Full wwPDB X-ray Structure Validation Report (i)

Oct 18, 2023 – 01:01 PM EDT

PDB ID	:	1WE1
Title	:	Crystal structure of heme oxygenase-1 from cyanobacterium Synechocystis sp. PCC6803 in complex with heme
Authors	:	Sugishima, M.; Migita, C.T.; Zhang, X.; Yoshida, T.; Fukuyama, K.
Deposited on	:	2004-05-21
Resolution	:	2.50 Å(reported)

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

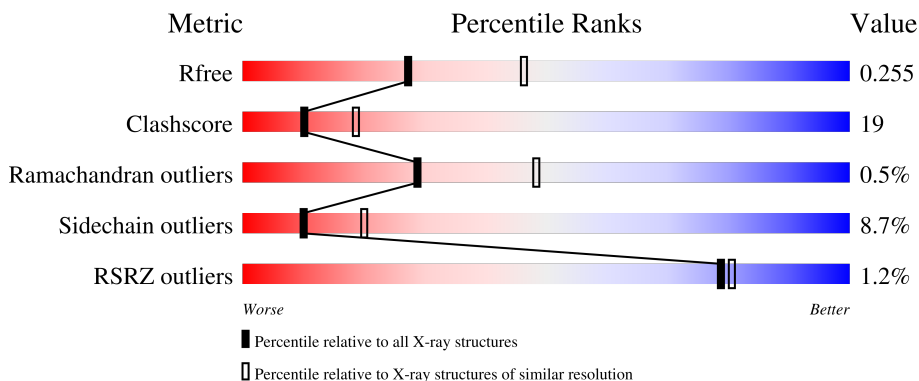|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.50 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	Percentile Ranks	Value
Rfree		0.255
Clashscore		19
Ramachandran outliers		0.5%
Sidechain outliers		8.7%
RSRZ outliers		1.2%

Worse — *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	240	% — 58% / 29% / 5% / 8%
1	B	240	% — 66% / 23% / · / 8%
1	C	240	58% / 31% / · / 8%
1	D	240	2% — 61% / 26% / 5% / 8%

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:

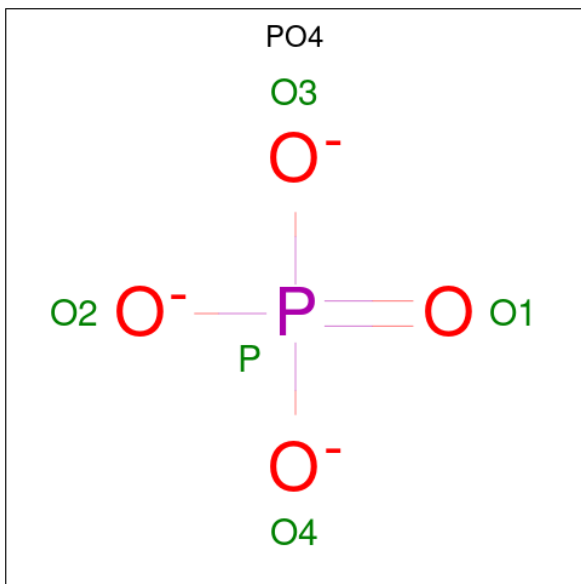| Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	IPA	C	1007	-	-	X	-
5	IPA	D	1008	-	-	X	-

2   Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7468 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 Heme oxygenase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1763	1118	301	334	10			
1	B	222	Total	C	N	O	S	0	0	0
			1764	1118	301	335	10			
1	C	222	Total	C	N	O	S	0	0	0
			1761	1116	301	335	9			
1	D	221	Total	C	N	O	S	0	0	0
			1752	1113	301	329	9			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Cl 2	0	0
3	B	1	Total 1	Cl 1	0	0
3	C	1	Total 1	Cl 1	0	0
3	D	1	Total 1	Cl 1	0	0

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

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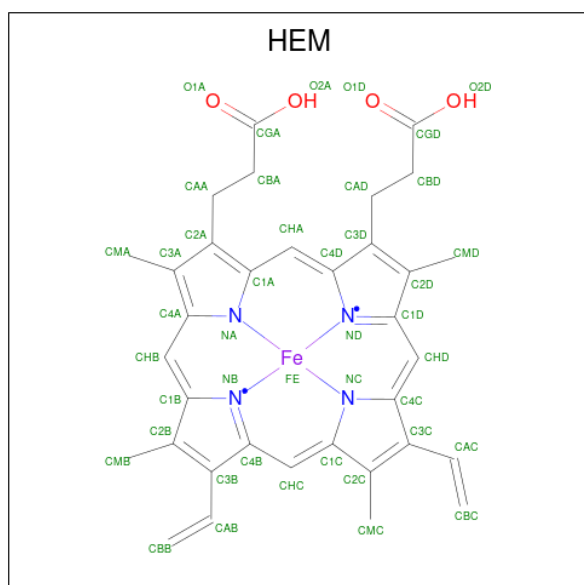
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
4	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 5 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).

IPA

C3

C2

C1

OH

O2

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 4	C 3	O 1	0	0
5	A	1	Total 4	C 3	O 1	0	0
5	B	1	Total 4	C 3	O 1	0	0
5	B	1	Total 4	C 3	O 1	0	0
5	C	1	Total 4	C 3	O 1	0	0
5	C	1	Total 4	C 3	O 1	0	0
5	D	1	Total 4	C 3	O 1	0	0
5	D	1	Total 4	C 3	O 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	53	Total 53	O 53	0	0
6	B	51	Total 51	O 51	0	0
6	C	65	Total 65	O 65	0	0
6	D	40	Total 40	O 40	0	0

W O R L D W I D E

PDB

PROTEIN DATA BANK

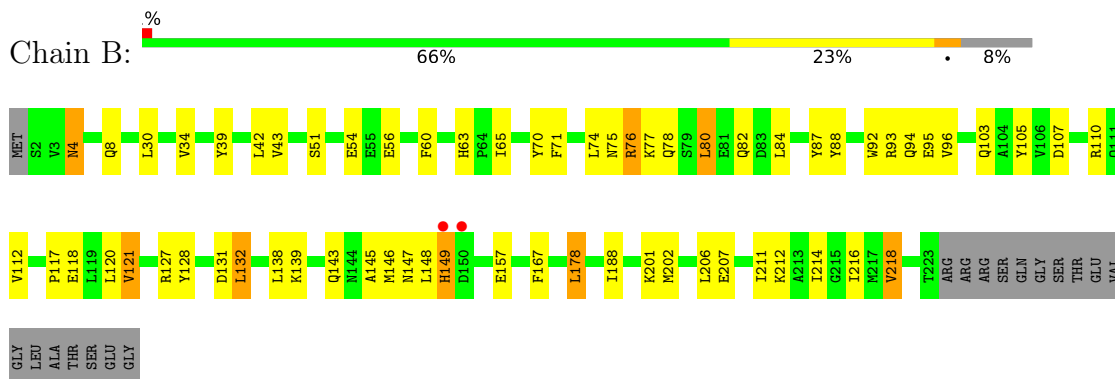# 3　Residue-property plots ⓘ

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: Heme oxygenase 1

- Molecule 1: Heme oxygenase 1

- Molecule 1: Heme oxygenase 1

T184 I188 V189 A197 M202 L206 K212 A213 I216 T223 ARG ARG SER GLN GLY SER THR GLU VAL GLY LEU ALA THR SER GLU GLY

• Molecule 1: Heme oxygenase 1

Chain D:

2%

61%　　　　26%　　5%　　8%

MET SER V3 N4 L5 E11 A20 E21 N22 K27 C28 F29 L30 V34 E35 K36 N37 R40 N45 V49 Y50 E54 E55 E56 M57 F60 K61 D62 H63 L66 S67 H68 I69 Y70 F71 P72 N75 R76 L80 Y87 Y88 N91 W92 R93 Q94 E95

V96 A101 Y105 R108 V109 R110 Q111 V112 T115 A116 P117 E118 L119 L120 Y128 L132 Q136 I137 L138 Q143 M146 N147 L148 H149 D150 Y171 R172 M175 N176 D177 L178 P179 I180 D181 Q182 E191 D194 A197 M198 F203 N204 E205 L206 E207

I211 T223 ARG ARG ARG SER GLN GLY SER THR GLU VAL GLY LEU ALA THR SER GLU GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	110.79Å 113.73Å 109.70Å 90.00° 112.26° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 40.06 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.4 (20.00-2.50) 89.6 (40.06-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.19 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.220 , 0.269 0.209 , 0.255	Depositor DCC
R_{free} test set	4675 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å^2)	48.7	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7468	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< \|L\| >$, $< L^2 >$ 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: PO4, IPA, CL, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#|Z|>5$	RMSZ	$\#|Z|>5$
1	A	0.40	0/1796	0.57	0/2419
1	B	0.42	0/1797	0.56	0/2420
1	C	0.40	0/1794	0.57	0/2417
1	D	0.39	0/1785	0.55	0/2404
All	All	0.40	0/7172	0.56	0/9660

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2   Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1763	0	1722	74	0
1	B	1764	0	1725	60	0
1	C	1761	0	1718	78	0
1	D	1752	0	1718	66	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1	0	0	0	0
4	A	43	0	30	1	0
4	B	43	0	30	1	0
4	C	43	0	30	0	0
4	D	43	0	30	2	0
5	A	8	0	16	3	0
5	B	8	0	16	3	0
5	C	8	0	16	4	0
5	D	8	0	16	6	0
6	A	53	0	0	4	0
6	B	51	0	0	0	0
6	C	65	0	0	1	0
6	D	40	0	0	1	0
All	All	7468	0	7067	270	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 19.

