHE
4	D	175	LYS

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Mol	Chain	Res	Type
5	E	28	SER
2	B	2	ALA
7	G	32	PRO
8	H	23	VAL
3	C	199	ILE
4	D	99	ILE
4	D	145	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	137/137 (100%)	121 (88%)	16 (12%)	5	23
3	C	242/243 (100%)	219 (90%)	23 (10%)	8	31
4	D	134/146 (92%)	126 (94%)	8 (6%)	17	50
5	E	25/25 (100%)	23 (92%)	2 (8%)	11	38
6	F	24/27 (89%)	17 (71%)	7 (29%)	0	2
7	G	28/28 (100%)	24 (86%)	4 (14%)	3	16
8	H	24/24 (100%)	19 (79%)	5 (21%)	1	7
All	All	798/814 (98%)	716 (90%)	82 (10%)	7	28

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	11	ARG
1	A	12	LEU
1	A	14	ILE
1	A	31	ASN
1	A	36	LEU
1	A	61	THR
1	A	81	LEU

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Mol	Chain	Res	Type
1	A	87	ARG
1	A	95	LEU
1	A	103	ARG
1	A	107	THR
1	A	151	VAL
1	A	164	LEU
1	A	200	LEU
1	A	211	ILE
1	A	215	LEU
2	B	6	LYS
2	B	20	LYS
2	B	25	ASN
2	B	34	ASN
2	B	39	VAL
2	B	64	GLU
2	B	73	LEU
2	B	75	ILE
2	B	79	TRP
2	B	95	LEU
2	B	96	LEU
2	B	103	SER
2	B	108	LEU
2	B	119	LYS
2	B	134	LEU
2	B	143	LEU
3	C	58	LEU
3	C	61	VAL
3	C	70	LEU
3	C	71	ASN
3	C	88	GLU
3	C	94	LEU
3	C	116	VAL
3	C	131	VAL
3	C	141	ASN
3	C	155	ARG
3	C	166	LYS
3	C	170	ASN
3	C	185	LYS
3	C	194	LYS
3	C	211	ILE
3	C	249	LEU
3	C	256	LYS

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Mol	Chain	Res	Type
3	C	264	LEU
3	C	267	LEU
3	C	270	LEU
3	C	271	MET
3	C	286	GLU
3	C	288	ASN
4	D	59	LYS
4	D	72	SER
4	D	125	LYS
4	D	133	TYR
4	D	154	THR
4	D	156	GLN
4	D	165	TRP
4	D	167	GLU
5	E	9	ILE
5	E	29	ILE
6	F	1	MET
6	F	2	THR
6	F	7	TYR
6	F	22	LEU
6	F	26	LEU
6	F	29	ILE
6	F	30	GLN
7	G	3	GLU
7	G	6	LEU
7	G	17	THR
7	G	21	LEU
8	H	2	GLU
8	H	6	LEU
8	H	14	VAL
8	H	18	SER
8	H	21	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	47	GLN
2	B	25	ASN
2	B	34	ASN
2	B	118	ASN
3	C	6	GLN

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Mol	Chain	Res	Type
3	C	59	GLN
3	C	60	GLN
3	C	71	ASN
3	C	110	GLN
3	C	123	GLN
3	C	141	ASN
3	C	196	GLN
3	C	234	ASN
3	C	242	GLN
3	C	250	GLN
3	C	288	ASN
4	D	82	GLN
4	D	118	ASN
4	D	132	GLN
4	D	156	GLN
4	D	159	ASN
7	G	27	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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
11	HEC	A	303	18	50,50,50	2.12	8 (16%)	68,82,82	1.47	8 (11%)
14	OPC	H	1002	-	53,53,54	2.14	14 (26%)	59,61,64	2.30	16 (27%)
10	HEM	A	301	1	50,50,50	1.81	8 (16%)	67,82,82	1.55	17 (25%)
13	CLA	B	201	18	69,73,73	1.88	16 (23%)	82,113,113	2.56	27 (32%)
16	SQD	D	201	-	52,54,54	3.24	23 (44%)	62,65,65	4.54	23 (37%)
12	UMQ	A	1104	-	35,35,35	1.40	3 (8%)	46,46,46	2.08	8 (17%)
17	BCR	G	101	-	41,41,41	2.81	12 (29%)	56,56,56	7.05	17 (30%)
12	UMQ	A	1103	-	35,35,35	1.50	4 (11%)	46,46,46	2.11	8 (17%)
15	FES	D	200	4	0,4,4	-	-	-	-	-
11	HEC	C	301	3	50,50,50	1.94	8 (16%)	68,82,82	1.64	14 (20%)
10	HEM	A	302	1	50,50,50	1.70	9 (18%)	67,82,82	1.24	7 (10%)
12	UMQ	A	1101	-	35,35,35	1.46	4 (11%)	46,46,46	2.16	9 (19%)
14	OPC	B	202	-	53,53,54	2.07	14 (26%)	59,61,64	2.43	13 (22%)
12	UMQ	A	1102	-	35,35,35	1.61	4 (11%)	46,46,46	2.25	11 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	HEC	A	303	18	1/1/3/7	8/14/54/54	-
14	OPC	H	1002	-	-	26/57/57/60	-
16	SQD	D	201	-	1/1/9/9	28/49/69/69	0/1/1/1
13	CLA	B	201	18	1/1/15/20	16/39/115/115	-
10	HEM	A	301	1	-	5/14/54/54	-
12	UMQ	A	1104	-	2/2/10/10	11/20/60/60	0/2/2/2
17	BCR	G	101	-	-	9/29/63/63	0/2/2/2
12	UMQ	A	1103	-	2/2/10/10	5/20/60/60	0/2/2/2
15	FES	D	200	4	-	-	0/1/1/1
11	HEC	C	301	3	1/1/3/7	8/14/54/54	-
10	HEM	A	302	1	-	3/14/54/54	-
12	UMQ	A	1101	-	2/2/10/10	12/20/60/60	0/2/2/2
14	OPC	B	202	-	-	22/57/57/60	-
12	UMQ	A	1102	-	2/2/10/10	11/20/60/60	0/2/2/2

All (127) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	D	201	SQD	C4-C3	12.70	1.85	1.52
17	G	101	BCR	C8-C9	-8.96	1.26	1.46
17	G	101	BCR	C23-C22	-8.54	1.27	1.46
11	C	301	HEC	C3D-C2D	7.89	1.53	1.36
11	A	303	HEC	C3D-C2D	7.52	1.53	1.36
10	A	301	HEM	C3D-C2D	7.19	1.52	1.36
10	A	302	HEM	C3D-C2D	6.92	1.51	1.36
12	A	1102	UMQ	C1'-C2'	-6.57	1.33	1.52
16	D	201	SQD	C17-C16	-6.23	1.20	1.51
12	A	1103	UMQ	C1'-C2'	-6.11	1.34	1.52
10	A	301	HEM	FE-ND	6.10	2.13	1.94
12	A	1104	UMQ	C1'-C2'	-6.07	1.34	1.52
11	A	303	HEC	FE-ND	6.05	2.13	1.94
16	D	201	SQD	C12-C11	-6.03	1.21	1.51
12	A	1101	UMQ	C1'-C2'	-5.98	1.35	1.52
14	B	202	OPC	CAG-CAH	-5.78	1.33	1.51
14	H	1002	OPC	CAG-CAH	-5.77	1.33	1.51
17	G	101	BCR	C24-C25	-5.13	1.27	1.45
14	B	202	OPC	OBJ-CBK	5.12	1.48	1.33
16	D	201	SQD	C18-C17	-5.05	1.26	1.51
17	G	101	BCR	C7-C6	-5.04	1.27	1.45
14	H	1002	OPC	CAQ-CAP	-4.97	1.34	1.52
16	D	201	SQD	C16-C15	-4.95	1.27	1.51
14	B	202	OPC	CAQ-CAP	-4.93	1.34	1.52
16	D	201	SQD	C11-C10	-4.91	1.27	1.51
16	D	201	SQD	C13-C12	-4.86	1.27	1.51
14	H	1002	OPC	OBJ-CBK	4.85	1.47	1.33
11	A	303	HEC	FE-NC	4.83	2.11	1.95
16	D	201	SQD	O48-C23	4.78	1.47	1.33
13	B	201	CLA	C3C-C2C	4.73	1.47	1.36
11	A	303	HEC	CBC-CAC	-4.68	1.31	1.51
14	H	1002	OPC	OAN-CAO	4.63	1.47	1.34
17	G	101	BCR	C12-C13	-4.59	1.36	1.46
17	G	101	BCR	C8-C7	-4.53	1.19	1.33
14	H	1002	OPC	CBP-CBQ	-4.52	1.33	1.52
17	G	101	BCR	C24-C23	-4.50	1.19	1.33
17	G	101	BCR	C19-C18	-4.50	1.36	1.46
12	A	1102	UMQ	O1'-C1'	4.46	1.47	1.40
16	D	201	SQD	O47-C7	4.42	1.46	1.34
13	B	201	CLA	CHC-C1C	4.37	1.47	1.38
11	A	303	HEC	CBB-CAB	-4.37	1.32	1.51
11	C	301	HEC	FE-NB	4.34	2.08	1.94
13	B	201	CLA	O2D-CGD	4.29	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	C	301	HEC	CBB-CAB	-4.24	1.33	1.51
13	B	201	CLA	O2A-CGA	4.22	1.45	1.33
12	A	1103	UMQ	O1'-C1'	4.19	1.47	1.40
13	B	201	CLA	OBD-CAD	4.14	1.29	1.22
12	A	1101	UMQ	O2'-C2'	-4.09	1.32	1.43
13	B	201	CLA	C3D-C4D	-4.09	1.35	1.44
14	B	202	OPC	CBP-CBQ	-4.07	1.35	1.52
16	D	201	SQD	C21-C20	-4.06	1.26	1.51
13	B	201	CLA	CHD-C1D	4.05	1.46	1.38
11	A	303	HEC	FE-NB	4.03	2.07	1.94
14	B	202	OPC	OAN-CAO	4.02	1.45	1.34
14	H	1002	OPC	CBP-CBO	-3.97	1.32	1.51
14	B	202	OPC	CAV-CAW	3.90	1.53	1.31
11	C	301	HEC	CBC-CAC	-3.88	1.35	1.51
13	B	201	CLA	CHD-C4C	3.83	1.47	1.39
12	A	1102	UMQ	O2'-C2'	-3.79	1.33	1.43
14	H	1002	OPC	CAV-CAW	3.75	1.53	1.31
14	H	1002	OPC	CAQ-CAR	-3.73	1.33	1.51
14	H	1002	OPC	CAR-CAS	-3.72	1.33	1.51
11	C	301	HEC	FE-ND	3.72	2.06	1.94
10	A	302	HEM	FE-ND	3.66	2.06	1.94
12	A	1103	UMQ	O2'-C2'	-3.64	1.33	1.43
12	A	1104	UMQ	O2'-C2'	-3.63	1.34	1.43
16	D	201	SQD	C36-C35	-3.59	1.33	1.51
16	D	201	SQD	C19-C18	-3.57	1.34	1.51
16	D	201	SQD	C34-C33	-3.53	1.34	1.51
14	B	202	OPC	CBB-CBC	-3.53	1.34	1.51
10	A	301	HEM	CMB-C2B	3.53	1.58	1.50
16	D	201	SQD	C20-C19	-3.52	1.34	1.51
16	D	201	SQD	C32-C31	-3.52	1.34	1.51
14	H	1002	OPC	CBC-CBD	-3.52	1.34	1.51
14	B	202	OPC	CBC-CBD	-3.52	1.34	1.51
14	B	202	OPC	CAQ-CAR	-3.50	1.34	1.51
16	D	201	SQD	C33-C32	-3.47	1.34	1.51
16	D	201	SQD	C35-C34	-3.46	1.34	1.51
13	B	201	CLA	CHC-C4B	3.45	1.47	1.39
14	H	1002	OPC	CBB-CBC	-3.41	1.34	1.51
16	D	201	SQD	C15-C14	-3.41	1.34	1.51
12	A	1101	UMQ	O1'-C1'	3.40	1.45	1.40
14	B	202	OPC	CBP-CBO	-3.38	1.35	1.51
12	A	1104	UMQ	O1'-C1'	3.36	1.45	1.40
13	B	201	CLA	CHB-C1B	3.36	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	D	201	SQD	C22-C21	-3.35	1.26	1.50
14	B	202	OPC	CAR-CAS	-3.34	1.35	1.51
16	D	201	SQD	C14-C13	-3.34	1.35	1.51
14	H	1002	OPC	CBQ-CBR	-3.32	1.31	1.50
13	B	201	CLA	C3D-C2D	3.17	1.47	1.39
14	H	1002	OPC	CBT-CBS	-3.03	1.33	1.50
10	A	302	HEM	CAC-C3C	2.89	1.55	1.47
16	D	201	SQD	C37-C36	-2.88	1.33	1.51
14	H	1002	OPC	CAG-NAF	-2.87	1.42	1.51
14	B	202	OPC	CBQ-CBR	-2.83	1.34	1.50
14	B	202	OPC	CBT-CBS	-2.72	1.35	1.50
13	B	201	CLA	C1D-C2D	2.72	1.50	1.45
17	G	101	BCR	C11-C10	-2.69	1.34	1.43
10	A	301	HEM	CMC-C2C	2.68	1.56	1.50
10	A	301	HEM	C2A-C3A	-2.62	1.32	1.38
14	B	202	OPC	CAG-NAF	-2.60	1.43	1.51
16	D	201	SQD	C38-C37	-2.49	1.32	1.50
17	G	101	BCR	C15-C14	-2.44	1.35	1.43
13	B	201	CLA	C1B-C2B	2.43	1.48	1.43
10	A	302	HEM	C3C-C2C	-2.42	1.32	1.37
16	D	201	SQD	O6-C1	2.37	1.44	1.40
10	A	302	HEM	CAB-C3B	2.36	1.53	1.47
10	A	301	HEM	CAB-C3B	2.35	1.53	1.47
10	A	302	HEM	CMA-C3A	2.33	1.55	1.50
17	G	101	BCR	C16-C17	-2.31	1.36	1.43
13	B	201	CLA	C4B-NB	-2.31	1.34	1.37
11	C	301	HEC	CMA-C3A	2.26	1.55	1.50
11	C	301	HEC	CMD-C2D	2.24	1.55	1.50
13	B	201	CLA	C1C-C2C	2.22	1.49	1.44
10	A	302	HEM	C3B-C2B	-2.21	1.32	1.37
10	A	301	HEM	CHB-C1B	-2.18	1.34	1.38
13	B	201	CLA	C4C-C3C	2.18	1.48	1.45
11	A	303	HEC	C3C-C2C	-2.16	1.33	1.38
10	A	301	HEM	CAC-C3C	2.13	1.53	1.47
11	C	301	HEC	C4B-C3B	2.13	1.48	1.45
12	A	1102	UMQ	O5'-C1'	2.08	1.47	1.41
11	A	303	HEC	O1D-CGD	2.06	1.28	1.22
12	A	1101	UMQ	O5'-C1'	2.05	1.47	1.41
17	G	101	BCR	C20-C21	-2.05	1.36	1.43
12	A	1103	UMQ	O5'-C1'	2.05	1.47	1.41
10	A	302	HEM	CMC-C2C	2.05	1.55	1.50
10	A	302	HEM	CMD-C2D	2.01	1.54	1.50

