



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 07:24 AM EDT

PDB ID : 7ASB
Title : Crystal structure of dimeric chlorite dismutase variant Q74E (CCld Q74E) from *Cyanothece* sp. PCC7425
Authors : Schmidt, D.; Mlynek, G.; Djinovic-Carugo, K.; Obinger, C.
Deposited on : 2020-10-27
Resolution : 1.40 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

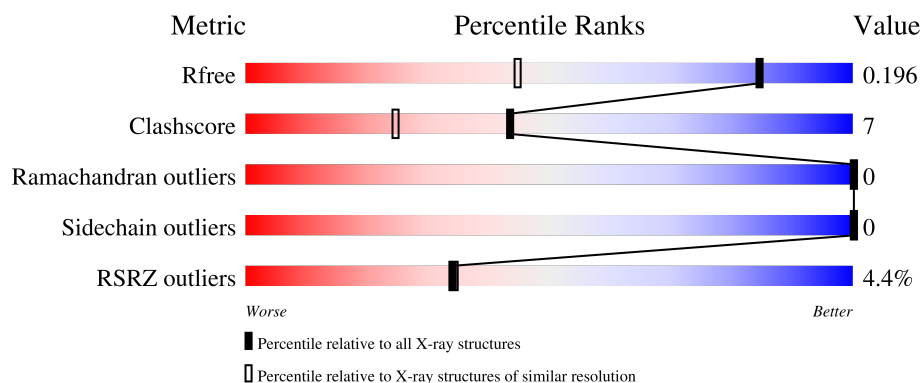
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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}	130704	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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	188	 4% 86% 10% . .
1	B	188	 4% 85% 11% . .

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
2	GOL	B	704	-	X	-	-
5	PEG	B	705	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6665 atoms, of which 3169 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 Chlorite dismutase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	181	Total	C	H	N	O	S	0	8	0
			3045	975	1517	276	272	5			
1	B	181	Total	C	H	N	O	S	0	6	0
			3045	976	1516	275	273	5			

There are 16 discrepancies between the modelled and reference sequences:

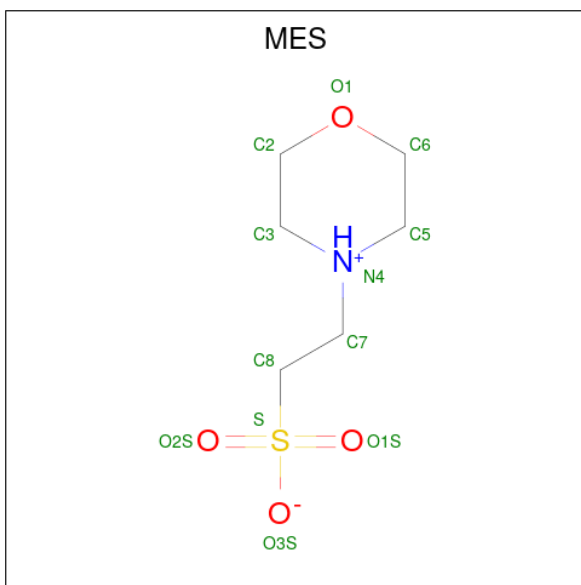
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP B8HNS6
A	-4	PRO	-	expression tag	UNP B8HNS6
A	-3	GLY	-	expression tag	UNP B8HNS6
A	-2	TYR	-	expression tag	UNP B8HNS6
A	-1	GLN	-	expression tag	UNP B8HNS6
A	0	ASP	-	expression tag	UNP B8HNS6
A	1	PRO	-	expression tag	UNP B8HNS6
A	74	GLU	GLN	engineered mutation	UNP B8HNS6
B	-5	GLY	-	expression tag	UNP B8HNS6
B	-4	PRO	-	expression tag	UNP B8HNS6
B	-3	GLY	-	expression tag	UNP B8HNS6
B	-2	TYR	-	expression tag	UNP B8HNS6
B	-1	GLN	-	expression tag	UNP B8HNS6
B	0	ASP	-	expression tag	UNP B8HNS6
B	1	PRO	-	expression tag	UNP B8HNS6
B	74	GLU	GLN	engineered mutation	UNP B8HNS6