All (270) 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:C:212:LYS:HE2	1:C:216:ILE:HD12	1.42	1.00
1:B:4:ASN:H	1:B:4:ASN:HD22	1.14	0.96
1:D:71:PHE:H	5:D:1008:IPA:H31	1.34	0.91
1:C:212:LYS:HD3	1:C:213:ALA:N	1.84	0.91
1:C:4:ASN:HD22	1:C:4:ASN:H	1.19	0.89
1:A:5:LEU:HD11	1:A:175:MET:HB3	1.55	0.87
1:C:118:GLU:O	1:C:121:VAL:HG13	1.76	0.85
1:A:118:GLU:O	1:A:121:VAL:HG12	1.79	0.83
1:D:50:TYR:O	1:D:54:GLU:HG3	1.79	0.82
1:B:139:LYS:HE2	1:B:143:GLN:NE2	1.98	0.78
1:B:78:GLN:HE21	1:B:82:GLN:HE21	1.31	0.77
1:D:40:ARG:HG3	1:D:87:TYR:HB3	1.67	0.77
1:D:91:ASN:HB3	1:D:94:GLN:OE1	1.83	0.76
1:D:71:PHE:N	5:D:1008:IPA:H31	2.00	0.76
1:A:209:ASN:H	1:A:209:ASN:HD22	1.34	0.75
1:C:4:ASN:HD22	1:C:4:ASN:N	1.85	0.74
1:B:4:ASN:HD22	1:B:4:ASN:N	1.81	0.74
1:D:92:TRP:O	1:D:96:VAL:HG23	1.87	0.74
1:D:108:ARG:NH2	1:D:191:GLU:OE1	2.21	0.74
1:A:209:ASN:HD22	1:A:209:ASN:N	1.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:GLU:O	1:B:121:VAL:HG13	1.87	0.73
1:C:110:ARG:HG3	1:C:110:ARG:HH11	1.52	0.73
1:C:34:VAL:HG12	1:C:145:ALA:HB1	1.70	0.73
1:B:92:TRP:O	1:B:96:VAL:HG23	1.89	0.72
1:A:157:GLU:HG2	6:A:1042:HOH:O	1.89	0.72
1:C:4:ASN:ND2	1:C:8:GLN:HE21	1.88	0.71
1:C:50:TYR:O	1:C:54:GLU:HG3	1.90	0.71
1:B:139:LYS:HE2	1:B:143:GLN:HE22	1.55	0.71
1:C:139:LYS:HE3	1:C:153:THR:HG21	1.73	0.71
1:A:121:VAL:HG11	1:A:188:ILE:HD13	1.71	0.71
1:B:110:ARG:HH11	1:B:110:ARG:HG3	1.54	0.71
1:A:5:LEU:CD1	1:A:175:MET:HB3	2.22	0.70
1:D:29:PHE:HA	1:D:34:VAL:HG12	1.72	0.70
1:A:204:ASN:ND2	1:B:94:GLN:HE22	1.91	0.69
1:C:139:LYS:HE2	1:C:143:GLN:OE1	1.92	0.69
1:A:112:VAL:HG12	1:A:120:LEU:HD13	1.75	0.68
1:B:78:GLN:HE21	1:B:82:GLN:NE2	1.91	0.68
1:C:8:GLN:HE22	1:C:182:GLN:HE22	1.40	0.68
1:C:58:ALA:O	1:C:61:LYS:HG2	1.93	0.68
1:C:112:VAL:HG12	1:C:120:LEU:HD13	1.74	0.68
1:C:35:GLU:HG3	1:C:213:ALA:CB	2.23	0.68
1:A:36:LYS:O	1:A:40:ARG:HB2	1.93	0.68
1:B:117:PRO:O	1:B:120:LEU:HB2	1.94	0.67
1:C:35:GLU:OE1	1:C:37:ASN:HB2	1.94	0.67
1:C:57:MET:HG2	5:C:1007:IPA:H31	1.75	0.67
1:B:207:GLU:O	1:B:211:ILE:HG12	1.96	0.66
1:C:125:TYR:CE1	1:C:129:LEU:HD23	2.31	0.65
1:D:178:LEU:HB3	1:D:180:ILE:HD12	1.78	0.65
1:C:139:LYS:HE3	1:C:153:THR:CG2	2.26	0.65
1:D:69:ILE:HD13	1:D:69:ILE:H	1.61	0.65
1:B:34:VAL:HG12	1:B:145:ALA:HB1	1.78	0.64
1:B:70:TYR:HA	5:B:1006:IPA:H31	1.78	0.64
1:B:4:ASN:H	1:B:4:ASN:ND2	1.89	0.64
1:C:92:TRP:O	1:C:96:VAL:HG23	1.98	0.64
1:A:223:THR:O	1:A:223:THR:HG22	1.97	0.63
1:B:214:ILE:O	1:B:218:VAL:HG12	1.99	0.63
1:D:116:ALA:HB1	1:D:118:GLU:OE2	1.98	0.63
1:D:3:VAL:O	1:D:4:ASN:HB3	1.98	0.63
1:D:110:ARG:HG3	1:D:110:ARG:HH11	1.62	0.63
1:D:63:HIS:O	1:D:67:SER:HB2	1.99	0.62
1:C:110:ARG:HD2	1:D:115:THR:HG21	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:VAL:CG1	1:A:188:ILE:HD13	2.30	0.62
1:B:112:VAL:HG23	1:B:120:LEU:HD22	1.80	0.61
1:B:139:LYS:HG2	1:B:143:GLN:HE21	1.65	0.61
1:C:212:LYS:HE2	1:C:216:ILE:CD1	2.26	0.61
1:A:75:ASN:HD21	5:A:1005:IPA:H33	1.66	0.60
1:C:74:LEU:O	1:C:76:ARG:NH2	2.35	0.59
1:B:74:LEU:HD21	1:B:167:PHE:CE2	2.36	0.59
1:C:9:LEU:HD23	1:C:189:VAL:HG22	1.83	0.59
1:A:146:MET:HB2	1:A:148:LEU:HD21	1.84	0.59
1:A:5:LEU:HD12	1:A:6:ALA:N	2.18	0.59
1:C:4:ASN:H	1:C:4:ASN:ND2	1.94	0.59
1:C:34:VAL:HG12	1:C:145:ALA:CB	2.33	0.59
1:A:4:ASN:CG	1:A:4:ASN:O	2.42	0.58
1:A:117:PRO:O	1:A:120:LEU:HB2	2.02	0.58
1:A:54:GLU:HG2	1:A:75:ASN:ND2	2.19	0.58
1:D:40:ARG:HG3	1:D:87:TYR:CB	2.33	0.58
1:D:35:GLU:HG2	1:D:37:ASN:H	1.68	0.58
1:A:204:ASN:HD22	1:B:94:GLN:HE22	1.52	0.57
1:C:168:LYS:HE2	1:C:172:ARG:NH2	2.19	0.57
1:A:125:TYR:CE1	1:A:129:LEU:HD23	2.39	0.57
1:A:57:MET:HG2	5:A:1005:IPA:H13	1.87	0.57
1:C:40:ARG:HG2	1:C:88:TYR:CE2	2.40	0.57
1:A:133:SER:HB3	4:A:300:HEM:HAD1	1.86	0.57
1:A:139:LYS:HE2	1:A:143:GLN:OE1	2.05	0.56
1:A:174:ALA:O	1:A:178:LEU:HD13	2.04	0.56
1:A:140:LYS:HE2	6:A:1049:HOH:O	2.06	0.56
1:A:3:VAL:HG13	1:A:182:GLN:HG2	1.86	0.56
1:A:34:VAL:HG12	1:A:145:ALA:CB	2.35	0.56
1:B:202:MET:O	1:B:206:LEU:HD13	2.06	0.56
1:B:112:VAL:HG23	1:B:120:LEU:CD2	2.36	0.56
1:A:35:GLU:OE2	1:A:37:ASN:HB2	2.06	0.56
1:C:136:GLN:O	1:C:140:LYS:HG3	2.05	0.56
1:D:45:ASN:O	1:D:49:VAL:HG23	2.07	0.55
1:D:128:TYR:CE2	5:D:1008:IPA:H11	2.42	0.55
1:D:172:ARG:O	1:D:175:MET:HB2	2.07	0.55
1:D:40:ARG:HG2	1:D:88:TYR:CE2	2.42	0.54
1:D:11:GLU:HB3	6:D:1046:HOH:O	2.07	0.54
1:D:108:ARG:HH22	1:D:191:GLU:CD	2.10	0.54
1:D:112:VAL:HG13	1:D:119:LEU:HB2	1.88	0.54
1:C:125:TYR:HE1	1:C:129:LEU:HD23	1.73	0.54
1:B:63:HIS:CD2	1:B:65:ILE:H	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:TYR:HE1	1:A:129:LEU:HD23	1.74	0.53
1:D:207:GLU:O	1:D:211:ILE:HG12	2.08	0.53
1:B:118:GLU:O	1:B:121:VAL:CG1	2.57	0.53
1:C:125:TYR:HB2	1:C:175:MET:HE3	1.91	0.53
1:C:180:ILE:HB	1:C:184:THR:OG1	2.09	0.53
1:A:209:ASN:N	1:A:209:ASN:ND2	2.55	0.53
1:A:207:GLU:O	1:A:211:ILE:HG12	2.09	0.52
1:D:36:LYS:O	1:D:40:ARG:HB2	2.10	0.52
1:C:45:ASN:OD1	1:C:102:GLY:HA3	2.10	0.52
1:B:92:TRP:HE3	1:B:96:VAL:CG2	2.23	0.52
1:D:22:ASN:HA	1:D:27:LYS:HE3	1.91	0.52
1:A:110:ARG:HG3	1:A:110:ARG:HH11	1.75	0.52
1:B:34:VAL:HG12	1:B:145:ALA:CB	2.38	0.52
1:D:56:GLU:O	1:D:60:PHE:HD1	1.92	0.51
1:D:178:LEU:HB3	1:D:180:ILE:CD1	2.40	0.51
1:A:80:LEU:HD13	1:A:155:PHE:CD2	2.44	0.51
1:C:110:ARG:HH11	1:C:110:ARG:CG	2.19	0.51
1:D:180:ILE:HD13	1:D:180:ILE:H	1.75	0.51
1:C:4:ASN:HD21	1:C:8:GLN:HE21	1.57	0.51
1:A:181:ASP:OD1	1:A:183:ALA:HB3	2.11	0.51
1:A:40:ARG:HG2	1:A:88:TYR:CE2	2.46	0.51
1:B:71:PHE:H	5:B:1006:IPA:C3	2.23	0.51
1:A:115:THR:HG21	1:B:110:ARG:HD2	1.93	0.51
1:C:148:LEU:HD11	1:C:151:GLY:O	2.11	0.50
1:B:71:PHE:H	5:B:1006:IPA:H2	1.76	0.50
1:A:40:ARG:HG3	1:A:87:TYR:HB3	1.93	0.50
1:A:3:VAL:HG12	1:A:8:GLN:HE22	1.76	0.50
1:C:212:LYS:HD3	1:C:212:LYS:C	2.31	0.50
1:B:87:TYR:CE2	1:B:146:MET:HE3	2.47	0.50
1:A:5:LEU:HD13	1:A:9:LEU:HD12	1.94	0.50
1:B:74:LEU:HD21	1:B:167:PHE:HE2	1.76	0.50
1:D:4:ASN:CG	1:D:4:ASN:O	2.50	0.50
1:D:40:ARG:CG	1:D:87:TYR:HB3	2.40	0.50
1:C:117:PRO:O	1:C:120:LEU:HB2	2.11	0.49
1:A:56:GLU:OE1	1:A:59:LYS:HE2	2.12	0.49
1:A:108:ARG:HG2	1:A:198:MET:HE1	1.94	0.49