All (178) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	G	101	BCR	C24-C23-C22	33.77	176.20	126.23
17	G	101	BCR	C7-C8-C9	29.62	170.05	126.23
16	D	201	SQD	C4-C3-C2	-19.42	76.74	110.83
17	G	101	BCR	C23-C24-C25	17.93	174.90	127.00
17	G	101	BCR	C8-C7-C6	17.39	173.47	127.00
16	D	201	SQD	C18-C17-C16	11.30	171.49	114.37
16	D	201	SQD	C12-C11-C10	10.96	169.79	114.37
16	D	201	SQD	C17-C16-C15	10.73	168.62	114.37
16	D	201	SQD	C13-C12-C11	10.66	168.26	114.37
16	D	201	SQD	O3-C3-C4	-9.56	87.85	110.38
16	D	201	SQD	C22-C21-C20	9.47	177.30	113.36
14	B	202	OPC	CAA-NAF-CBG	-8.89	85.62	108.98
14	B	202	OPC	CAA-NAF-CAE	-8.49	86.67	108.98
14	H	1002	OPC	CAA-NAF-CAE	-8.46	86.75	108.98
14	H	1002	OPC	CAA-NAF-CBG	-8.24	87.33	108.98
12	A	1103	UMQ	O1'-C1'-C2'	7.70	119.96	108.27
12	A	1101	UMQ	O1'-C1'-C2'	7.55	119.74	108.27
13	B	201	CLA	CMD-C2D-C1D	7.17	137.35	124.73
12	A	1102	UMQ	O1'-C1'-C2'	7.16	119.14	108.27
12	A	1104	UMQ	O1'-C1'-C2'	7.12	119.08	108.27
13	B	201	CLA	C2B-C1B-NB	6.43	117.00	110.33
12	A	1104	UMQ	O5'-C1'-C2'	6.36	123.44	110.37
16	D	201	SQD	C3-C4-C5	-6.33	98.76	110.23
13	B	201	CLA	C2C-C1C-NC	6.04	116.33	109.98
13	B	201	CLA	O2D-CGD-CBD	5.94	121.61	111.23
13	B	201	CLA	C3B-C2B-C1B	-5.90	100.22	107.17
14	B	202	OPC	CAA-NAF-CAG	-5.68	87.35	109.91
14	H	1002	OPC	CAA-NAF-CAG	-5.63	87.55	109.91
12	A	1104	UMQ	C1'-C2'-C3'	5.52	121.63	110.01
11	C	301	HEC	CAB-C3B-C4B	5.43	131.86	124.79
11	A	303	HEC	C1D-ND-C4D	5.30	111.49	105.21
12	A	1102	UMQ	O5'-C1'-O1'	5.27	122.49	110.04
14	B	202	OPC	OAN-CAO-CAP	5.20	122.72	111.48
12	A	1101	UMQ	O5'-C1'-C2'	5.14	120.93	110.37
12	A	1101	UMQ	O2'-C2'-C1'	5.05	122.12	110.08
12	A	1101	UMQ	C1'-C2'-C3'	4.93	120.39	110.01
12	A	1103	UMQ	O5'-C1'-C2'	4.93	120.49	110.37
12	A	1103	UMQ	C1'-C2'-C3'	4.89	120.30	110.01
12	A	1102	UMQ	CA-O1'-C1'	4.88	122.01	113.68
12	A	1104	UMQ	CA-O1'-C1'	4.87	121.99	113.68
12	A	1102	UMQ	C1'-C2'-C3'	4.84	120.19	110.01
16	D	201	SQD	O5-C5-C4	4.84	118.41	109.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	D	201	SQD	O7-S-C6	4.81	113.94	106.76
12	A	1103	UMQ	O2'-C2'-C1'	4.71	121.30	110.08
12	A	1103	UMQ	CA-O1'-C1'	4.68	121.67	113.68
13	B	201	CLA	O2D-CGD-O1D	-4.60	114.89	123.85
14	B	202	OPC	CAR-CAQ-CAP	4.58	129.97	113.13
17	G	101	BCR	C8-C9-C10	4.53	126.13	119.01
13	B	201	CLA	C3D-C2D-C1D	-4.52	99.66	105.83
16	D	201	SQD	O47-C7-C8	4.51	121.24	111.48
13	B	201	CLA	CHD-C4C-C3C	-4.49	118.22	124.77
13	B	201	CLA	O2A-CGA-CBA	4.48	125.50	111.83
14	H	1002	OPC	CBG-NAF-CAE	4.41	120.57	108.98
12	A	1104	UMQ	O2'-C2'-C1'	4.37	120.49	110.08
11	C	301	HEC	C1D-ND-C4D	4.35	110.36	105.21
10	A	301	HEM	C4D-ND-C1D	4.35	110.36	105.21
16	D	201	SQD	O9-S-C6	4.34	113.24	106.76
12	A	1102	UMQ	O2'-C2'-C1'	4.33	120.40	110.08
14	B	202	OPC	CBG-NAF-CAE	4.32	120.32	108.98
13	B	201	CLA	C3C-C4C-NC	4.22	115.83	110.43
13	B	201	CLA	C1C-C2C-C3C	-4.12	102.65	106.98
12	A	1103	UMQ	O5'-C1'-O1'	4.02	119.54	110.04
17	G	101	BCR	C38-C26-C25	-3.96	120.17	124.48
12	A	1101	UMQ	O5'-C1'-O1'	3.92	119.31	110.04
10	A	301	HEM	CHB-C4A-NA	3.90	130.92	123.86
12	A	1102	UMQ	O5'-C1'-C2'	3.89	118.37	110.37
14	B	202	OPC	OAN-CAO-OAD	-3.88	114.62	123.70
12	A	1101	UMQ	CA-O1'-C1'	3.86	120.28	113.68
13	B	201	CLA	CMB-C2B-C1B	3.84	131.26	125.42
13	B	201	CLA	C3B-C4B-NB	3.83	113.95	110.53
12	A	1102	UMQ	O2'-C2'-C3'	3.83	119.40	110.38
11	C	301	HEC	CAB-C3B-C2B	-3.77	120.63	127.56
13	B	201	CLA	C1D-ND-C4D	-3.75	103.68	106.31
13	B	201	CLA	CHD-C1D-ND	-3.70	119.60	124.80
16	D	201	SQD	O6-C1-C2	3.63	113.79	108.27
17	G	101	BCR	C34-C9-C10	-3.61	116.97	122.82
17	G	101	BCR	C3-C4-C5	-3.57	107.69	114.06
13	B	201	CLA	C4-C3-C5	3.56	121.41	115.23
13	B	201	CLA	C3D-C4D-ND	3.52	115.72	109.99
10	A	302	HEM	C1D-C2D-C3D	-3.52	103.28	106.98
13	B	201	CLA	O2A-CGA-O1A	-3.42	115.08	123.63
12	A	1103	UMQ	O2'-C2'-C3'	3.40	118.40	110.38
17	G	101	BCR	C32-C1-C6	-3.39	104.92	110.24
11	A	303	HEC	CBA-CAA-C2A	-3.36	103.23	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	301	HEC	CBC-CAC-C3C	3.34	121.47	112.42
14	H	1002	OPC	OAN-CAO-CAP	3.32	118.67	111.48
13	B	201	CLA	C2D-C1D-ND	3.32	113.41	110.13
11	A	303	HEC	CMD-C2D-C1D	3.24	130.10	125.03
13	B	201	CLA	CAA-CBA-CGA	-3.23	104.03	113.21
12	A	1104	UMQ	O2'-C2'-C3'	3.18	117.88	110.38
10	A	302	HEM	C4D-ND-C1D	3.15	108.94	105.21
12	A	1104	UMQ	O5'-C1'-O1'	3.15	117.48	110.04
16	D	201	SQD	C15-C14-C13	3.08	129.96	114.37
11	C	301	HEC	CHC-C4B-C3B	3.07	130.88	125.23
11	A	303	HEC	C3C-C4C-NC	-3.03	106.79	110.15
12	A	1101	UMQ	O2'-C2'-C3'	3.02	117.50	110.38
14	H	1002	OPC	OBJ-CBK-CBL	2.95	120.84	111.83
11	C	301	HEC	CHA-C1A-NA	2.95	127.67	124.45
11	A	303	HEC	CAB-C3B-C4B	2.90	128.56	124.79
10	A	301	HEM	CAD-CBD-CGD	-2.89	106.01	113.67
17	G	101	BCR	C33-C5-C6	-2.85	121.38	124.48
14	B	202	OPC	OBJ-CBK-CBL	2.84	120.50	111.83
13	B	201	CLA	CHB-C4A-NA	2.84	128.50	124.40
13	B	201	CLA	C4C-C3C-C2C	-2.83	102.77	106.89
12	A	1102	UMQ	O1-C1-C2	2.78	114.92	108.09
16	D	201	SQD	C14-C13-C12	2.77	128.38	114.37
14	B	202	OPC	CBG-NAF-CAG	2.77	120.90	109.91
10	A	301	HEM	C4C-C3C-C2C	2.75	109.20	106.81
14	B	202	OPC	CBU-CBT-CBS	2.74	127.95	112.60
16	D	201	SQD	O4-C4-C3	-2.72	103.98	110.38
12	A	1102	UMQ	C3-C4-C5	2.67	115.06	110.23
11	A	303	HEC	CAD-C3D-C4D	2.63	129.28	124.70
13	B	201	CLA	CHB-C1B-NB	-2.63	120.11	124.05
16	D	201	SQD	C45-O47-C7	-2.61	111.54	117.80
10	A	301	HEM	C3B-C2B-C1B	-2.61	104.45	106.41
16	D	201	SQD	O9-S-O7	-2.58	105.44	113.82
10	A	301	HEM	CMA-C3A-C4A	-2.57	121.51	125.42
14	H	1002	OPC	CAR-CAS-CAT	2.57	127.36	114.37
14	H	1002	OPC	OAI-CAH-CAG	2.57	122.01	109.65
14	H	1002	OPC	CBO-CBP-CBQ	2.56	126.18	113.86
16	D	201	SQD	O48-C23-C24	2.56	119.64	111.83
16	D	201	SQD	C16-C15-C14	2.56	127.30	114.37
10	A	301	HEM	CAD-C3D-C4D	2.53	129.11	124.70
10	A	301	HEM	C4D-C3D-C2D	-2.53	103.20	106.89
11	C	301	HEC	C1D-C2D-C3D	-2.53	104.32	106.98
12	A	1101	UMQ	C1-O1-C4'	-2.52	111.99	117.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	302	HEM	CHC-C4B-NB	2.50	127.11	124.42
12	A	1101	UMQ	C1'-O5'-C5'	-2.49	108.86	113.72
11	C	301	HEC	CHC-C4B-NB	-2.48	121.30	124.37
17	G	101	BCR	C2-C1-C6	2.48	114.04	110.44
11	A	303	HEC	C2A-C1A-NA	-2.47	107.94	110.32
14	H	1002	OPC	CAE-NAF-CAG	2.47	119.71	109.91
10	A	302	HEM	CAA-CBA-CGA	2.46	120.19	113.67
11	C	301	HEC	CBD-CAD-C3D	-2.46	105.74	112.53
10	A	301	HEM	C4A-C3A-C2A	2.43	109.60	106.82
16	D	201	SQD	O3-C3-C2	-2.42	104.67	110.38
14	B	202	OPC	CAR-CAS-CAT	2.41	126.55	114.37
17	G	101	BCR	C1-C6-C5	-2.41	119.35	122.64
10	A	301	HEM	C4B-C3B-C2B	2.39	109.48	107.28
14	H	1002	OPC	CBV-CBU-CBT	-2.38	102.42	113.86
10	A	301	HEM	CHB-C4A-C3A	-2.34	120.64	127.43
10	A	301	HEM	CHD-C4C-NC	2.33	126.99	124.45
10	A	301	HEM	CBA-CAA-C2A	-2.33	106.08	112.53
14	H	1002	OPC	CAQ-CAP-CAO	2.33	122.23	113.69
17	G	101	BCR	C11-C10-C9	2.31	130.52	127.28
10	A	301	HEM	CBB-CAB-C3B	-2.31	116.00	127.53
14	H	1002	OPC	CAQ-CAR-CAS	2.30	126.01	114.37
14	H	1002	OPC	CBG-NAF-CAG	2.29	119.01	109.91
17	G	101	BCR	C24-C25-C26	-2.28	116.29	121.56
11	C	301	HEC	CBA-CAA-C2A	-2.27	106.25	112.53
14	B	202	OPC	CAM-OAN-CAO	-2.26	112.38	117.80
13	B	201	CLA	CHC-C1C-C2C	-2.26	120.53	126.95
16	D	201	SQD	O47-C7-O49	-2.25	118.44	123.70
10	A	302	HEM	C3B-C2B-C1B	2.24	108.09	106.41
11	C	301	HEC	CHD-C4C-NC	2.24	127.92	123.86
10	A	302	HEM	CAD-CBD-CGD	-2.23	107.74	113.67
11	C	301	HEC	CHC-C1C-NC	2.23	127.90	123.86
14	H	1002	OPC	CBP-CBQ-CBR	2.23	125.07	112.60
12	A	1103	UMQ	C1-O1-C4'	-2.20	112.75	117.98
13	B	201	CLA	CMC-C2C-C1C	2.18	128.44	125.03
10	A	301	HEM	CHC-C4B-NB	2.18	126.77	124.42
13	B	201	CLA	CAA-C2A-C3A	-2.18	107.12	113.00
17	G	101	BCR	C38-C26-C27	2.17	118.21	113.60
17	G	101	BCR	C10-C11-C12	-2.15	116.97	123.20
11	C	301	HEC	C3B-C4B-NB	-2.15	107.81	110.17
16	D	201	SQD	C1-C2-C3	2.15	114.52	110.01
14	H	1002	OPC	CBW-CBV-CBU	-2.12	103.63	114.37
11	C	301	HEC	O1D-CGD-CBD	-2.12	116.36	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	G	101	BCR	C20-C19-C18	-2.11	120.58	126.36
10	A	301	HEM	CAA-CBA-CGA	-2.08	108.14	113.67
11	A	303	HEC	CAB-C3B-C2B	-2.08	123.73	127.56
10	A	302	HEM	O2A-CGA-CBA	2.08	120.58	114.00
14	B	202	OPC	CBP-CBO-CBN	2.05	124.75	114.37
10	A	301	HEM	CHA-C1A-NA	2.05	127.58	123.86
13	B	201	CLA	CMD-C2D-C3D	-2.05	122.99	127.69
12	A	1102	UMQ	C3'-C4'-C5'	2.04	115.44	110.93
12	A	1102	UMQ	O3'-C3'-C2'	-2.03	105.59	110.38
12	A	1104	UMQ	C1-O1-C4'	-2.01	113.22	117.98