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



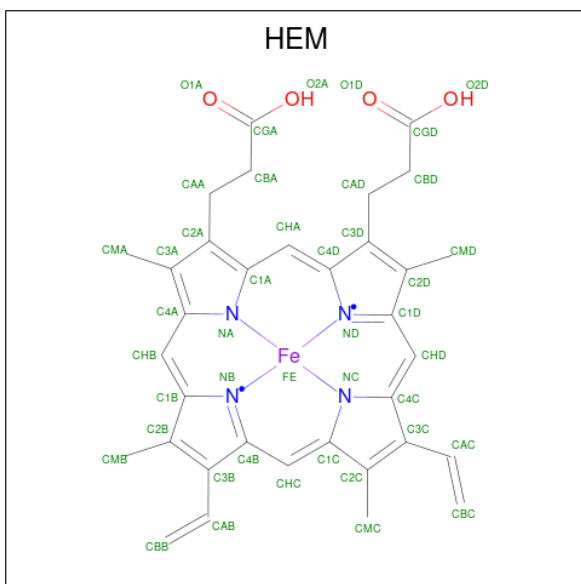
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			9	3	3	3		
2	A	1	Total	C	H	O	0	0
			9	3	3	3		
2	A	1	Total	C	H	O	0	0
			9	3	3	3		
2	A	1	Total	C	H	O	0	0
			9	3	3	3		
2	B	1	Total	C	H	O	0	0
			9	3	3	3		
2	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



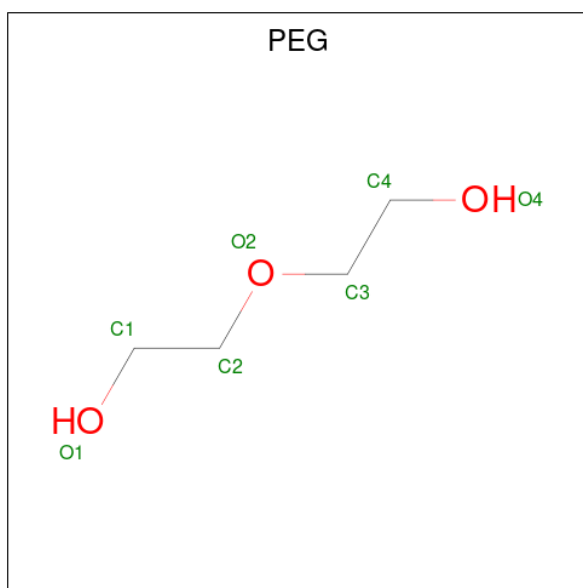
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



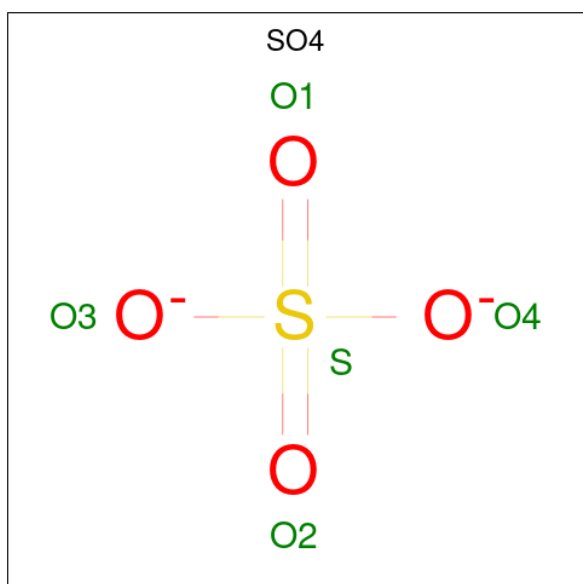
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0
4	B	1	Total 73	C 34	Fe 1	H 30	N 4	O 4	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			17	4	10	3		
5	A	1	Total	C	H	O	0	0
			17	4	10	3		
5	B	1	Total	C	H	O	0	0
			17	4	10	3		
5	B	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		


- Molecule 7 is water.