1:C:125:TYR:HB2	1:C:175:MET:CE	2.42	0.49
1:A:40:ARG:HG2	1:A:88:TYR:CZ	2.47	0.49
1:D:112:VAL:HG12	1:D:120:LEU:HD13	1.95	0.49
1:D:54:GLU:HG2	1:D:128:TYR:OH	2.12	0.49
1:A:33:VAL:O	1:A:33:VAL:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:PHE:O	5:C:1007:IPA:H12	2.13	0.48
1:A:143:GLN:HA	1:A:148:LEU:HD23	1.95	0.48
1:A:210:LEU:O	1:A:214:ILE:HG13	2.13	0.48
1:B:56:GLU:O	1:B:60:PHE:HD1	1.97	0.48
1:C:143:GLN:HA	1:C:148:LEU:HB3	1.96	0.48
1:A:15:LYS:HB3	6:A:1022:HOH:O	2.13	0.48
1:A:93:ARG:HB3	1:C:197:ALA:CB	2.44	0.48
1:A:5:LEU:HD11	1:A:175:MET:SD	2.54	0.47
1:C:5:LEU:HD22	1:C:9:LEU:HG	1.96	0.47
1:D:36:LYS:HA	1:D:146:MET:HE1	1.95	0.47
1:A:47:TYR:CE1	1:A:81:GLU:HG2	2.49	0.47
1:B:4:ASN:ND2	1:B:8:GLN:HE21	2.13	0.47
1:A:3:VAL:HG12	1:A:8:GLN:NE2	2.30	0.47
1:A:92:TRP:CZ2	1:A:93:ARG:HD2	2.50	0.47
1:A:44:GLY:O	1:A:47:TYR:HB3	2.15	0.47
1:B:112:VAL:CG2	1:B:120:LEU:HD22	2.45	0.47
1:C:149:HIS:ND1	1:C:150:ASP:N	2.62	0.47
1:C:174:ALA:O	1:C:178:LEU:HD13	2.15	0.47
1:B:63:HIS:HD2	1:B:65:ILE:H	1.62	0.47
1:C:121:VAL:HG22	1:C:188:ILE:HG21	1.96	0.46
1:D:34:VAL:CG2	1:D:146:MET:HG3	2.46	0.46
1:D:143:GLN:HG2	1:D:148:LEU:O	2.16	0.46
1:A:97:LYS:H	1:A:97:LYS:HD3	1.80	0.46
1:D:5:LEU:HD12	1:D:5:LEU:C	2.36	0.46
1:D:20:ALA:HB1	4:D:300:HEM:HAB	1.97	0.46
1:A:97:LYS:HD3	1:A:97:LYS:N	2.31	0.46
1:B:78:GLN:NE2	1:B:82:GLN:HE21	2.08	0.46
1:C:66:LEU:HD21	1:C:117:PRO:O	2.15	0.46
1:C:10:ARG:HG3	1:C:10:ARG:HH11	1.81	0.46
1:C:40:ARG:HG3	1:C:87:TYR:HB3	1.98	0.46
1:A:5:LEU:HD12	1:A:5:LEU:C	2.36	0.46
1:A:34:VAL:HG12	1:A:145:ALA:HB1	1.98	0.46
1:C:93:ARG:HG2	1:D:197:ALA:HB2	1.98	0.45
1:B:206:LEU:HD12	1:B:206:LEU:N	2.31	0.45
1:B:121:VAL:HG22	1:B:188:ILE:HG21	1.99	0.45
1:C:56:GLU:O	1:C:60:PHE:HD1	2.00	0.45
1:D:66:LEU:CD1	1:D:118:GLU:HA	2.47	0.45
1:B:214:ILE:O	1:B:218:VAL:CG1	2.63	0.45
1:C:110:ARG:CG	1:C:110:ARG:NH1	2.80	0.45
1:D:180:ILE:HD13	1:D:180:ILE:N	2.32	0.45
1:A:62:ASP:OD1	1:A:62:ASP:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:ARG:HD2	1:D:115:THR:CG2	2.46	0.44
1:D:203:PHE:CE2	4:D:300:HEM:HBB1	2.52	0.44
1:B:39:TYR:O	1:B:42:LEU:HB3	2.17	0.44
1:B:54:GLU:HG2	1:B:75:ASN:ND2	2.32	0.44
1:C:69:ILE:HD13	1:C:121:VAL:HB	1.98	0.44
1:B:4:ASN:N	1:B:4:ASN:ND2	2.54	0.44
1:B:103:GLN:NE2	1:B:107:ASP:OD2	2.48	0.44
1:C:74:LEU:O	1:C:76:ARG:HG2	2.18	0.44
1:D:57:MET:HG2	5:D:1008:IPA:H32	2.00	0.44
1:D:171:TYR:O	1:D:175:MET:HG2	2.17	0.44
1:A:112:VAL:HG13	1:A:119:LEU:HB2	2.00	0.44
1:C:54:GLU:OE2	1:C:76:ARG:N	2.46	0.43
1:D:138:LEU:HD22	5:D:1004:IPA:H2	2.00	0.43
1:A:78:GLN:CD	1:A:78:GLN:H	2.22	0.43
1:A:213:ALA:O	1:A:217:MET:HG2	2.18	0.43
1:D:57:MET:HG2	5:D:1008:IPA:H13	2.00	0.43
1:A:41:LYS:HE2	6:A:1056:HOH:O	2.18	0.43
1:C:76:ARG:HG2	1:C:76:ARG:HH21	1.83	0.43
1:C:36:LYS:O	1:C:40:ARG:HB2	2.19	0.43
1:B:127:ARG:O	1:B:131:ASP:CG	2.57	0.43
1:C:44:GLY:O	1:C:47:TYR:HB3	2.19	0.43
1:C:153:THR:HG23	1:C:153:THR:O	2.18	0.43
1:C:103:GLN:NE2	1:C:107:ASP:OD2	2.47	0.43
1:C:202:MET:O	1:C:206:LEU:HD22	2.19	0.43
1:D:70:TYR:CE2	1:D:72:PRO:HD3	2.54	0.43
1:A:15:LYS:O	1:A:18:SER:HB3	2.19	0.42
1:A:146:MET:HB2	1:A:148:LEU:CD2	2.48	0.42
1:D:111:GLN:HE22	1:D:115:THR:CG2	2.32	0.42
1:A:191:GLU:O	1:A:194:ASP:HB2	2.18	0.42
1:B:65:ILE:HG23	1:B:178:LEU:HG	2.01	0.42
1:D:194:ASP:O	1:D:198:MET:HG3	2.19	0.42
1:C:98:ILE:HD13	1:C:99:SER:O	2.19	0.42
1:D:62:ASP:O	1:D:63:HIS:C	2.58	0.42
1:A:34:VAL:HG12	1:A:145:ALA:HB3	2.00	0.42
1:A:204:ASN:HD22	1:B:94:GLN:NE2	2.17	0.42
1:B:92:TRP:HE3	1:B:96:VAL:HG21	1.85	0.42
1:C:40:ARG:HG3	1:C:87:TYR:CB	2.50	0.42
1:D:54:GLU:OE2	1:D:75:ASN:HA	2.20	0.42
1:B:201:LYS:HB2	1:B:201:LYS:HE3	1.78	0.42
1:C:75:ASN:HD21	5:C:1007:IPA:H33	1.85	0.42
1:D:143:GLN:HA	1:D:148:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:LEU:O	1:B:88:TYR:HB2	2.20	0.42
1:D:66:LEU:HD21	1:D:117:PRO:O	2.19	0.42
1:A:148:LEU:O	1:A:149:HIS:C	2.58	0.42
1:C:121:VAL:HG22	1:C:188:ILE:CG2	2.50	0.42
1:B:212:LYS:NZ	1:B:216:ILE:HD12	2.35	0.41
1:C:48:PHE:CE1	1:C:98:ILE:HB	2.55	0.41
1:D:3:VAL:HB	1:D:176:ASN:O	2.19	0.41
1:A:168:LYS:HE2	1:A:172:ARG:HH11	1.85	0.41
1:C:168:LYS:NZ	6:C:1012:HOH:O	2.52	0.41
1:D:61:LYS:HE3	1:D:70:TYR:OH	2.20	0.41
1:D:63:HIS:O	1:D:67:SER:CB	2.66	0.41
1:B:76:ARG:HG2	1:B:76:ARG:HH11	1.85	0.41
1:C:54:GLU:OE2	1:C:75:ASN:HA	2.20	0.41
1:A:30:LEU:HD12	1:A:30:LEU:HA	1.78	0.41
1:A:71:PHE:C	1:A:73:GLU:H	2.23	0.41
1:B:51:SER:OG	1:B:77:LYS:HE2	2.20	0.41
1:C:92:TRP:CG	1:C:93:ARG:N	2.89	0.41
1:B:74:LEU:O	1:B:76:ARG:HG2	2.20	0.41
1:C:40:ARG:HG2	1:C:88:TYR:CZ	2.55	0.41
1:D:36:LYS:HB2	1:D:146:MET:HE3	2.03	0.41
1:D:172:ARG:HA	1:D:175:MET:HG3	2.01	0.41
1:B:34:VAL:O	1:B:34:VAL:HG13	2.21	0.41
1:D:136:GLN:HA	1:D:136:GLN:NE2	2.35	0.41
1:A:40:ARG:CD	1:A:87:TYR:HB3	2.50	0.41
1:C:9:LEU:HD23	1:C:9:LEU:HA	1.85	0.41
1:A:75:ASN:HD21	5:A:1005:IPA:C3	2.33	0.41
1:B:43:VAL:HG13	1:B:80:LEU:HD12	2.03	0.41
1:B:74:LEU:HD21	1:B:132:LEU:HD21	2.02	0.41
1:C:63:HIS:CG	1:C:64:PRO:HD2	2.56	0.41
1:C:63:HIS:HB3	1:C:66:LEU:HB2	2.02	0.41
1:C:84:LEU:HA	1:C:84:LEU:HD23	1.87	0.41
1:C:71:PHE:H	5:C:1007:IPA:H2	1.86	0.40
1:A:5:LEU:HD11	1:A:175:MET:CB	2.38	0.40
1:B:87:TYR:HE2	1:B:146:MET:HE3	1.87	0.40
1:A:172:ARG:HG2	1:A:172:ARG:HH21	1.86	0.40
1:B:92:TRP:CE3	1:B:96:VAL:HG21	2.56	0.40
1:B:138:LEU:CD2	4:B:300:HEM:HBC2	2.52	0.40
1:C:55:GLU:O	1:C:58:ALA:HB3	2.21	0.40
1:C:178:LEU:HD12	1:C:178:LEU:HA	1.90	0.40
1:D:110:ARG:HH11	1:D:110:ARG:CG	2.31	0.40
1:D:178:LEU:O	1:D:180:ILE:HD13	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:GLU:HG3	1:B:128:TYR:OH	2.21	0.40
1:D:69:ILE:HA	1:D:71:PHE:CE2	2.57	0.40
1:D:76:ARG:HB3	1:D:80:LEU:CD2	2.52	0.40
1:D:101:ALA:HB3	1:D:205:GLU:OE2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	220/240 (92%)	203 (92%)	16 (7%)	1 (0%)	29	48
1	B	220/240 (92%)	213 (97%)	6 (3%)	1 (0%)	29	48
1	C	220/240 (92%)	208 (94%)	11 (5%)	1 (0%)	29	48
1	D	219/240 (91%)	204 (93%)	14 (6%)	1 (0%)	29	48
All	All	879/960 (92%)	828 (94%)	47 (5%)	4 (0%)	29	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	149	HIS
1	C	135	GLY
1	D	4	ASN
1	A	182	GLN