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	A	303	HEC	NA
11	C	301	HEC	NA
12	A	1101	UMQ	C2'
12	A	1101	UMQ	C1'
12	A	1102	UMQ	C2'
12	A	1102	UMQ	C1'
12	A	1103	UMQ	C2'
12	A	1103	UMQ	C1'
12	A	1104	UMQ	C2'
12	A	1104	UMQ	C1'
13	B	201	CLA	C8
16	D	201	SQD	C5

All (164) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	A	1102	UMQ	C3'-C4'-O1-C1
12	A	1103	UMQ	CB-CA-O1'-C1'
12	A	1104	UMQ	O5'-C1'-O1'-CA
13	B	201	CLA	O2A-C1-C2-C3
14	B	202	OPC	NAF-CAG-CAH-OAI
14	B	202	OPC	CBO-CBP-CBQ-CBR
14	H	1002	OPC	CAL-OAK-PAJ-OBH
14	H	1002	OPC	CAL-OAK-PAJ-OAB
14	H	1002	OPC	CAL-OAK-PAJ-OAI
14	H	1002	OPC	NAF-CAG-CAH-OAI
14	H	1002	OPC	CBO-CBP-CBQ-CBR
16	D	201	SQD	C2-C1-O6-C44

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Mol	Chain	Res	Type	Atoms
16	D	201	SQD	O5-C1-O6-C44
16	D	201	SQD	O47-C45-C46-O48
16	D	201	SQD	O5-C5-C6-S
16	D	201	SQD	C5-C6-S-O7
16	D	201	SQD	C5-C6-S-O8
16	D	201	SQD	C5-C6-S-O9
17	G	101	BCR	C6-C7-C8-C9
17	G	101	BCR	C22-C23-C24-C25
11	C	301	HEC	C2B-C3B-CAB-CBB
11	C	301	HEC	C4B-C3B-CAB-CBB
13	B	201	CLA	CBD-CGD-O2D-CED
16	D	201	SQD	C31-C32-C33-C34
16	D	201	SQD	C33-C34-C35-C36
11	A	303	HEC	C4D-C3D-CAD-CBD
14	H	1002	OPC	CAQ-CAR-CAS-CAT
11	A	303	HEC	C2B-C3B-CAB-CBB
16	D	201	SQD	C12-C13-C14-C15
16	D	201	SQD	C13-C14-C15-C16
12	A	1101	UMQ	O5-C5-C6-O6
12	A	1102	UMQ	O5'-C5'-C6'-O6'
11	C	301	HEC	C2C-C3C-CAC-CBC
12	A	1101	UMQ	O5'-C5'-C6'-O6'
12	A	1102	UMQ	C4-C5-C6-O6
12	A	1103	UMQ	O5'-C1'-O1'-CA
12	A	1104	UMQ	O5-C5-C6-O6
16	D	201	SQD	C10-C11-C12-C13
16	D	201	SQD	C16-C17-C18-C19
16	D	201	SQD	C9-C10-C11-C12
12	A	1102	UMQ	C2'-C1'-O1'-CA
12	A	1104	UMQ	C4-C5-C6-O6
17	G	101	BCR	C7-C8-C9-C34
12	A	1102	UMQ	O5-C5-C6-O6
17	G	101	BCR	C7-C8-C9-C10
12	A	1101	UMQ	C4-C5-C6-O6
16	D	201	SQD	C8-C7-O47-C45
14	H	1002	OPC	OAN-CAM-CBI-OBJ
12	A	1101	UMQ	C4'-C5'-C6'-O6'
11	C	301	HEC	C4C-C3C-CAC-CBC
13	B	201	CLA	C6-C7-C8-C10
14	B	202	OPC	CAP-CAO-OAN-CAM
13	B	201	CLA	C15-C16-C17-C18
12	A	1102	UMQ	O1'-CA-CB-CC

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Mol	Chain	Res	Type	Atoms
11	A	303	HEC	C4B-C3B-CAB-CBB
13	B	201	CLA	O1D-CGD-O2D-CED
14	B	202	OPC	CBL-CBK-OBJ-CBI
12	A	1102	UMQ	C4'-C5'-C6'-O6'
13	B	201	CLA	C8-C10-C11-C12
14	B	202	OPC	OAD-CAO-OAN-CAM
16	D	201	SQD	O49-C7-O47-C45
14	B	202	OPC	CAH-CAG-NAF-CBG
12	A	1101	UMQ	C2'-C1'-O1'-CA
13	B	201	CLA	C10-C11-C12-C13
11	A	303	HEC	C2D-C3D-CAD-CBD
14	B	202	OPC	CBK-CBL-CBM-CBN
16	D	201	SQD	C23-C24-C25-C26
14	B	202	OPC	OCC-CBK-OBJ-CBI
14	B	202	OPC	OAK-CAL-CAM-OAN
14	H	1002	OPC	CAH-CAG-NAF-CBG
12	A	1101	UMQ	CB-CC-CD-CF
14	B	202	OPC	CBM-CBN-CBO-CBP
14	B	202	OPC	CAZ-CBA-CBB-CBC
12	A	1104	UMQ	CB-CC-CD-CF
12	A	1101	UMQ	CA-CB-CC-CD
13	B	201	CLA	C3A-C2A-CAA-CBA
14	H	1002	OPC	CBW-CBX-CBY-CBZ
14	B	202	OPC	CAY-CAZ-CBA-CBB
14	H	1002	OPC	CBX-CBY-CBZ-CCA
16	D	201	SQD	C26-C27-C28-C29
12	A	1104	UMQ	CD-CF-CG-CH
14	H	1002	OPC	CBM-CBN-CBO-CBP
12	A	1102	UMQ	CH-CI-CJ-CK
14	B	202	OPC	CAS-CAT-CAU-CAV
17	G	101	BCR	C37-C22-C23-C24
17	G	101	BCR	C21-C22-C23-C24
13	B	201	CLA	C4-C3-C5-C6
14	B	202	OPC	CAH-CAG-NAF-CAA
12	A	1101	UMQ	CH-CI-CJ-CK
14	H	1002	OPC	CBL-CBM-CBN-CBO
14	H	1002	OPC	CBS-CBT-CBU-CBV
13	B	201	CLA	C2-C3-C5-C6
13	B	201	CLA	C1A-C2A-CAA-CBA
14	H	1002	OPC	CAS-CAT-CAU-CAV
16	D	201	SQD	C25-C26-C27-C28
14	H	1002	OPC	CAL-CAM-CBI-OBJ

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Mol	Chain	Res	Type	Atoms
16	D	201	SQD	C28-C29-C30-C31
14	B	202	OPC	CBT-CBU-CBV-CBW
12	A	1104	UMQ	CF-CG-CH-CI
14	H	1002	OPC	CAX-CAY-CAZ-CBA
12	A	1104	UMQ	O5'-C5'-C6'-O6'
14	H	1002	OPC	CAW-CAX-CAY-CAZ
16	D	201	SQD	C24-C23-O48-C46
12	A	1104	UMQ	CH-CI-CJ-CK
13	B	201	CLA	C3-C5-C6-C7
16	D	201	SQD	C24-C25-C26-C27
13	B	201	CLA	C4B-C3B-CAB-CBB
10	A	301	HEM	C3D-CAD-CBD-CGD
14	B	202	OPC	CBC-CBD-CBE-CBF
14	B	202	OPC	OAK-CAL-CAM-CBI
14	B	202	OPC	CAR-CAS-CAT-CAU
16	D	201	SQD	C44-C45-C46-O48
12	A	1104	UMQ	O1'-CA-CB-CC
13	B	201	CLA	C2B-C3B-CAB-CBB
17	G	101	BCR	C23-C24-C25-C26
14	H	1002	OPC	CBU-CBV-CBW-CBX
16	D	201	SQD	O6-C44-C45-O47
16	D	201	SQD	O10-C23-O48-C46
12	A	1103	UMQ	CF-CG-CH-CI
10	A	302	HEM	C2C-C3C-CAC-CBC
12	A	1103	UMQ	CA-CB-CC-CD
14	H	1002	OPC	OAK-CAL-CAM-OAN
14	H	1002	OPC	CBV-CBW-CBX-CBY
14	B	202	OPC	CBL-CBM-CBN-CBO
12	A	1101	UMQ	CF-CG-CH-CI
14	B	202	OPC	CBP-CBQ-CBR-CBS
14	H	1002	OPC	CAM-CAL-OAK-PAJ
12	A	1104	UMQ	CC-CD-CF-CG
14	B	202	OPC	CAL-CAM-CBI-OBJ
14	H	1002	OPC	CBP-CBQ-CBR-CBS
13	B	201	CLA	C6-C7-C8-C9
16	D	201	SQD	C15-C16-C17-C18
11	A	303	HEC	C3D-CAD-CBD-CGD
14	H	1002	OPC	CBC-CBD-CBE-CBF
16	D	201	SQD	O6-C44-C45-C46
16	D	201	SQD	C45-C44-O6-C1
12	A	1101	UMQ	CB-CA-O1'-C1'
12	A	1102	UMQ	CB-CA-O1'-C1'

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Mol	Chain	Res	Type	Atoms
14	H	1002	OPC	OAK-CAL-CAM-CBI
10	A	301	HEM	C4C-C3C-CAC-CBC
10	A	302	HEM	C4C-C3C-CAC-CBC
17	G	101	BCR	C11-C10-C9-C34
17	G	101	BCR	C11-C10-C9-C8
11	C	301	HEC	CAA-CBA-CGA-O2A
11	C	301	HEC	CAD-CBD-CGD-O2D
11	C	301	HEC	CAA-CBA-CGA-O1A
13	B	201	CLA	C11-C12-C13-C15
11	C	301	HEC	CAD-CBD-CGD-O1D
12	A	1102	UMQ	CC-CD-CF-CG
10	A	301	HEM	CAA-CBA-CGA-O2A
11	A	303	HEC	CAA-CBA-CGA-O2A
12	A	1104	UMQ	CG-CH-CI-CJ
10	A	301	HEM	C2C-C3C-CAC-CBC
10	A	301	HEM	CAA-CBA-CGA-O1A
11	A	303	HEC	CAA-CBA-CGA-O1A
12	A	1102	UMQ	C5'-C4'-O1-C1
12	A	1103	UMQ	CG-CH-CI-CJ
12	A	1101	UMQ	CC-CD-CF-CG
11	A	303	HEC	CAD-CBD-CGD-O2D
14	B	202	OPC	CBR-CBS-CBT-CBU
12	A	1101	UMQ	CI-CJ-CK-CL
10	A	302	HEM	C1A-C2A-CAA-CBA
14	H	1002	OPC	CBY-CBZ-CCA-CCB
14	H	1002	OPC	CBR-CBS-CBT-CBU

There are no ring outliers.