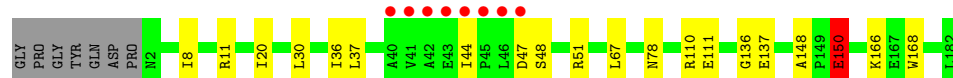
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	139	Total	O	0	0
			139	139		
7	B	133	Total	O	0	0
			133	133		

3 Residue-property plots [i](#)


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

- Molecule 1: Chlorite dismutase

Chain A: 



- Molecule 1: Chlorite dismutase

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	51.16Å 52.74Å 54.77Å 107.41° 99.14° 108.98°	Depositor
Resolution (Å)	30.98 – 1.40 50.11 – 1.24	Depositor EDS
% Data completeness (in resolution range)	92.5 (30.98-1.40) 76.3 (50.11-1.24)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.24 (at 1.24Å)	Xtriage
Refinement program	PHENIX dev_3885	Depositor
R, R_{free}	0.162 , 0.193 0.165 , 0.196	Depositor DCC
R_{free} test set	1981 reflections (1.54%)	wwPDB-VP
Wilson B-factor (Å ²)	12.9	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6665	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.77% 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: HEM, GOL, SO4, PEG, MES

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	0.90	5/1593 (0.3%)	1.24	3/2149 (0.1%)
1	B	0.80	4/1583 (0.3%)	0.94	6/2137 (0.3%)
All	All	0.85	9/3176 (0.3%)	1.10	9/4286 (0.2%)

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
1	A	0	1
1	B	0	1
All	All	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	150	GLU	CG-CD	16.18	1.76	1.51
1	A	150	GLU	CB-CG	10.19	1.71	1.52
1	A	150	GLU	CD-OE1	-7.76	1.17	1.25
1	B	95	GLN	CG-CD	7.41	1.68	1.51
1	B	180	LYS	CE-NZ	7.05	1.66	1.49
1	B	172	GLU	CB-CG	-6.08	1.40	1.52
1	A	150	GLU	N-CA	5.72	1.57	1.46
1	A	168	TRP	CB-CG	-5.63	1.40	1.50
1	B	95	GLN	CB-CG	5.50	1.67	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	GLU	OE1-CD-OE2	-35.06	81.23	123.30
1	A	150	GLU	CG-CD-OE1	20.63	159.55	118.30
1	B	127	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	B	99	MET	CG-SD-CE	-5.85	90.84	100.20
1	A	150	GLU	CG-CD-OE2	-5.47	107.35	118.30
1	B	104	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	B	168	TRP	CB-CG-CD1	-5.16	120.29	127.00
1	B	51	ARG	CG-CD-NE	-5.08	101.13	111.80
1	B	51	ARG	NE-CZ-NH2	-5.05	117.78	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	150	GLU	Sidechain
1	B	95	GLN	Sidechain

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	1528	1517	1465	20	0
1	B	1529	1516	1494	18	0
2	A	24	12	32	3	0
2	B	12	11	13	3	0
3	A	12	13	13	0	0
4	A	43	30	30	0	0
4	B	43	30	30	0	0
5	A	14	20	20	3	0
5	B	14	20	20	7	0
6	A	5	0	0	0	0
7	A	139	0	0	3	0
7	B	133	0	0	12	0
All	All	3496	3169	3117	43	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 7.