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	184/200 (92%)	166 (90%)	18 (10%)	8	15
1	B	185/200 (92%)	170 (92%)	15 (8%)	11	23
1	C	184/200 (92%)	169 (92%)	15 (8%)	11	22
1	D	182/200 (91%)	166 (91%)	16 (9%)	10	19
All	All	735/800 (92%)	671 (91%)	64 (9%)	10	20

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	30	LEU
1	A	33	VAL
1	A	35	GLU
1	A	61	LYS
1	A	62	ASP
1	A	66	LEU
1	A	80	LEU
1	A	93	ARG
1	A	97	LYS
1	A	105	TYR
1	A	111	GLN
1	A	120	LEU
1	A	150	ASP
1	A	182	GLN
1	A	194	ASP
1	A	206	LEU
1	A	209	ASN
1	B	4	ASN
1	B	30	LEU
1	B	76	ARG
1	B	80	LEU
1	B	93	ARG
1	B	95	GLU
1	B	105	TYR
1	B	121	VAL
1	B	132	LEU
1	B	147	ASN
1	B	148	LEU
1	B	149	HIS

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Mol	Chain	Res	Type
1	B	157	GLU
1	B	178	LEU
1	B	218	VAL
1	C	4	ASN
1	C	5	LEU
1	C	14	LYS
1	C	30	LEU
1	C	66	LEU
1	C	80	LEU
1	C	85	GLN
1	C	91	ASN
1	C	98	ILE
1	C	105	TYR
1	C	120	LEU
1	C	121	VAL
1	C	147	ASN
1	C	153	THR
1	C	178	LEU
1	D	5	LEU
1	D	30	LEU
1	D	34	VAL
1	D	37	ASN
1	D	69	ILE
1	D	94	GLN
1	D	105	TYR
1	D	108	ARG
1	D	111	GLN
1	D	120	LEU
1	D	132	LEU
1	D	148	LEU
1	D	180	ILE
1	D	182	GLN
1	D	194	ASP
1	D	206	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	8	GLN
1	A	75	ASN
1	A	94	GLN

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Mol	Chain	Res	Type
1	A	123	HIS
1	A	147	ASN
1	A	204	ASN
1	A	209	ASN
1	B	4	ASN
1	B	37	ASN
1	B	63	HIS
1	B	75	ASN
1	B	82	GLN
1	B	85	GLN
1	B	143	GLN
1	B	144	ASN
1	B	147	ASN
1	C	4	ASN
1	C	37	ASN
1	C	75	ASN
1	C	85	GLN
1	C	94	GLN
1	C	147	ASN
1	C	173	GLN
1	C	182	GLN
1	D	8	GLN
1	D	37	ASN
1	D	75	ASN
1	D	82	GLN
1	D	85	GLN
1	D	91	ASN
1	D	111	GLN
1	D	136	GLN
1	D	144	ASN
1	D	169	ASN
1	D	182	GLN

5.3.3　RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 5 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
5	IPA	C	1007	-	3,3,3	0.52	0	3,3,3	0.53	0
2	PO4	B	241	-	4,4,4	1.65	0	6,6,6	0.44	0
5	IPA	B	1006	-	3,3,3	0.47	0	3,3,3	0.41	0
4	HEM	C	300	1,6	41,50,50	1.87	12 (29%)	45,82,82	1.33	8 (17%)
5	IPA	C	1003	-	3,3,3	0.41	0	3,3,3	0.38	0
5	IPA	A	1005	-	3,3,3	0.45	0	3,3,3	0.39	0
4	HEM	A	300	1,6	41,50,50	1.90	13 (31%)	45,82,82	1.29	6 (13%)
4	HEM	D	300	1,6	41,50,50	1.89	12 (29%)	45,82,82	1.36	6 (13%)
4	HEM	B	300	1,6	41,50,50	2.01	13 (31%)	45,82,82	1.30	8 (17%)
5	IPA	A	1001	-	3,3,3	0.42	0	3,3,3	0.39	0
5	IPA	B	1002	-	3,3,3	0.40	0	3,3,3	0.37	0
5	IPA	D	1008	-	3,3,3	0.40	0	3,3,3	0.40	0
2	PO4	A	241	-	4,4,4	1.60	0	6,6,6	0.44	0
5	IPA	D	1004	-	3,3,3	0.42	0	3,3,3	0.41	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
4	HEM	D	300	1,6	-	6/12/54/54	-
4	HEM	A	300	1,6	-	4/12/54/54	-
4	HEM	C	300	1,6	-	6/12/54/54	-
4	HEM	B	300	1,6	-	6/12/54/54	-