14 monomers are involved in 94 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	303	HEC	6	0
14	H	1002	OPC	23	0
10	A	301	HEM	10	0
13	B	201	CLA	4	0
16	D	201	SQD	11	0
12	A	1104	UMQ	4	0
17	G	101	BCR	11	0
12	A	1103	UMQ	1	0
15	D	200	FES	2	0
11	C	301	HEC	6	0
10	A	302	HEM	9	0

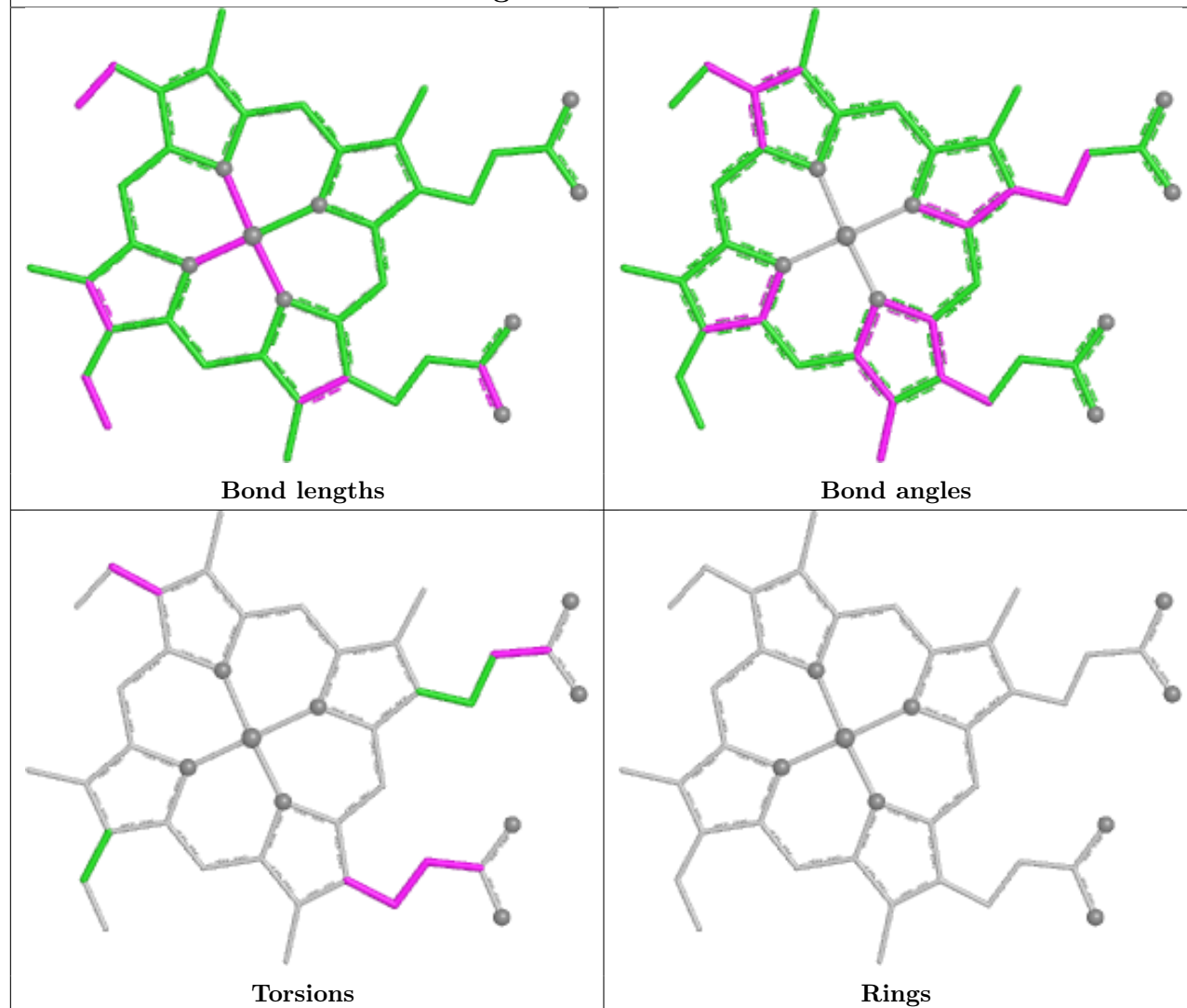
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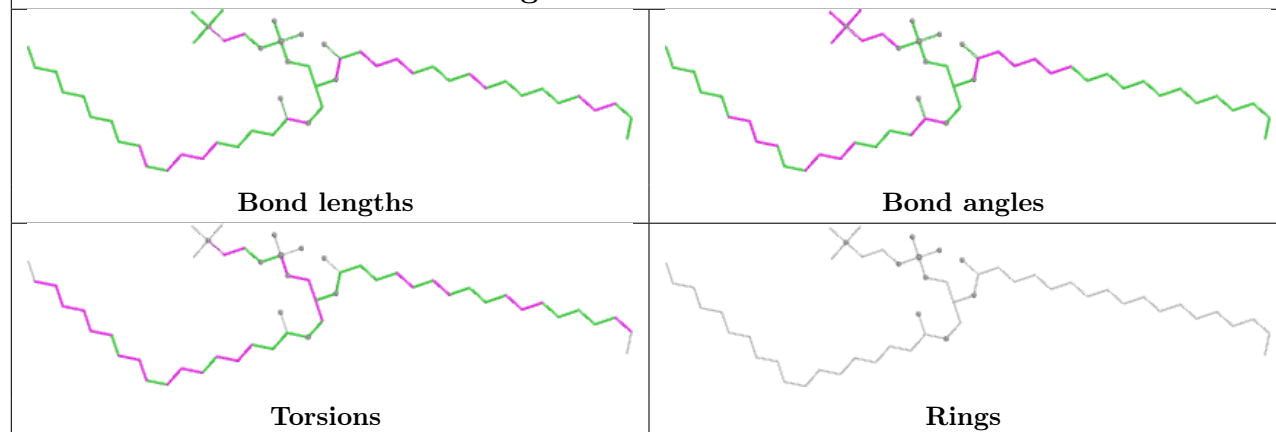
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	1101	UMQ	6	0
14	B	202	OPC	2	0
12	A	1102	UMQ	2	0

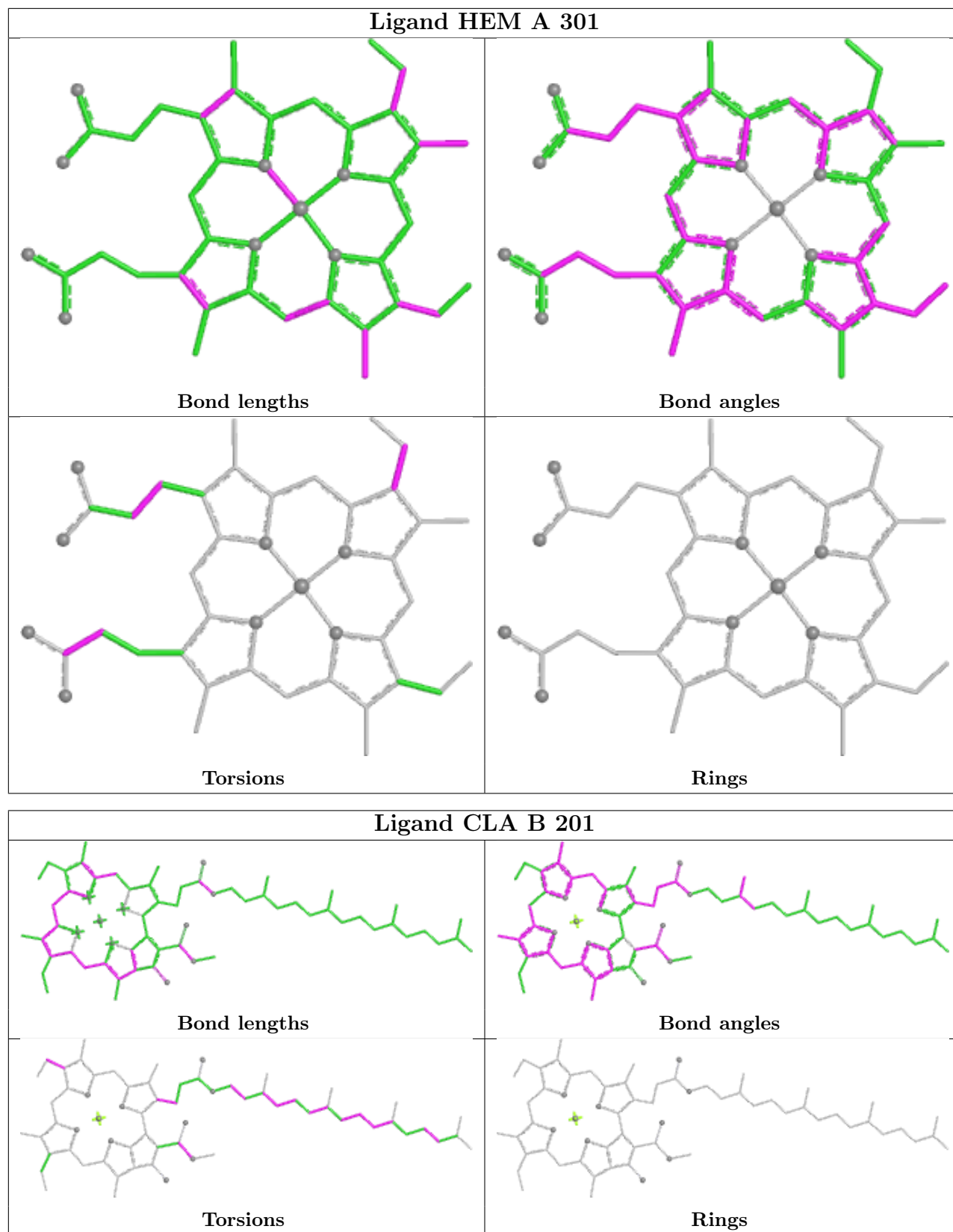
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