All (43) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:GLU:CD	1:A:150:GLU:CG	1.76	1.47
1:B:13:GLY:H	5:B:705:PEG:H11	1.31	0.95
1:B:114:HIS:O	7:B:801:HOH:O	1.85	0.94
2:B:704:GOL:O1	7:B:802:HOH:O	1.86	0.93
1:B:118:GLY:N	7:B:801:HOH:O	2.06	0.81
1:A:148:ALA:HB1	1:A:150:GLU:OE1	1.82	0.80
1:B:13:GLY:N	5:B:705:PEG:H11	2.01	0.74
1:B:11:ARG:HH11	1:B:47:ASP:HB3	1.55	0.70
1:B:12:THR:HB	5:B:705:PEG:H12	1.78	0.66
1:B:14:GLN:HG3	5:B:705:PEG:H41	1.86	0.57
1:B:115:THR:C	7:B:801:HOH:O	2.43	0.57
1:A:150:GLU:CG	1:A:150:GLU:OE2	2.45	0.56
1:B:118:GLY:CA	7:B:801:HOH:O	2.50	0.56
2:B:704:GOL:H11	7:B:861:HOH:O	2.05	0.55
1:A:150:GLU:CD	1:A:150:GLU:CB	2.74	0.55
1:A:8:ILE:HD13	1:A:51:ARG:HG2	1.88	0.54
1:B:13:GLY:H	5:B:705:PEG:C1	2.13	0.53
1:A:36:ILE:O	1:A:37:LEU:HD23	2.08	0.53
1:A:8:ILE:CD1	1:A:51:ARG:HG2	2.40	0.52
1:A:44:ILE:HG22	1:A:48:SER:OG	2.10	0.51
1:B:37:LEU:HD12	1:B:41:VAL:HG21	1.94	0.49
1:B:115:THR:O	7:B:801:HOH:O	2.20	0.49
1:B:20:ILE:HD12	1:B:30:LEU:HA	1.94	0.48
1:A:67:LEU:HD22	2:A:205:GOL:C1	2.45	0.46
2:B:704:GOL:C1	7:B:861:HOH:O	2.62	0.46
1:A:78[B]:ASN:OD1	7:A:301:HOH:O	2.20	0.46
1:A:20:ILE:HD12	1:A:30:LEU:HA	1.98	0.45
7:A:310:HOH:O	5:B:701:PEG:C2	2.64	0.45
1:B:115:THR:CA	7:B:801:HOH:O	2.65	0.45
1:A:136:GLY:O	5:A:207:PEG:C4	2.66	0.44
1:B:118:GLY:HA3	7:B:801:HOH:O	2.15	0.44
1:A:136:GLY:O	5:A:207:PEG:H41	2.18	0.44
1:A:8:ILE:CD1	1:A:51:ARG:CG	2.95	0.44
1:A:67:LEU:HD22	2:A:205:GOL:H12	2.01	0.43
1:A:11:ARG:HG3	1:A:47:ASP:HB3	1.99	0.42
7:A:310:HOH:O	5:B:701:PEG:H21	2.19	0.42
1:B:157:GLU:OE1	7:B:803:HOH:O	2.21	0.42
1:A:111:GLU:OE2	1:A:166:LYS:HG2	2.20	0.42
1:A:137:GLU:OE1	5:A:207:PEG:H12	2.20	0.42
1:B:115:THR:HA	7:B:801:HOH:O	2.19	0.42
1:A:110:ARG:HG2	1:A:110:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:ILE:O	1:B:44:ILE:HG13	2.21	0.41
1:A:36:ILE:HD12	2:A:202:GOL:H11	2.03	0.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	185/188 (98%)	181 (98%)	4 (2%)	0	100	100
1	B	184/188 (98%)	180 (98%)	4 (2%)	0	100	100
All	All	369/376 (98%)	361 (98%)	8 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	161/159 (101%)	161 (100%)	0	100	100
1	B	160/159 (101%)	160 (100%)	0	100	100
All	All	321/318 (101%)	321 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