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	300	HEM	CBB-CAB	5.19	1.56	1.30
4	A	300	HEM	CBB-CAB	5.11	1.55	1.30
4	C	300	HEM	CBB-CAB	5.08	1.55	1.30
4	D	300	HEM	CBB-CAB	4.93	1.54	1.30
4	B	300	HEM	CBD-CGD	-4.52	1.40	1.50
4	D	300	HEM	CBD-CGD	-4.41	1.40	1.50
4	B	300	HEM	C3C-C2C	-4.15	1.34	1.40
4	C	300	HEM	CBC-CAC	4.10	1.56	1.29
4	D	300	HEM	CBC-CAC	4.07	1.56	1.29
4	B	300	HEM	CBC-CAC	4.04	1.56	1.29
4	A	300	HEM	CBC-CAC	4.02	1.56	1.29
4	A	300	HEM	CBD-CGD	-3.70	1.42	1.50
4	C	300	HEM	CBD-CGD	-3.70	1.42	1.50
4	B	300	HEM	CBA-CGA	-3.70	1.42	1.50
4	A	300	HEM	C3C-C2C	-3.68	1.35	1.40
4	A	300	HEM	CBA-CGA	-3.60	1.42	1.50
4	C	300	HEM	CBA-CGA	-3.54	1.42	1.50
4	D	300	HEM	CBA-CGA	-3.51	1.42	1.50
4	D	300	HEM	C3C-CAC	3.39	1.54	1.47
4	C	300	HEM	C3C-CAC	3.20	1.54	1.47
4	D	300	HEM	C3C-C2C	-3.18	1.36	1.40
4	C	300	HEM	C3C-C2C	-3.16	1.36	1.40
4	B	300	HEM	C4D-ND	-2.97	1.35	1.40
4	A	300	HEM	C3C-CAC	2.77	1.53	1.47
4	B	300	HEM	C3C-CAC	2.75	1.53	1.47
4	A	300	HEM	C4D-ND	-2.73	1.35	1.40
4	B	300	HEM	CHB-C1B	2.65	1.41	1.35
4	A	300	HEM	CHA-C4D	2.65	1.41	1.35
4	D	300	HEM	O1A-CGA	2.58	1.30	1.22
4	B	300	HEM	O1A-CGA	2.57	1.30	1.22
4	A	300	HEM	CBD-CAD	2.47	1.59	1.52
4	C	300	HEM	O1A-CGA	2.47	1.30	1.22
4	C	300	HEM	CHA-C4D	2.46	1.41	1.35
4	D	300	HEM	C4D-ND	-2.44	1.36	1.40
4	B	300	HEM	C4D-C3D	2.42	1.49	1.45
4	A	300	HEM	O1A-CGA	2.32	1.29	1.22
4	B	300	HEM	CHA-C4D	2.32	1.40	1.35
4	A	300	HEM	CHB-C1B	2.32	1.40	1.35
4	C	300	HEM	CHB-C1B	2.27	1.40	1.35
4	C	300	HEM	CBD-CAD	2.26	1.59	1.52
4	C	300	HEM	C2C-C1C	2.23	1.47	1.42
4	A	300	HEM	C4D-C3D	2.21	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	300	HEM	CBD-CAD	2.20	1.59	1.52
4	B	300	HEM	CBD-CAD	2.18	1.58	1.52
4	C	300	HEM	C4D-ND	-2.18	1.36	1.40
4	A	300	HEM	O1D-CGD	2.14	1.29	1.22
4	D	300	HEM	CHA-C4D	2.13	1.40	1.35
4	D	300	HEM	O1D-CGD	2.12	1.29	1.22
4	B	300	HEM	C2C-C1C	2.07	1.47	1.42
4	D	300	HEM	C4D-C3D	2.00	1.48	1.45

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	300	HEM	O2A-CGA-CBA	3.03	123.76	114.03
4	D	300	HEM	CBB-CAB-C3B	-2.97	112.85	127.62
4	A	300	HEM	O2A-CGA-CBA	2.96	123.54	114.03
4	D	300	HEM	O2A-CGA-CBA	2.91	123.38	114.03
4	B	300	HEM	O2A-CGA-CBA	2.89	123.31	114.03
4	B	300	HEM	CBB-CAB-C3B	-2.80	113.69	127.62
4	A	300	HEM	CMC-C2C-C3C	2.77	129.86	124.68
4	A	300	HEM	CBB-CAB-C3B	-2.67	114.32	127.62
4	D	300	HEM	CMC-C2C-C3C	2.63	129.60	124.68
4	C	300	HEM	CBB-CAB-C3B	-2.60	114.68	127.62
4	C	300	HEM	CMC-C2C-C3C	2.49	129.34	124.68
4	B	300	HEM	C4B-CHC-C1C	2.48	125.83	122.56
4	C	300	HEM	O1A-CGA-CBA	-2.41	115.35	123.08
4	D	300	HEM	CMA-C3A-C4A	-2.40	124.77	128.46
4	B	300	HEM	CMC-C2C-C3C	2.31	129.01	124.68
4	C	300	HEM	C4C-CHD-C1D	2.30	125.59	122.56
4	C	300	HEM	CMA-C3A-C4A	-2.27	124.98	128.46
4	A	300	HEM	CMA-C3A-C4A	-2.26	124.98	128.46
4	A	300	HEM	O1A-CGA-CBA	-2.25	115.87	123.08
4	B	300	HEM	O1A-CGA-CBA	-2.23	115.92	123.08
4	D	300	HEM	CMA-C3A-C2A	2.23	129.14	124.94
4	C	300	HEM	O2D-CGD-CBD	2.22	121.17	114.03
4	D	300	HEM	O1A-CGA-CBA	-2.18	116.09	123.08
4	B	300	HEM	CMA-C3A-C4A	-2.15	125.16	128.46
4	C	300	HEM	CMA-C3A-C2A	2.15	129.00	124.94
4	B	300	HEM	O2D-CGD-CBD	2.07	120.68	114.03
4	A	300	HEM	CMA-C3A-C2A	2.06	128.83	124.94
4	B	300	HEM	CMA-C3A-C2A	2.02	128.75	124.94

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	300	HEM	C2B-C3B-CAB-CBB
4	B	300	HEM	C2B-C3B-CAB-CBB
4	D	300	HEM	C2B-C3B-CAB-CBB
4	C	300	HEM	C2B-C3B-CAB-CBB
4	A	300	HEM	C4B-C3B-CAB-CBB
4	B	300	HEM	C4B-C3B-CAB-CBB
4	D	300	HEM	C4B-C3B-CAB-CBB
4	A	300	HEM	CAA-CBA-CGA-O2A
4	A	300	HEM	CAA-CBA-CGA-O1A
4	C	300	HEM	CAA-CBA-CGA-O1A
4	C	300	HEM	CAA-CBA-CGA-O2A
4	B	300	HEM	CAD-CBD-CGD-O2D
4	B	300	HEM	CAD-CBD-CGD-O1D
4	D	300	HEM	CAA-CBA-CGA-O2A
4	D	300	HEM	CAA-CBA-CGA-O1A
4	D	300	HEM	CAD-CBD-CGD-O2D
4	C	300	HEM	CAD-CBD-CGD-O2D
4	C	300	HEM	C4B-C3B-CAB-CBB
4	B	300	HEM	CAA-CBA-CGA-O2A
4	B	300	HEM	CAA-CBA-CGA-O1A
4	C	300	HEM	CAD-CBD-CGD-O1D
4	D	300	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.
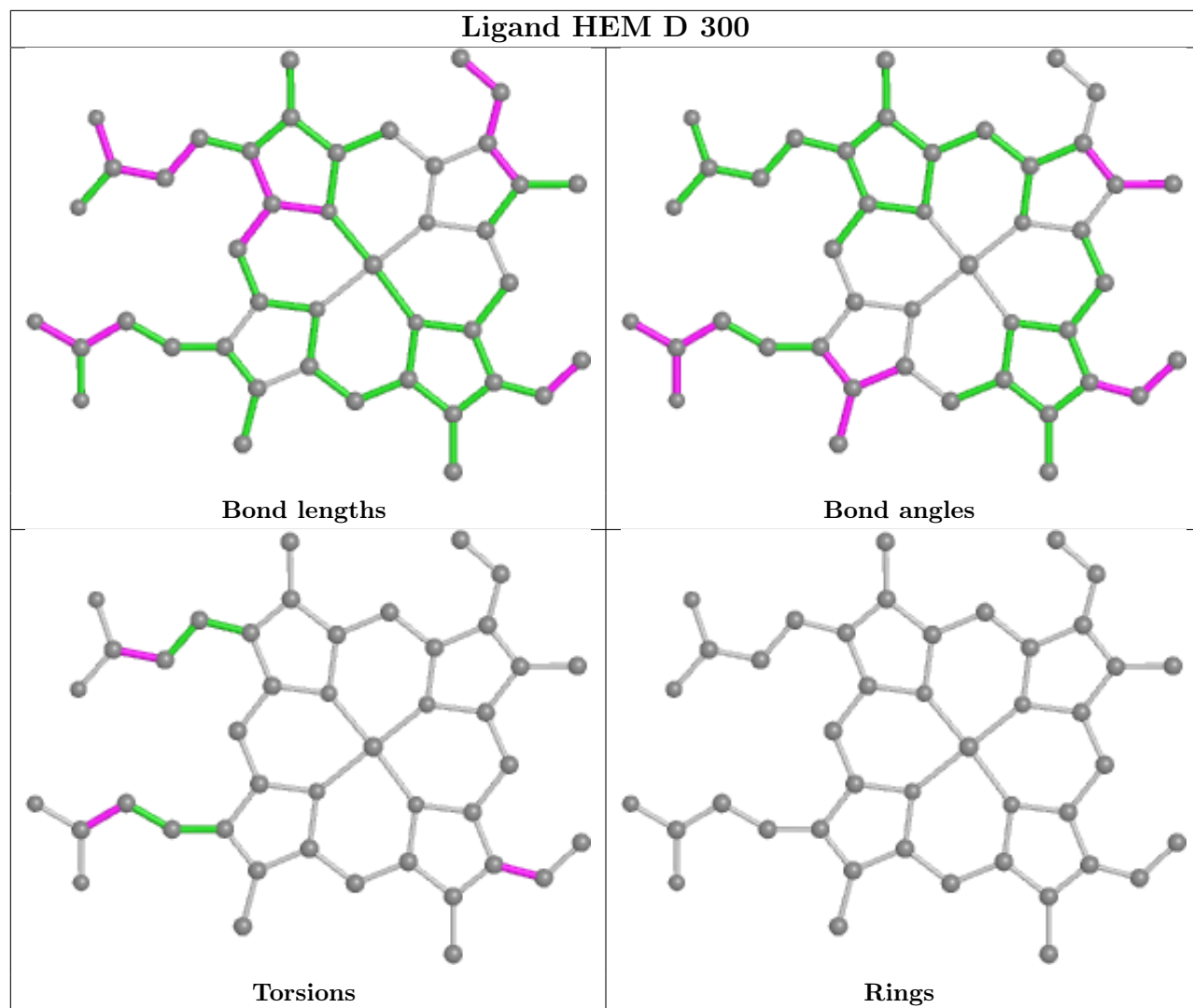
8 monomers are involved in 20 short contacts:

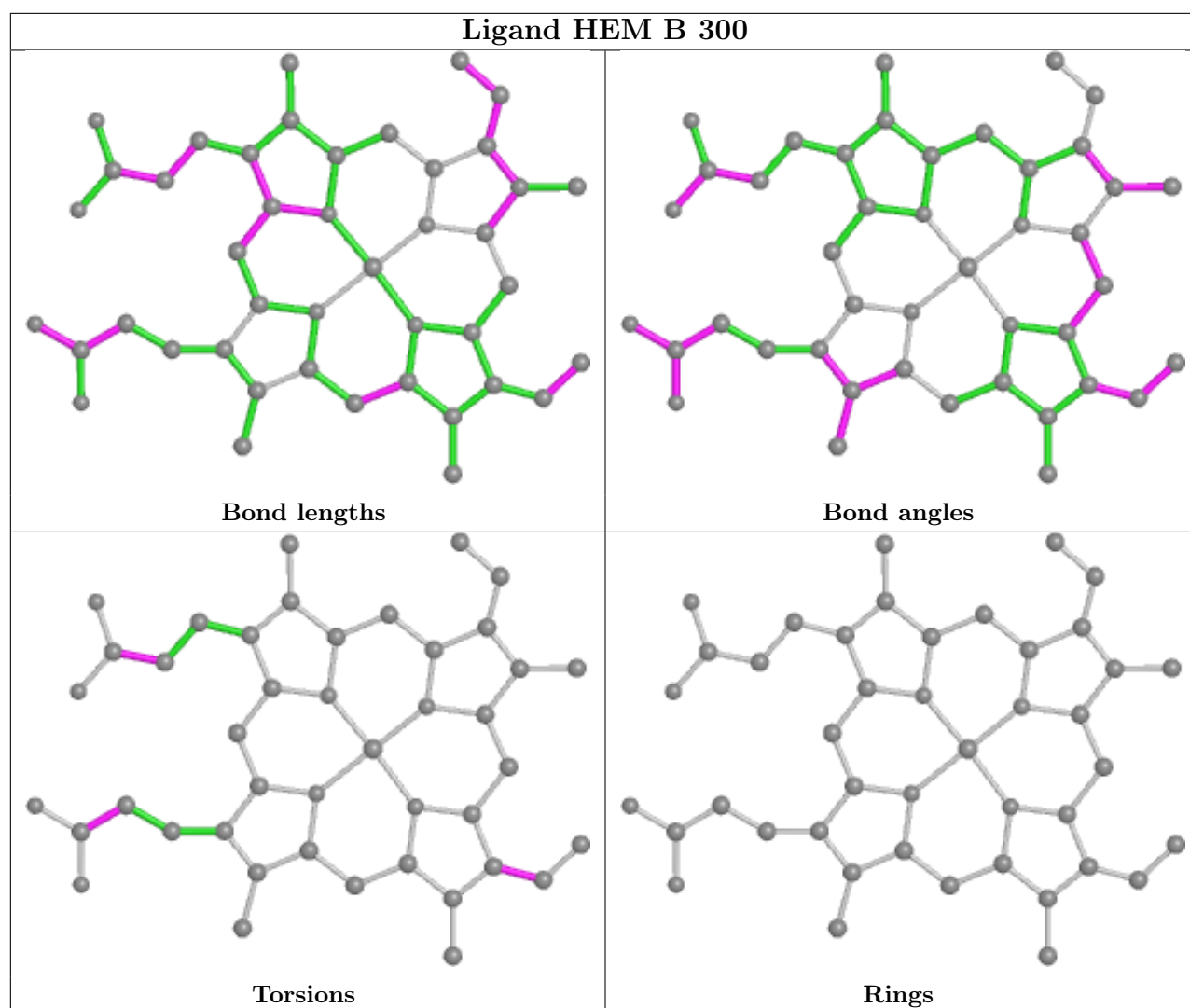| Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1007	IPA	4	0
5	B	1006	IPA	3	0
5	A	1005	IPA	3	0
4	A	300	HEM	1	0
4	D	300	HEM	2	0
4	B	300	HEM	1	0
5	D	1008	IPA	5	0
5	D	1004	IPA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand HEM C 300

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 300

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM D 300

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM B 300

Bond lengths

Bond angles

Torsions

Rings
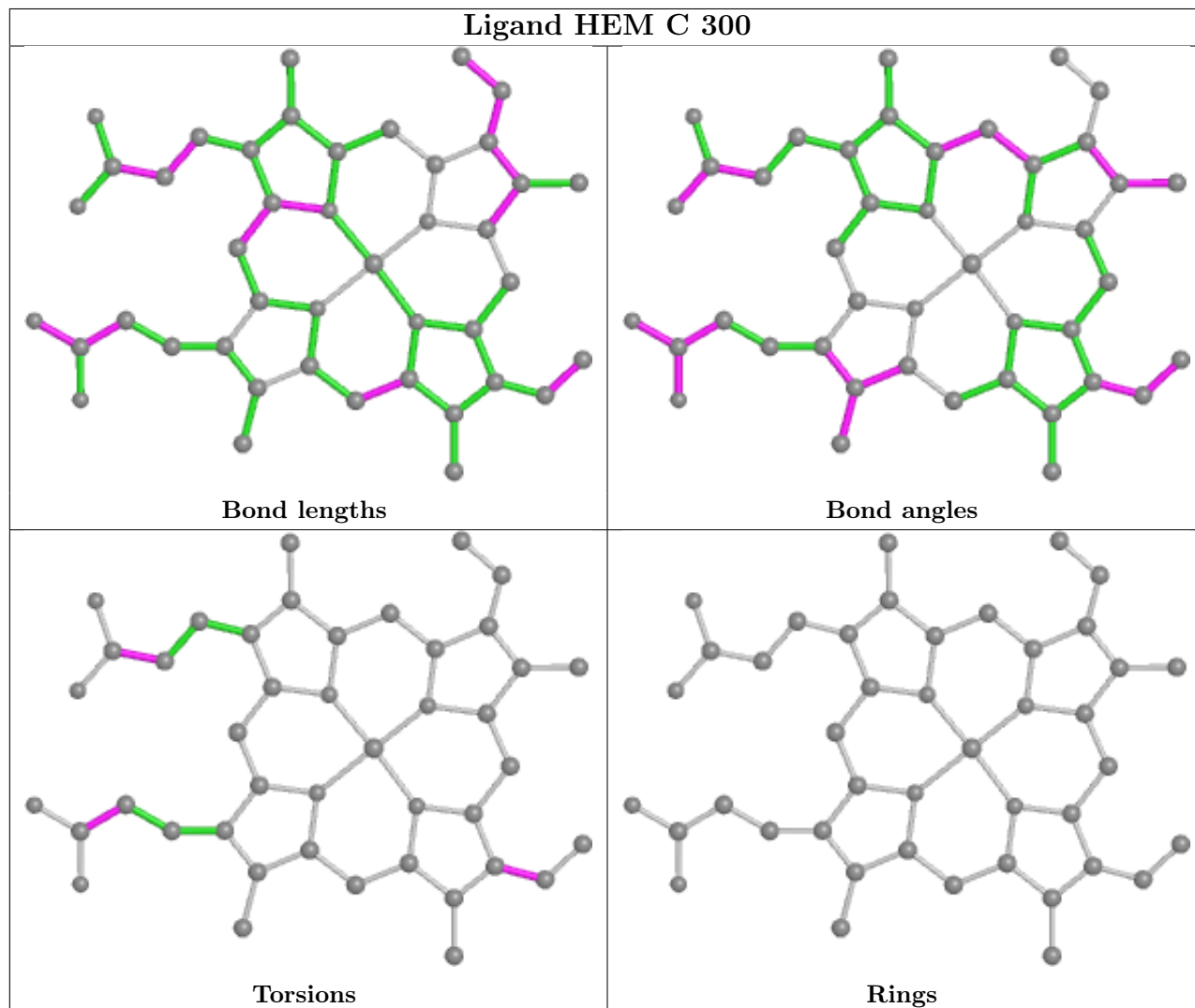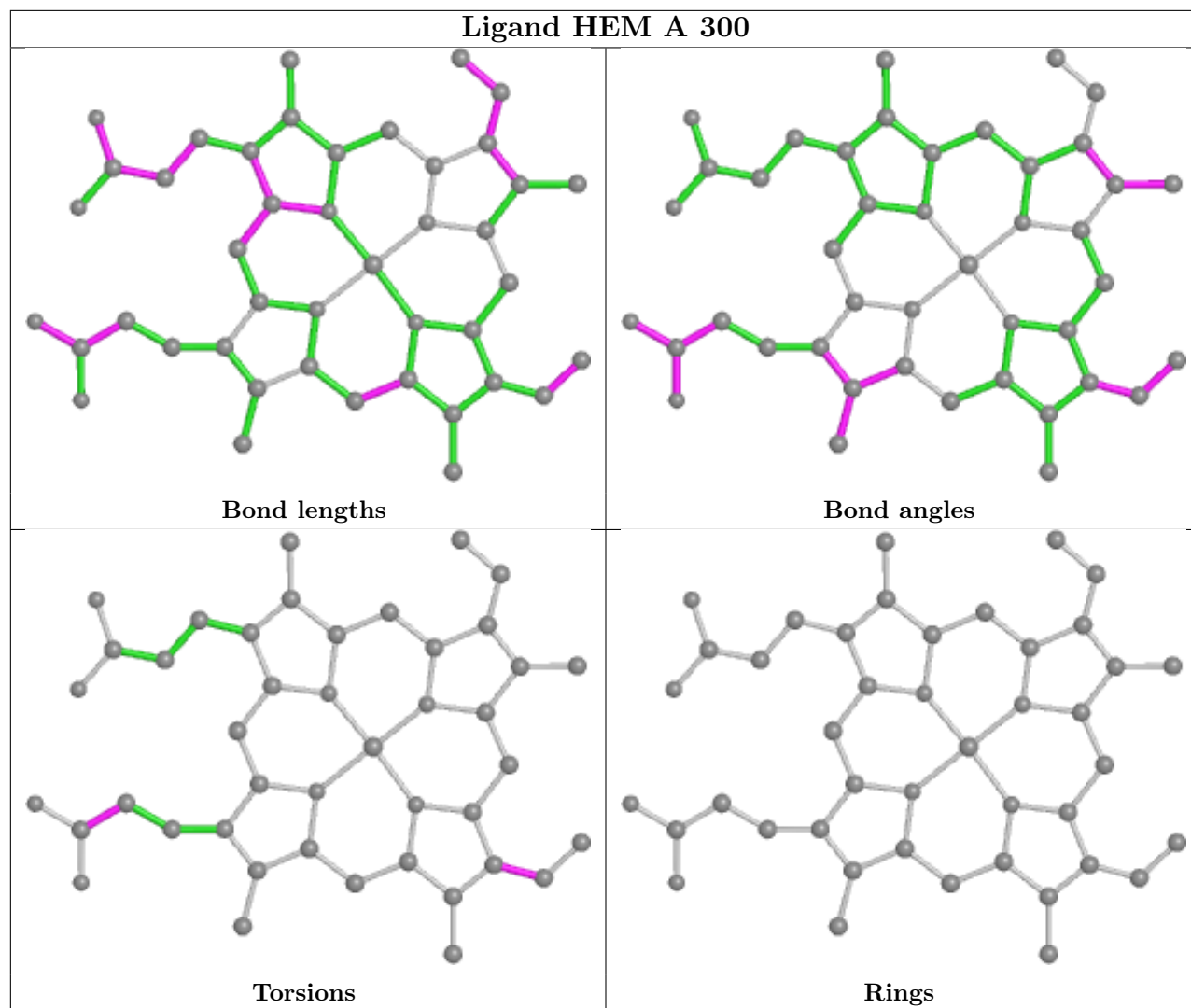
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6　Fit of model and data ⓘ