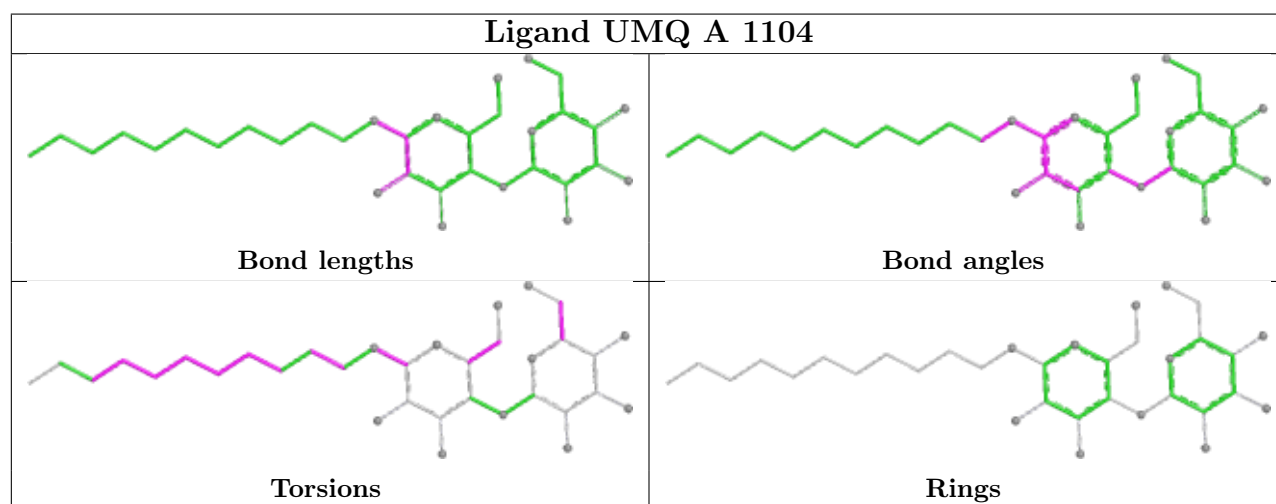
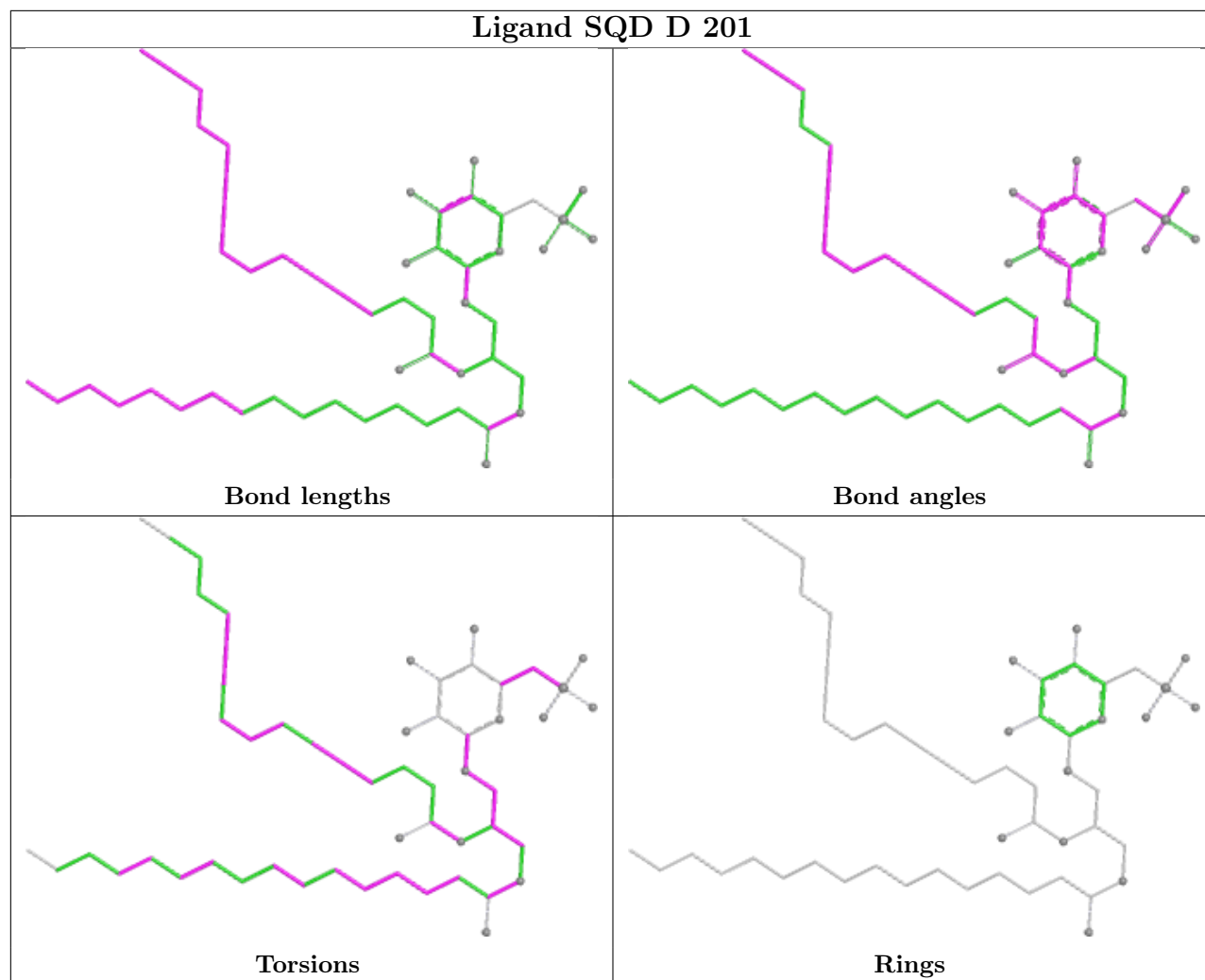
Ligand HEC A 303

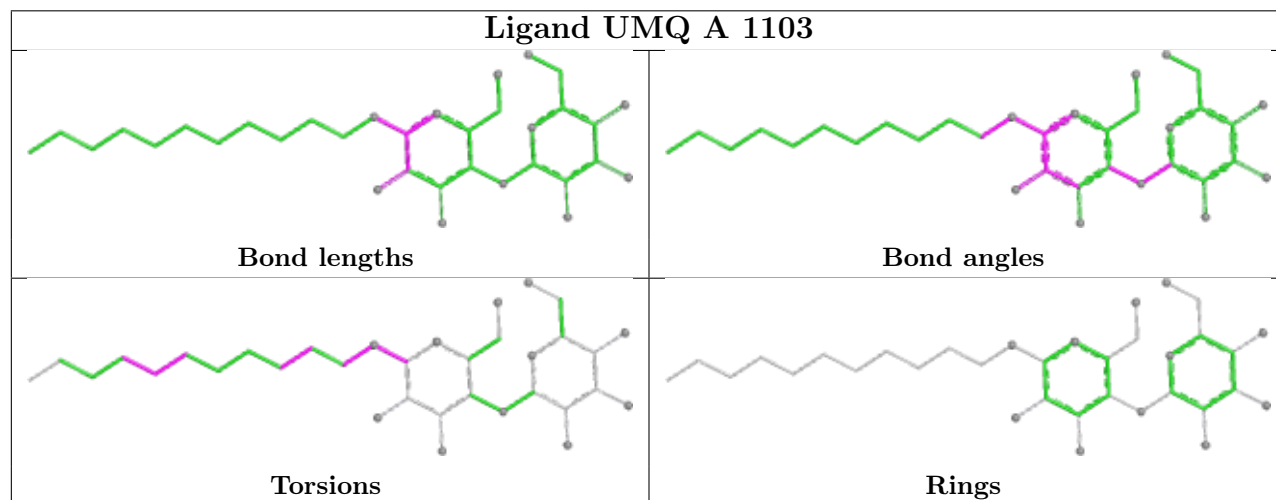
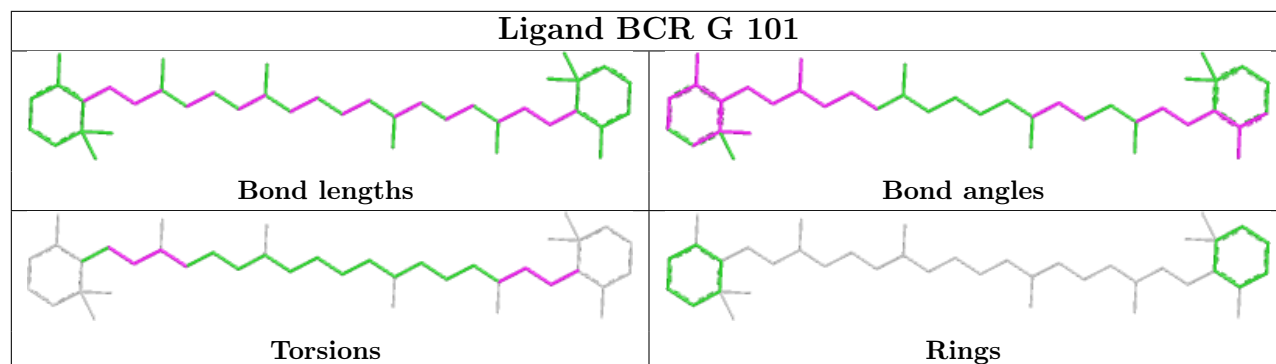


Ligand OPC H 1002

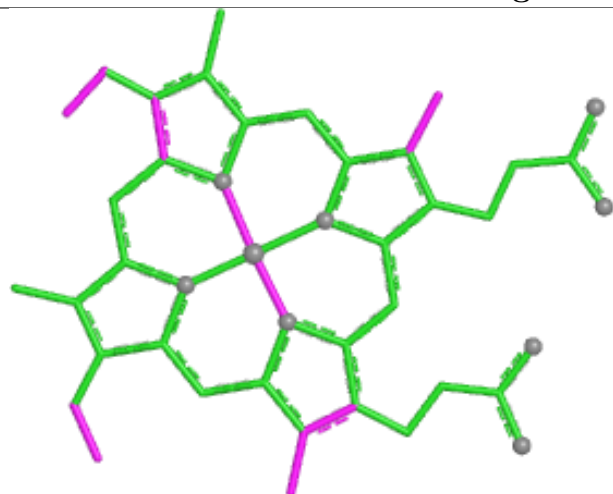




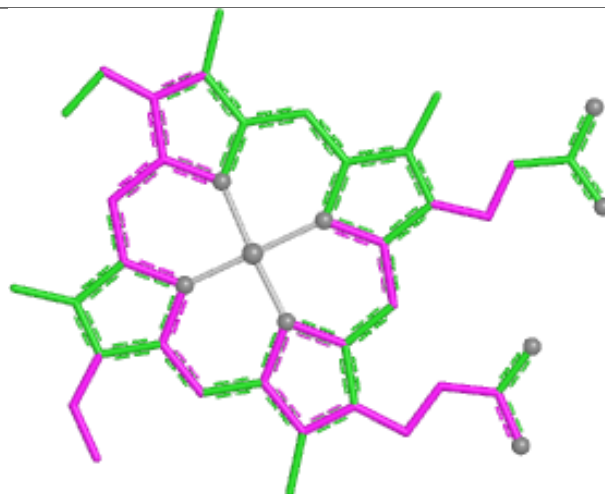




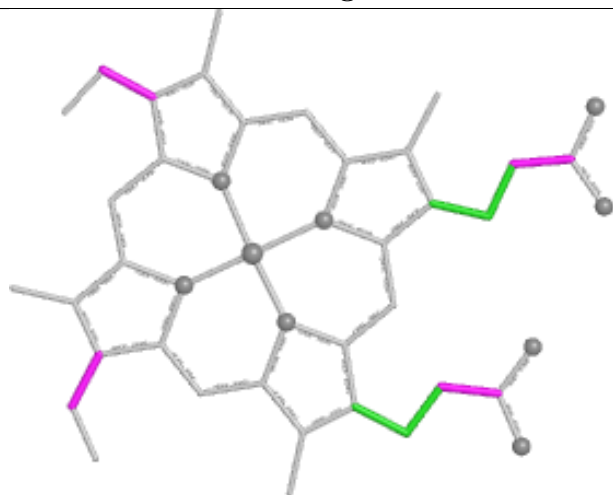
Ligand HEC C 301



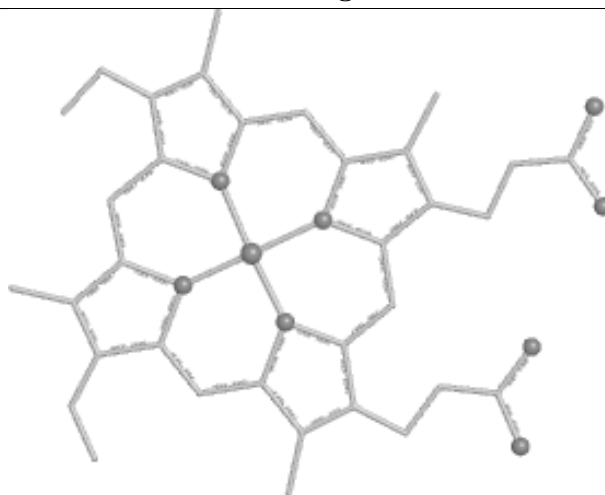
Bond lengths



Bond angles

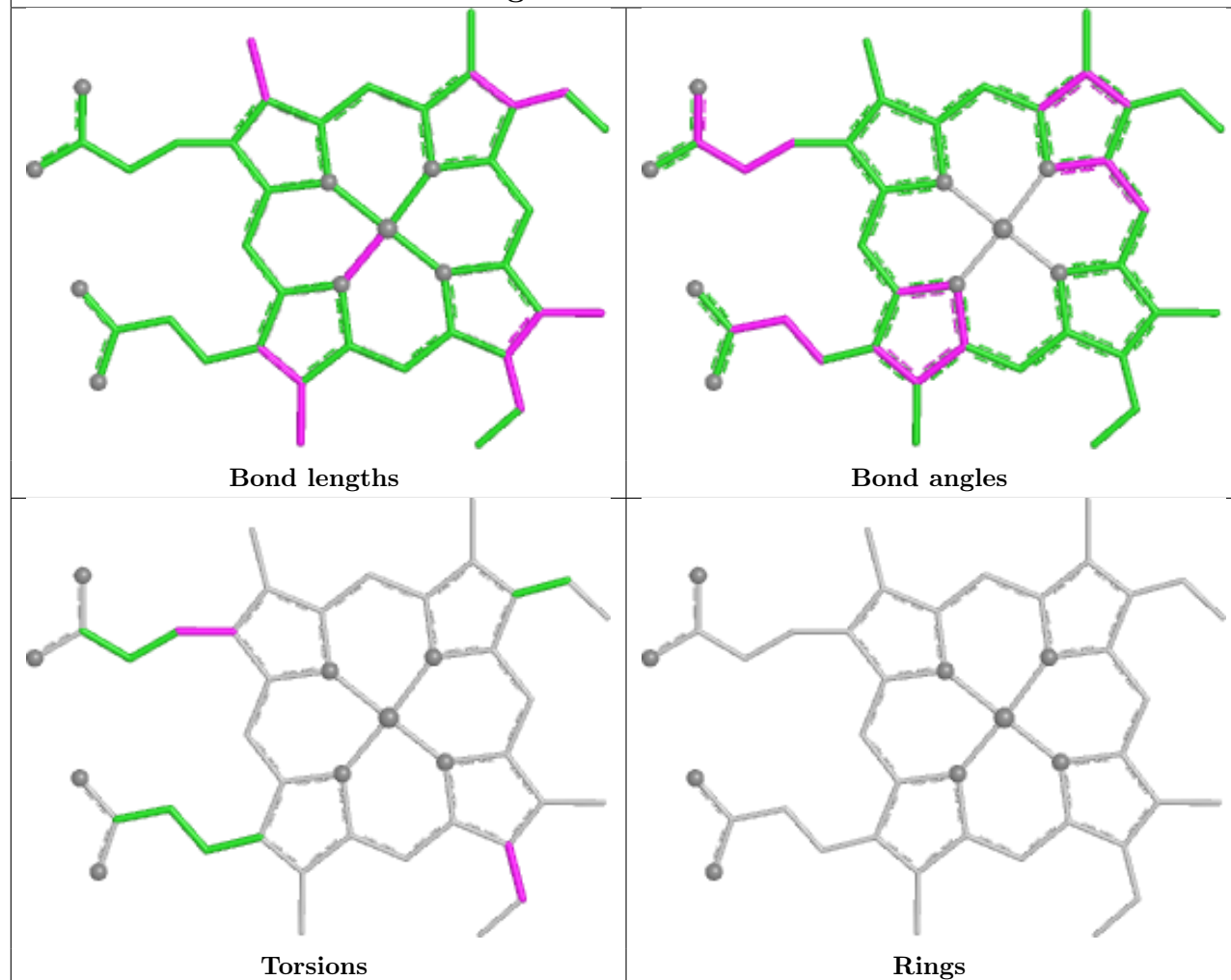


Torsions

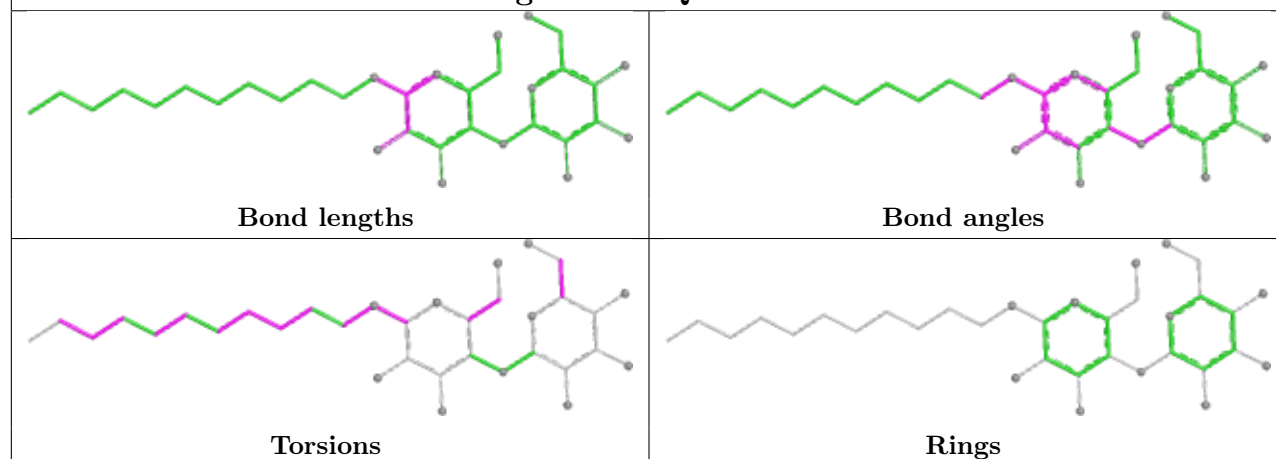


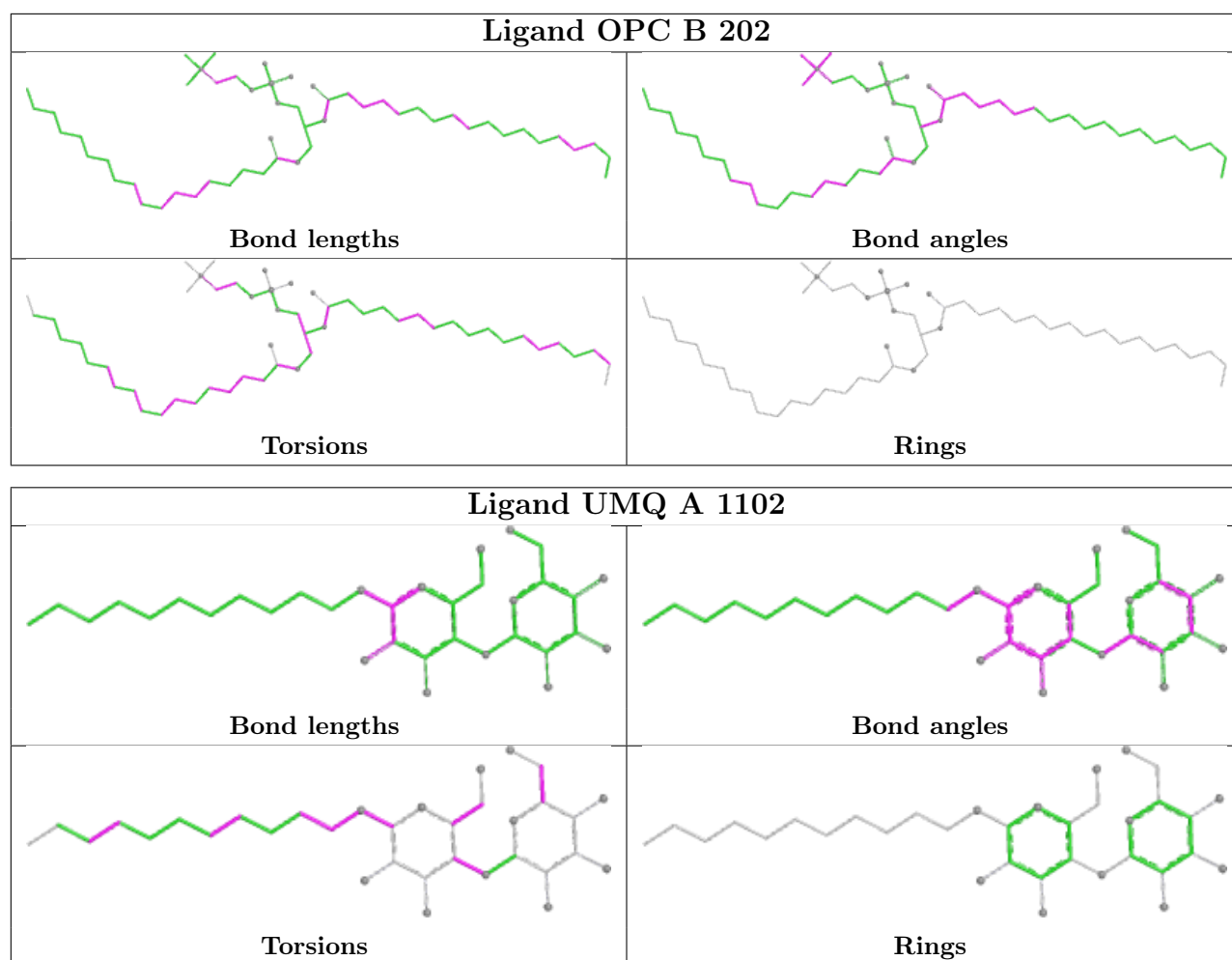
Rings

Ligand HEM A 302



Ligand UMQ A 1101





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%)	-0.39	2 (0%) 81 61	21, 41, 72, 160	0
2	B	160/160 (100%)	0.09	2 (1%) 75 53	32, 57, 103, 135	0
3	C	288/289 (99%)	1.64	87 (30%) 1 1	10, 54, 114, 130	1 (0%)
4	D	166/179 (92%)	2.20	86 (51%) 0 0	38, 91, 125, 171	0
5	E	32/32 (100%)	0.46	2 (6%) 26 13	60, 75, 106, 122	0
6	F	32/35 (91%)	0.50	5 (15%) 5 3	47, 69, 124, 139	0
7	G	37/37 (100%)	0.25	4 (10%) 11 6	42, 57, 123, 131	0
8	H	29/29 (100%)	0.12	2 (6%) 23 12	40, 52, 76, 118	0
All	All	959/976 (98%)	0.85	190 (19%) 3 2	10, 57, 115, 171	1 (0%)

All (190) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	40	VAL	10.7
4	D	149	ALA	8.6
4	D	173	GLY	7.6
4	D	50	VAL	6.0
6	F	1	MET	5.9
3	C	254	ARG	5.4
4	D	17	GLN	5.4
3	C	181	THR	5.4
4	D	105	ASN	5.3
3	C	88	GLU	5.2
4	D	172	THR	5.1
3	C	256	LYS	4.9
3	C	230	ALA	4.8
4	D	49	ALA	4.8
3	C	145	GLY	4.7
4	D	80	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
3	C	140	LYS	4.5
4	D	160	ILE	4.3
4	D	75	ALA	4.3
4	D	175	LYS	4.3
3	C	249	LEU	4.2
4	D	87	ASP	4.2
4	D	85	LYS	4.2
3	C	250	GLN	4.1
3	C	136	PRO	4.1
3	C	241	GLY	4.1
4	D	41	TYR	4.0
3	C	226	LYS	3.9
3	C	251	ASP	3.9
4	D	91	ILE	3.8
4	D	171	ARG	3.7
4	D	166	THR	3.7
4	D	46	SER	3.7
4	D	84	LEU	3.7
4	D	86	GLY	3.7
4	D	177	TRP	3.7
4	D	164	PRO	3.7
3	C	142	ILE	3.7
4	D	42	PHE	3.7
4	D	170	PHE	3.7
3	C	147	TYR	3.6
4	D	178	TRP	3.6
3	C	41	LEU	3.6
4	D	111	LEU	3.6
4	D	54	THR	3.6
3	C	207	VAL	3.5
3	C	252	PRO	3.5
3	C	39	SER	3.5
7	G	1	MET	3.5
4	D	43	ILE	3.5
3	C	234	ASN	3.5
3	C	206	THR	3.4
4	D	82	GLN	3.4
3	C	7	GLN	3.4
4	D	45	PRO	3.4
3	C	225	VAL	3.4
3	C	192	ASN	3.3
1	A	112	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
3	C	165	GLU	3.3
8	H	1	MET	3.3
4	D	148	LEU	3.3
3	C	258	MET	3.3
4	D	106	ALA	3.3
3	C	220	SER	3.2
4	D	159	ASN	3.2
6	F	2	THR	3.2
4	D	92	VAL	3.2
3	C	222	GLY	3.2
1	A	1	MET	3.2
3	C	171	VAL	3.2
3	C	168	ASN	3.1
3	C	221	GLU	3.1
3	C	141	ASN	3.1
4	D	88	PRO	3.1
3	C	100	ASP	3.1
3	C	135	ASN	3.0
4	D	168	THR	3.0
4	D	44	PRO	3.0
3	C	111	ASP	3.0
4	D	90	TYR	3.0
3	C	80	GLU	3.0
4	D	174	GLU	3.0
3	C	217	LEU	2.9
4	D	103	GLY	2.9
3	C	144	PHE	2.9
4	D	55	THR	2.9
4	D	155	VAL	2.9
3	C	214	GLY	2.9
4	D	40	LYS	2.9
3	C	143	HIS	2.9
3	C	139	ASP	2.9
4	D	114	VAL	2.9
4	D	14	GLY	2.9
4	D	73	HIS	2.8
3	C	253	ASN	2.8
4	D	59	LYS	2.8
4	D	179	VAL	2.8
4	D	10	VAL	2.8
8	H	29	LEU	2.8
4	D	13	MET	2.7

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Mol	Chain	Res	Type	RSRZ
3	C	257	TRP	2.7
3	C	247	ILE	2.7
4	D	120	ALA	2.7
6	F	31	GLY	2.7
3	C	182	LYS	2.7
3	C	213	ALA	2.7
4	D	150	LEU	2.7
4	D	156	GLN	2.7
3	C	177	THR	2.7
4	D	70	LEU	2.7
3	C	240	PHE	2.6
4	D	142	GLY	2.6
7	G	37	GLY	2.6
4	D	109	THR	2.6
4	D	119	ALA	2.6
4	D	102	TYR	2.6
3	C	146	LYS	2.6
3	C	287	MET	2.6
6	F	32	ALA	2.6
4	D	157	ASP	2.6
3	C	61	VAL	2.6
5	E	1	MET	2.5
4	D	145	PRO	2.5
7	G	27	GLN	2.5
2	B	1	MET	2.5
4	D	89	THR	2.5
3	C	211	ILE	2.5
3	C	9	TYR	2.5
2	B	74	GLU	2.5
3	C	262	ILE	2.4
3	C	255	VAL	2.4
4	D	123	LYS	2.4
3	C	64	ASP	2.4
3	C	134	PRO	2.4
3	C	176	ALA	2.4
3	C	59	GLN	2.4
4	D	52	GLY	2.4
4	D	76	GLY	2.4
4	D	38	LEU	2.4
4	D	112	GLY	2.4
3	C	246	GLU	2.4
4	D	37	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
3	C	201	THR	2.3
3	C	32	ALA	2.3
4	D	15	ARG	2.3
4	D	36	TYR	2.3
3	C	95	LYS	2.3
4	D	113	CYS	2.3
4	D	144	ALA	2.3
4	D	56	ALA	2.3
3	C	54	TYR	2.3
3	C	229	GLU	2.3
7	G	32	PRO	2.3
3	C	138	THR	2.3
4	D	68	LYS	2.3
3	C	195	TYR	2.2
3	C	233	ASN	2.2
4	D	79	VAL	2.2
4	D	158	ASP	2.2
4	D	48	GLY	2.2
3	C	89	ARG	2.2
6	F	30	GLN	2.2
4	D	169	ASP	2.2
3	C	42	PRO	2.2
3	C	260	ALA	2.2
4	D	65	LYS	2.2
4	D	140	ILE	2.2
4	D	162	LEU	2.2
3	C	112	ASN	2.2
4	D	143	PRO	2.2
4	D	47	GLY	2.1
3	C	244	ASP	2.1
3	C	215	PRO	2.1
3	C	68	VAL	2.1
4	D	110	HIS	2.1
3	C	79	PRO	2.1
3	C	45	VAL	2.1
3	C	231	LEU	2.1
4	D	78	ARG	2.1
5	E	32	ILE	2.1
3	C	110	GLN	2.1
3	C	242	GLN	2.1
3	C	85	ALA	2.0
3	C	190	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
3	C	82	PHE	2.0
4	D	101	ASP	2.0
3	C	191	GLY	2.0
4	D	151	CYS	2.0
3	C	269	GLN	2.0
3	C	248	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