6.1　Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9
1	A	222/240 (92%)	-0.15	3 (1%) 75	77	34, 51, 72, 91	0
1	B	222/240 (92%)	-0.29	2 (0%) 84	86	33, 46, 61, 88	0
1	C	222/240 (92%)	-0.21	1 (0%) 91	91	32, 50, 68, 91	0
1	D	221/240 (92%)	-0.07	5 (2%) 60	63	39, 55, 82, 88	0
All	All	887/960 (92%)	-0.18	11 (1%) 79	80	32, 50, 73, 91	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	149	HIS	3.7
1	A	150	ASP	3.5
1	B	150	ASP	3.3
1	C	150	ASP	3.0
1	D	150	ASP	3.0
1	D	149	HIS	2.7
1	D	180	ILE	2.6
1	B	149	HIS	2.5
1	D	179	PRO	2.3
1	A	148	LEU	2.2
1	D	3	VAL	2.1

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

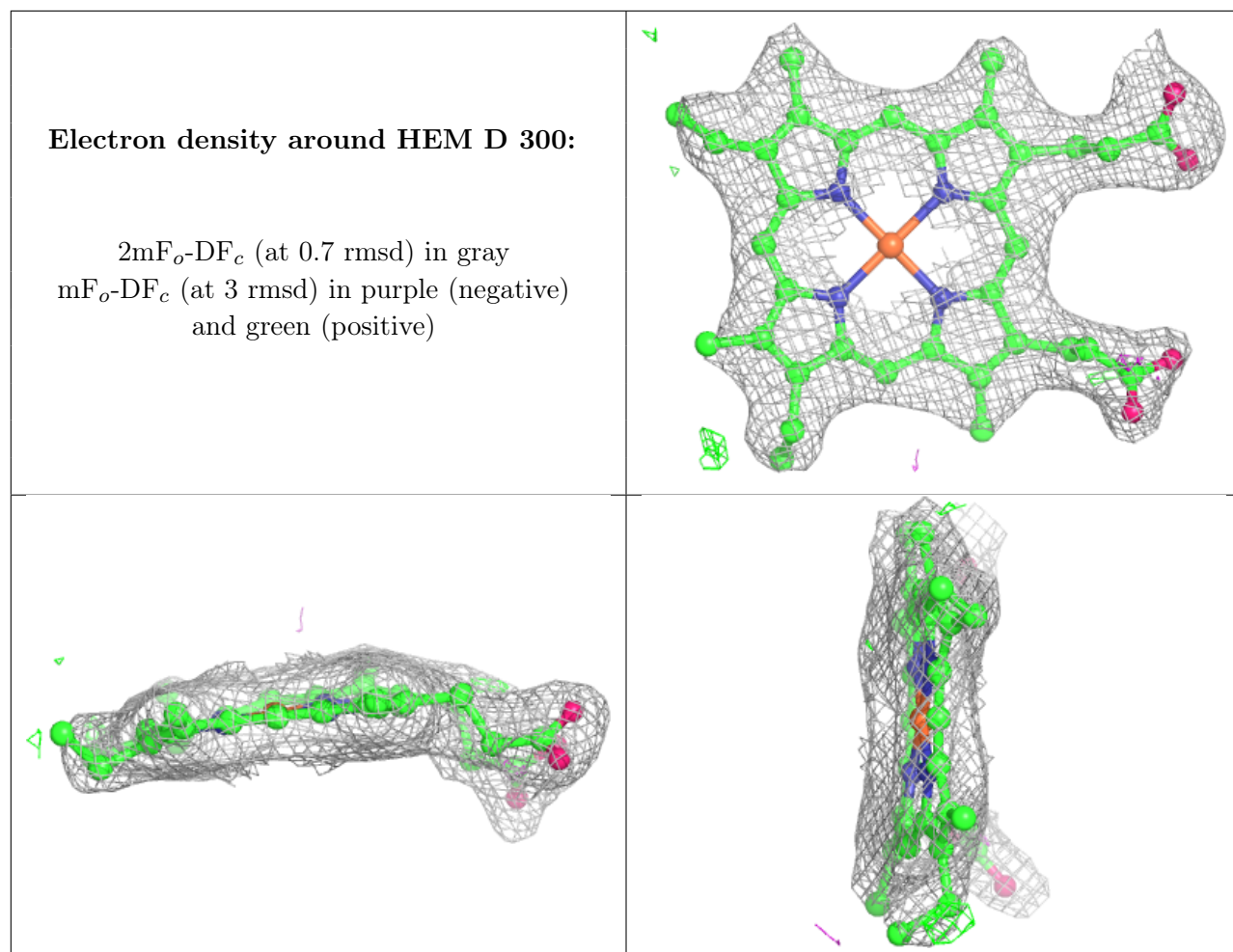There are no non-standard protein/DNA/RNA residues in this entry.

6.3　Carbohydrates ⓘ

There are no monosaccharides in this entry.

WORLDWIDE
wwPDB
PROTEIN DATA BANK

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.
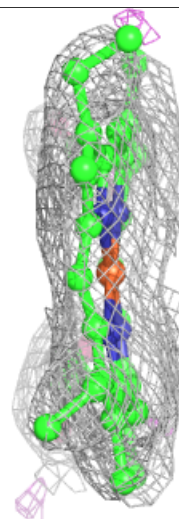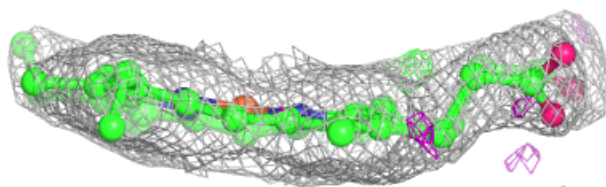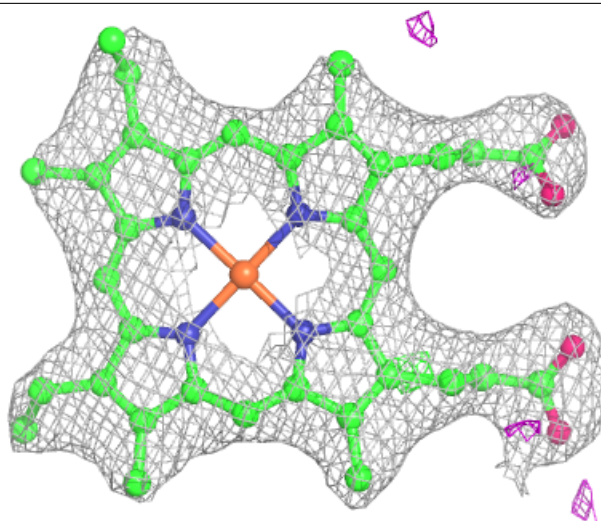
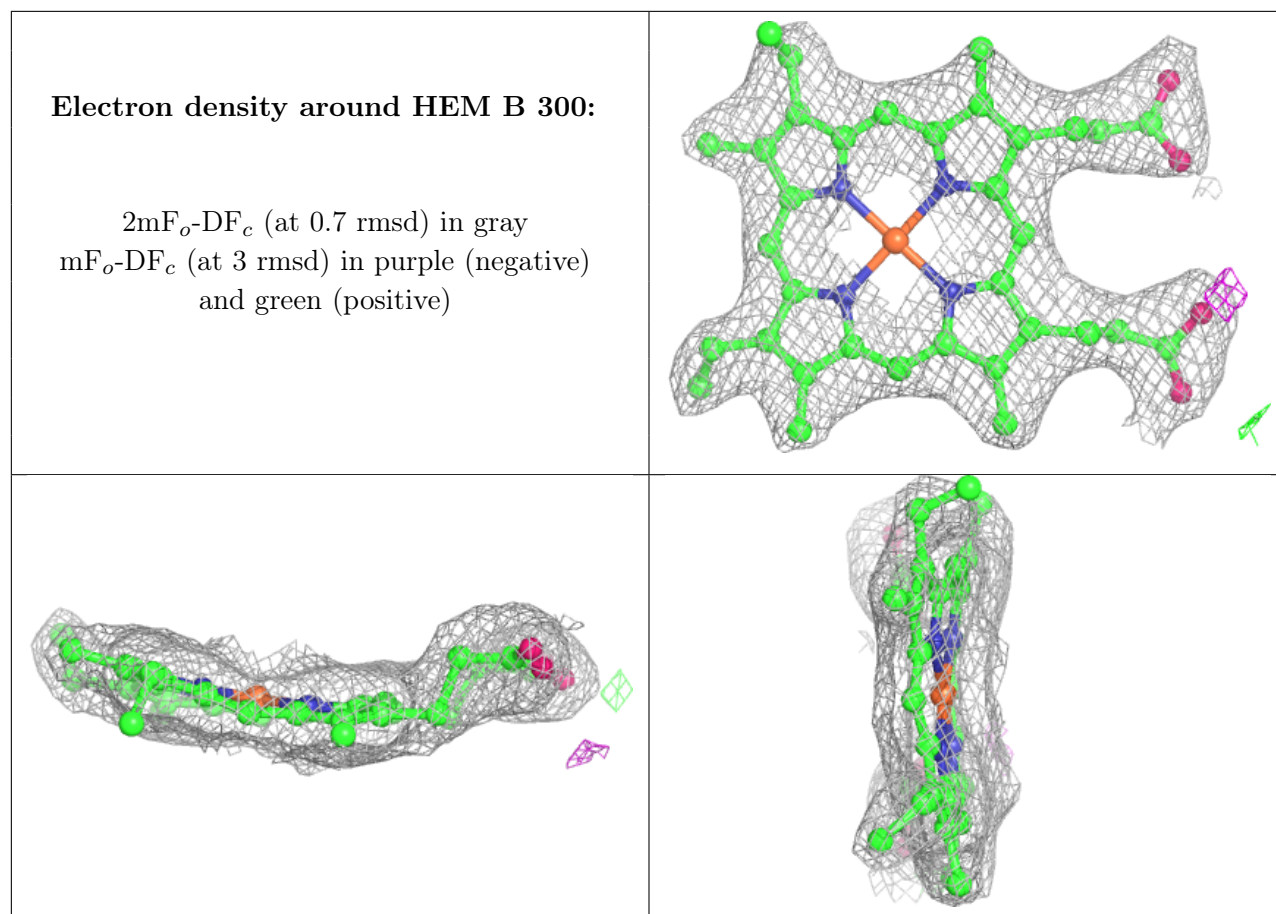| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	IPA	C	1007	4/4	0.70	0.34	71,72,72,74	0
3	CL	D	241	1/1	0.78	0.26	84,84,84,84	0
5	IPA	D	1004	4/4	0.81	0.33	78,79,80,80	0
3	CL	C	241	1/1	0.85	0.39	95,95,95,95	0
5	IPA	D	1008	4/4	0.86	0.22	61,63,64,64	0
3	CL	A	243	1/1	0.88	0.22	83,83,83,83	0
3	CL	A	242	1/1	0.89	0.36	87,87,87,87	0
3	CL	B	242	1/1	0.89	0.25	87,87,87,87	0
5	IPA	A	1005	4/4	0.89	0.19	58,59,60,60	0
2	PO4	A	241	5/5	0.90	0.16	96,97,97,97	0
5	IPA	A	1001	4/4	0.90	0.29	84,84,84,84	0
5	IPA	C	1003	4/4	0.92	0.18	71,71,71,72	0
5	IPA	B	1002	4/4	0.93	0.23	64,65,65,65	0
5	IPA	B	1006	4/4	0.96	0.18	59,59,59,60	0
4	HEM	D	300	43/43	0.97	0.15	41,46,61,67	0
4	HEM	A	300	43/43	0.97	0.15	44,48,62,70	0
4	HEM	B	300	43/43	0.97	0.14	36,40,50,58	0
4	HEM	C	300	43/43	0.98	0.14	36,41,49,55	0
2	PO4	B	241	5/5	0.98	0.11	59,61,62,62	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.
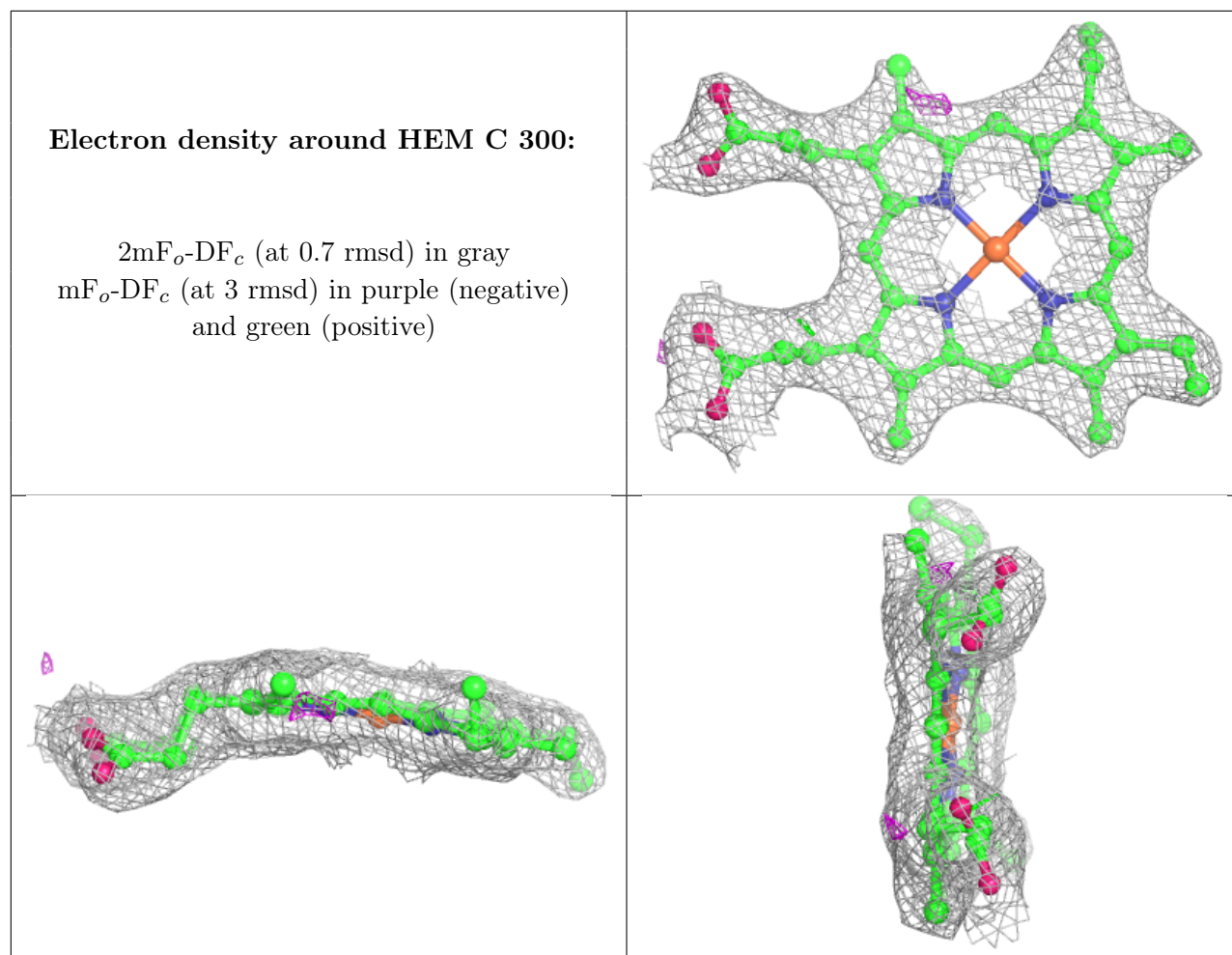
Electron density around HEM D 300:

$2mF_o$-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 300:

$2mF_o$-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 B 300:

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

Electron density around HEM C 300:

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

6.5   Other polymers ⓘ

There are no such residues in this entry.