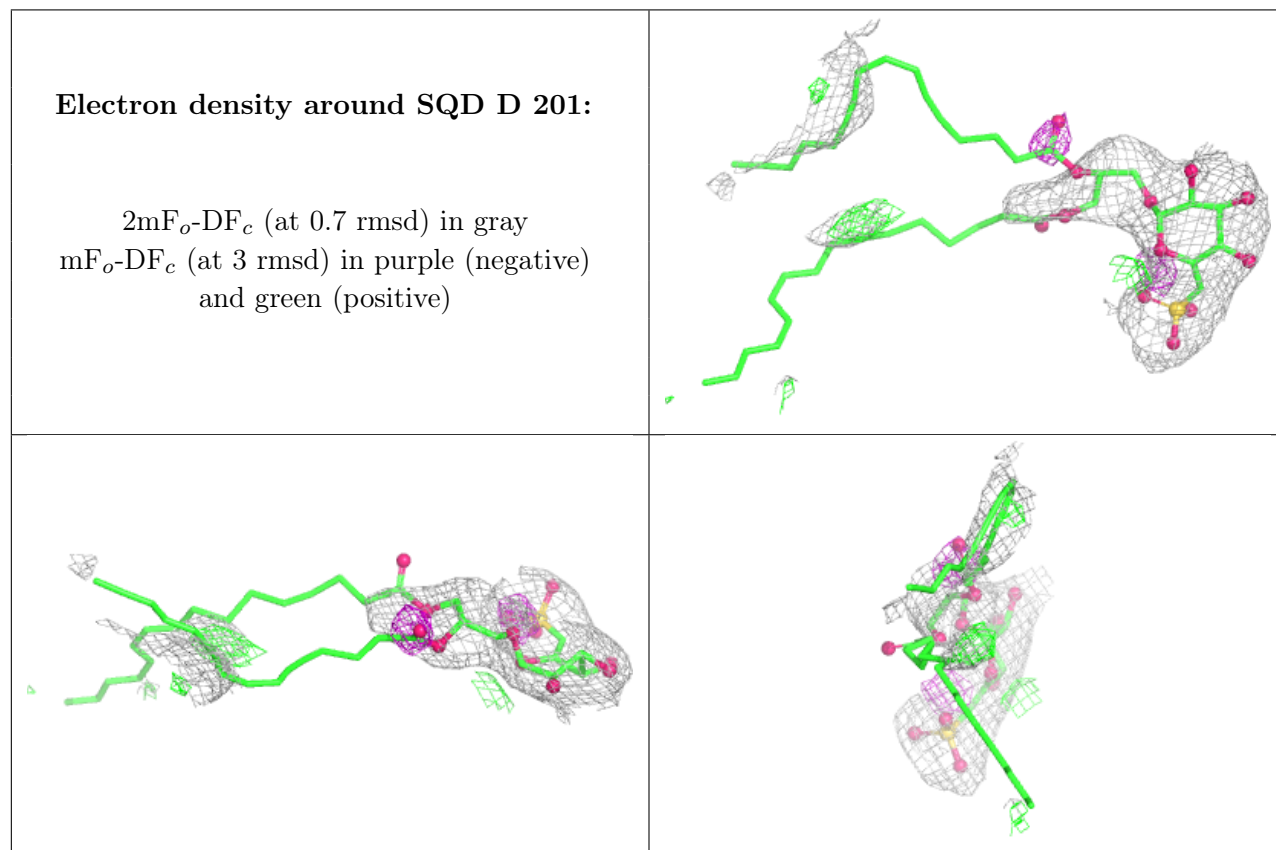
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

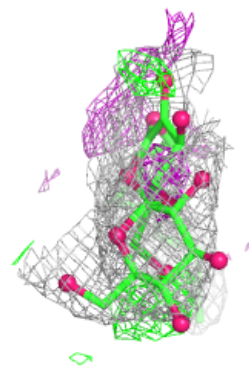
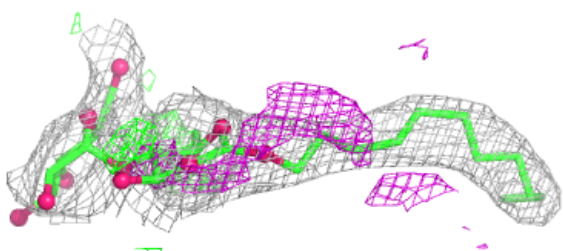
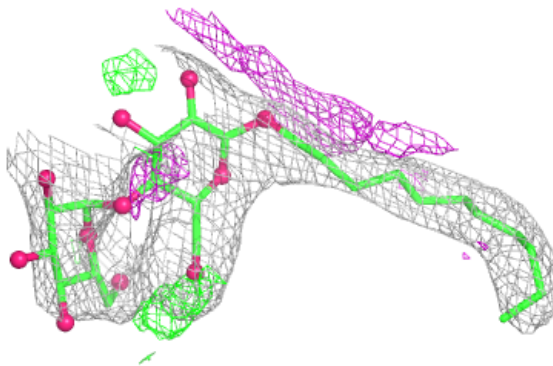
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	SQD	D	201	54/54	0.76	0.31	67,164,194,196	0
12	UMQ	A	1101	34/34	0.77	0.22	35,109,146,149	0
12	UMQ	A	1104	34/34	0.80	0.21	86,134,171,175	0
17	BCR	G	101	40/40	0.83	0.24	33,70,131,136	0
12	UMQ	A	1102	34/34	0.84	0.18	62,119,148,149	0
14	OPC	H	1002	54/55	0.85	0.23	41,93,187,196	0
14	OPC	B	202	54/55	0.88	0.20	48,82,157,162	0
12	UMQ	A	1103	34/34	0.88	0.17	76,112,134,135	0
13	CLA	B	201	65/65	0.95	0.11	41,60,91,99	0
15	FES	D	200	4/4	0.95	0.10	96,101,102,113	0
9	CD	B	161	1/1	0.96	0.06	166,166,166,166	0
10	HEM	A	302	43/43	0.97	0.09	9,34,57,74	0
11	HEC	C	301	43/43	0.97	0.10	29,54,89,97	0
11	HEC	A	303	43/43	0.98	0.07	26,59,68,76	0
10	HEM	A	301	43/43	0.98	0.08	9,32,51,75	0
9	CD	A	1001	1/1	0.99	0.04	65,65,65,65	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.

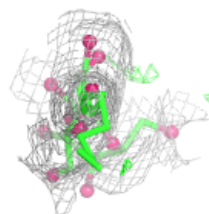
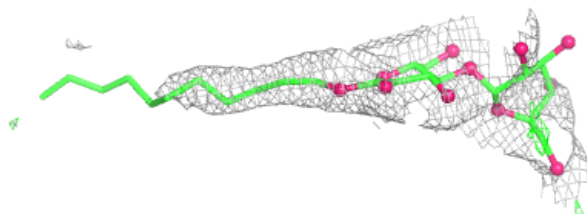
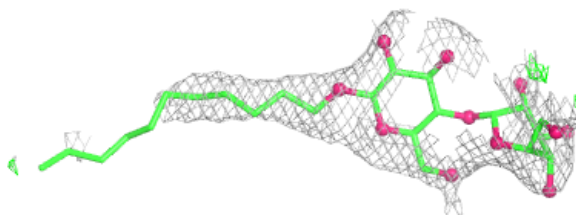


Electron density around UMQ A 1101:

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

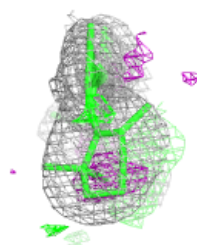
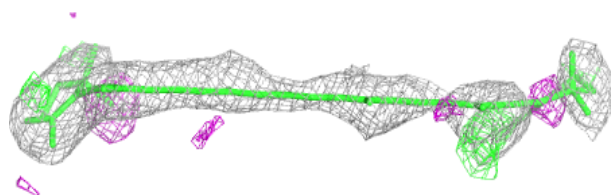
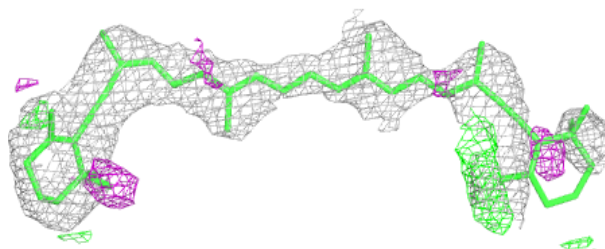
**Electron density around UMQ A 1104:**

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

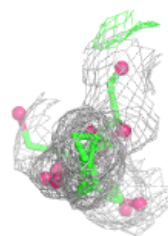
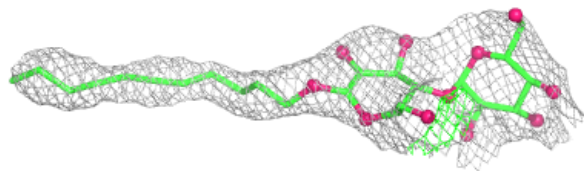
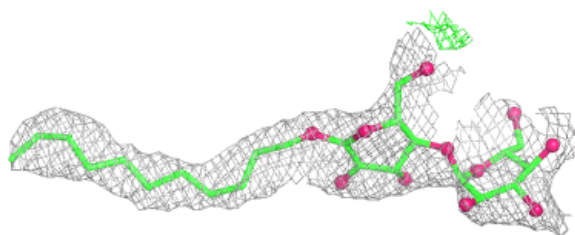


Electron density around BCR G 101:

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

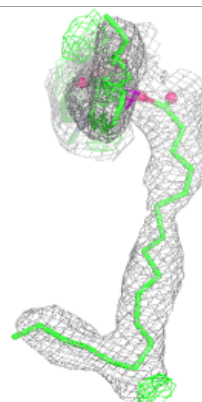
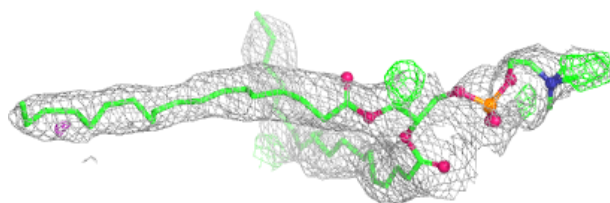
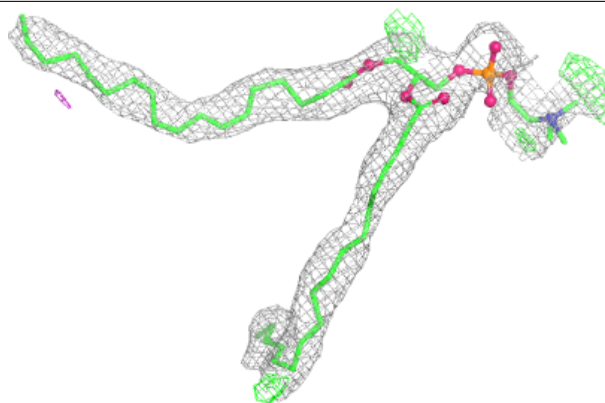
**Electron density around UMQ A 1102:**

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

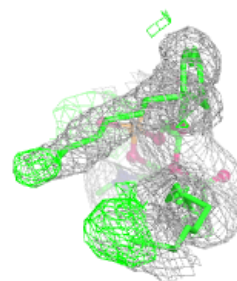
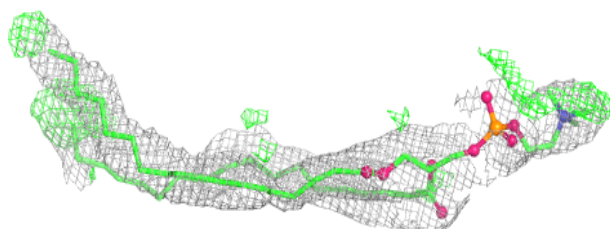
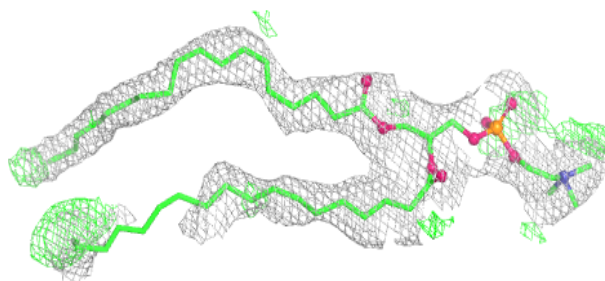


Electron density around OPC H 1002:

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

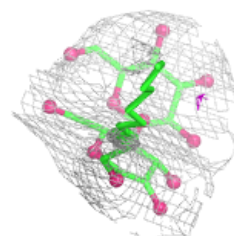
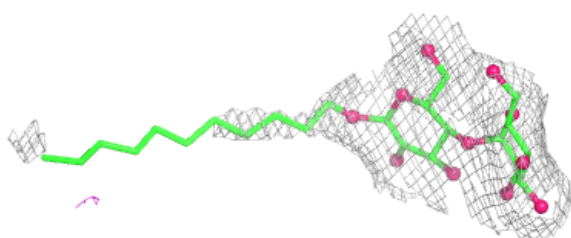
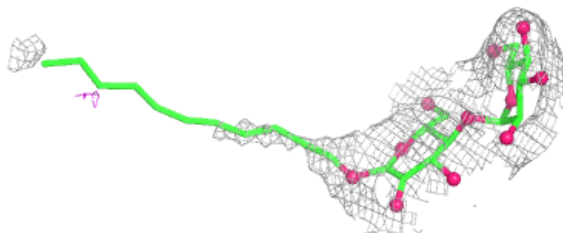
**Electron density around OPC B 202:**

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

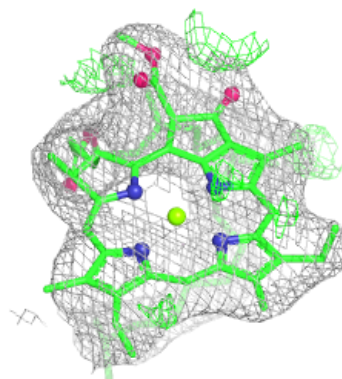
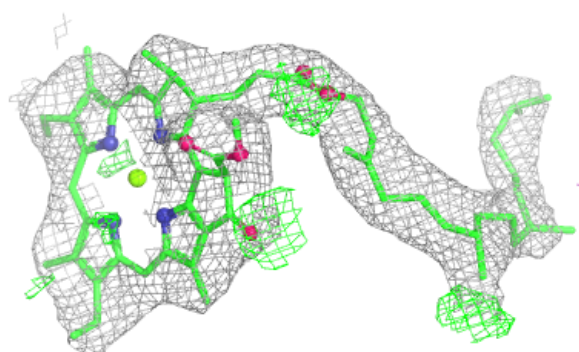
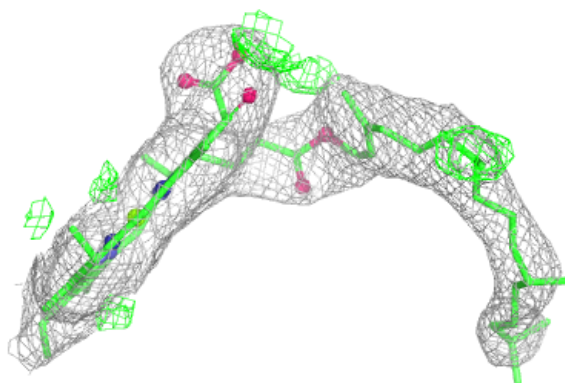


Electron density around UMQ A 1103:

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

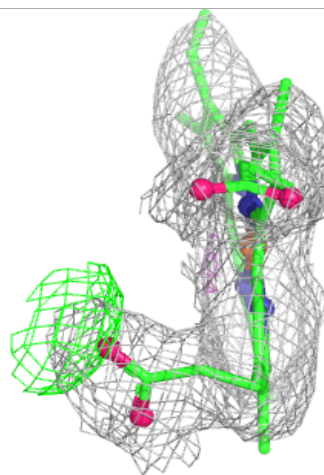
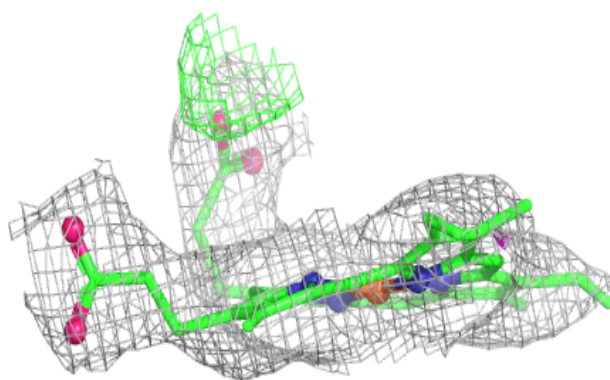
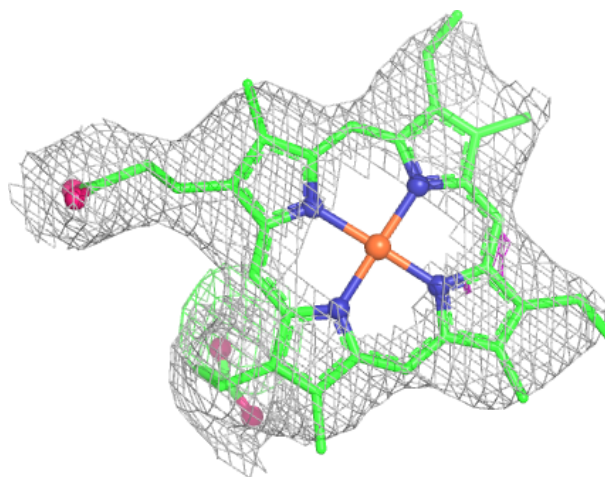
**Electron density around CLA B 201:**

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



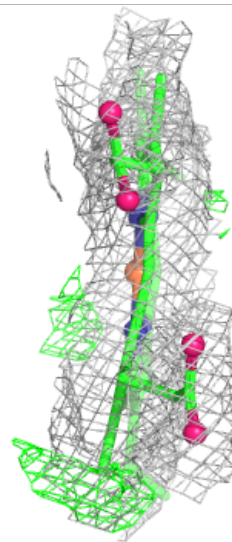
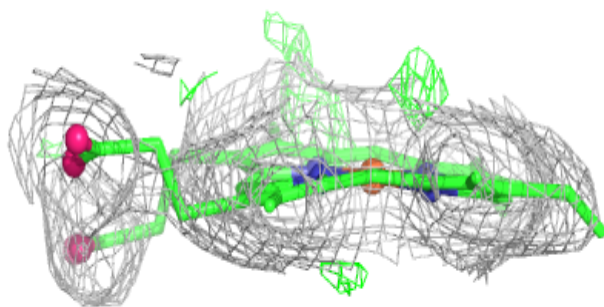
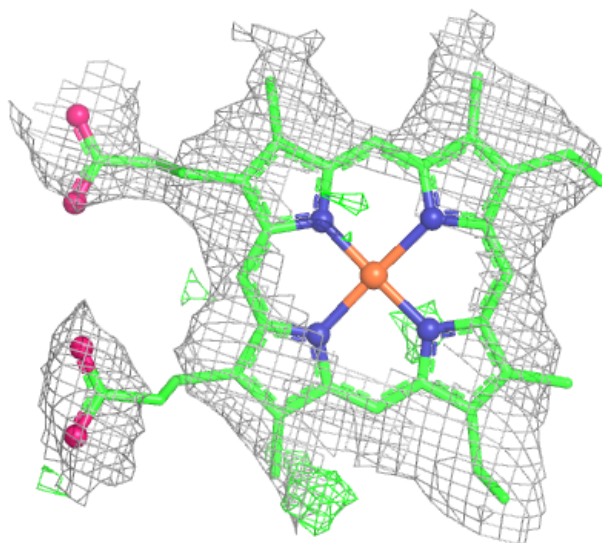
Electron density around HEM A 302:

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



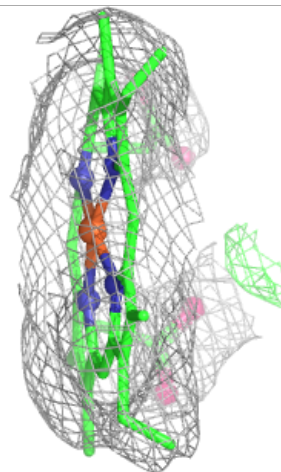
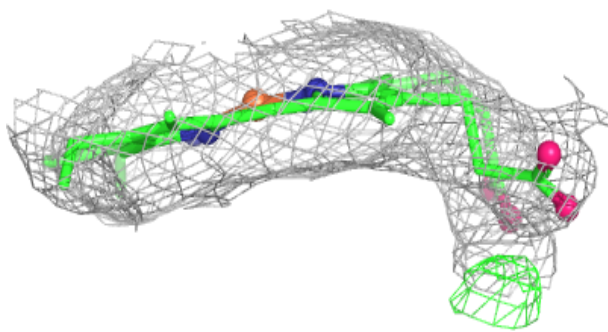
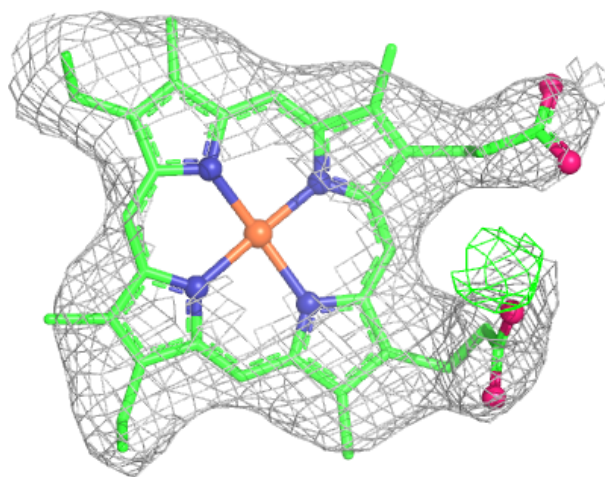
Electron density around HEC C 301:

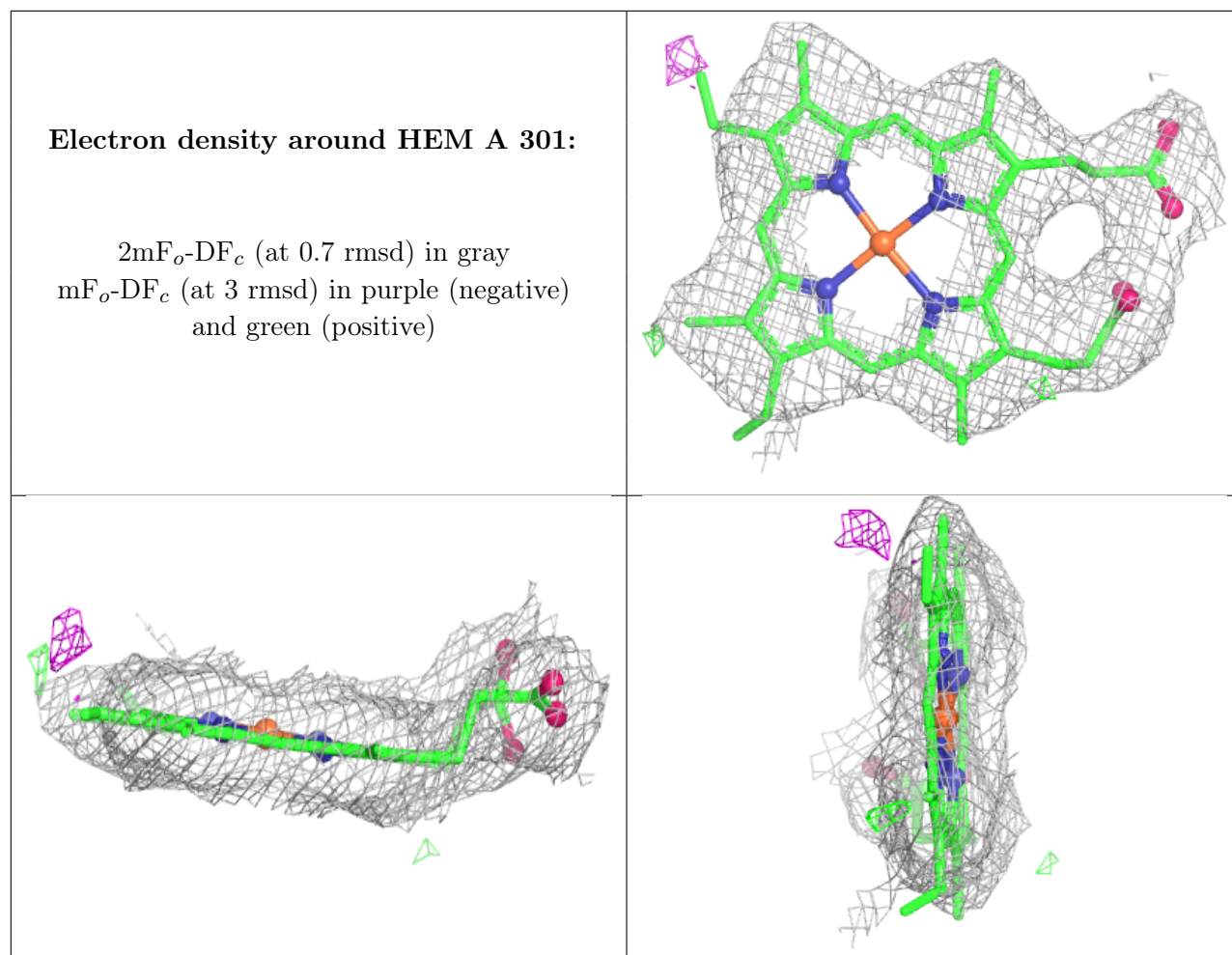
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC 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 ⓘ

There are no such residues in this entry.