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 ⓘ

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	HEM	A	204	7,1	42,50,50	1.91	8 (19%)	46,82,82	1.85	15 (32%)
2	GOL	A	205	-	5,5,5	0.99	0	5,5,5	1.11	1 (20%)
2	GOL	A	202	-	5,5,5	1.09	1 (20%)	5,5,5	0.98	1 (20%)
4	HEM	B	703	7,1	42,50,50	1.82	9 (21%)	46,82,82	2.04	14 (30%)
2	GOL	B	702	-	5,5,5	1.35	1 (20%)	5,5,5	0.99	0
2	GOL	B	704	-	5,5,5	3.25	4 (80%)	5,5,5	0.90	0
5	PEG	A	207	-	6,6,6	0.50	0	5,5,5	0.31	0
2	GOL	A	201	-	5,5,5	0.65	0	5,5,5	1.01	1 (20%)
3	MES	A	203	-	12,12,12	1.99	1 (8%)	15,16,16	1.17	1 (6%)
5	PEG	B	705	-	6,6,6	0.47	0	5,5,5	0.56	0
2	GOL	A	206	-	5,5,5	0.85	0	5,5,5	1.07	0
6	SO4	A	208	-	4,4,4	0.22	0	6,6,6	0.07	0
5	PEG	A	209	-	6,6,6	0.49	0	5,5,5	0.31	0
5	PEG	B	701	-	6,6,6	0.52	0	5,5,5	0.26	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	A	204	7,1	-	4/12/54/54	-
2	GOL	A	205	-	-	0/4/4/4	-
2	GOL	A	202	-	-	0/4/4/4	-
4	HEM	B	703	7,1	-	2/12/54/54	-
2	GOL	B	702	-	-	1/4/4/4	-
2	GOL	B	704	-	-	4/4/4/4	-
5	PEG	A	207	-	-	2/4/4/4	-
2	GOL	A	201	-	-	4/4/4/4	-
3	MES	A	203	-	-	0/6/14/14	0/1/1/1
5	PEG	B	705	-	-	3/4/4/4	-
2	GOL	A	206	-	-	2/4/4/4	-
5	PEG	A	209	-	-	3/4/4/4	-
5	PEG	B	701	-	-	2/4/4/4	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	204	HEM	C3C-C2C	-6.45	1.31	1.40
3	A	203	MES	C8-S	-6.28	1.68	1.77
4	B	703	HEM	C3C-C2C	-6.25	1.31	1.40
2	B	704	GOL	O2-C2	-5.64	1.27	1.43
4	A	204	HEM	C1A-NA	5.32	1.47	1.36
4	B	703	HEM	C3C-C4C	4.60	1.48	1.41
4	A	204	HEM	C3C-C4C	4.31	1.47	1.41
2	B	704	GOL	O1-C1	-2.97	1.30	1.42
4	A	204	HEM	C4A-NA	2.82	1.42	1.36
4	B	703	HEM	C1A-NA	2.70	1.41	1.36
2	B	702	GOL	O2-C2	-2.70	1.35	1.43
4	B	703	HEM	CAB-C3B	2.52	1.54	1.47
4	B	703	HEM	C3B-C2B	-2.48	1.32	1.37
2	B	704	GOL	C1-C2	-2.48	1.42	1.51
2	B	704	GOL	C3-C2	2.43	1.61	1.51
4	B	703	HEM	O2D-CGD	-2.42	1.22	1.30
4	B	703	HEM	FE-ND	2.27	2.10	1.98
4	A	204	HEM	FE-ND	2.25	2.10	1.98
4	A	204	HEM	CHB-C1B	2.23	1.40	1.34
2	A	202	GOL	O2-C2	-2.19	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	703	HEM	C4D-C3D	-2.16	1.41	1.45
4	A	204	HEM	CAB-C3B	2.07	1.52	1.47
4	A	204	HEM	C3D-C2D	-2.04	1.32	1.36
4	B	703	HEM	C3C-CAC	2.03	1.52	1.47

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	703	HEM	C4B-CHC-C1C	6.47	131.10	122.56
4	B	703	HEM	C4C-CHD-C1D	4.79	128.88	122.56
4	B	703	HEM	CHC-C4B-C3B	4.31	131.16	124.57
4	A	204	HEM	C4B-CHC-C1C	4.07	127.93	122.56
4	A	204	HEM	C4C-CHD-C1D	4.00	127.84	122.56
4	B	703	HEM	C4B-C3B-C2B	3.92	110.88	107.28
4	B	703	HEM	C3B-C4B-NB	-3.75	106.77	109.47
4	A	204	HEM	CHB-C1B-NB	3.38	128.56	124.37
4	A	204	HEM	CHC-C4B-C3B	3.19	129.45	124.57
4	A	204	HEM	C3B-C4B-NB	-3.16	107.20	109.47
4	A	204	HEM	CMA-C3A-C4A	-3.00	124.06	128.46
4	A	204	HEM	C4B-C3B-C2B	3.00	110.04	107.28
4	B	703	HEM	C3C-C4C-NC	-2.68	105.88	110.94
4	B	703	HEM	CHA-C4D-C3D	2.65	130.11	125.23
4	B	703	HEM	CMA-C3A-C4A	-2.63	124.61	128.46
4	B	703	HEM	C3D-C4D-ND	-2.55	107.38	110.17
4	A	204	HEM	CBD-CAD-C3D	-2.53	105.53	112.53
4	A	204	HEM	CBB-CAB-C3B	-2.44	115.34	127.53
4	A	204	HEM	O1D-CGD-CBD	-2.43	115.39	123.09
4	A	204	HEM	CHA-C4D-C3D	2.39	129.64	125.23
4	B	703	HEM	O1A-CGA-CBA	-2.33	115.72	123.09
4	A	204	HEM	CAA-CBA-CGA	-2.32	107.58	113.83
4	B	703	HEM	CHC-C4B-NB	-2.29	121.97	124.44
4	A	204	HEM	CMC-C2C-C3C	2.21	129.11	124.68
4	A	204	HEM	CHB-C1B-C2B	-2.20	120.71	126.94
2	A	201	GOL	C3-C2-C1	-2.18	103.82	111.80
4	B	703	HEM	CAD-C3D-C4D	-2.17	120.91	124.70
3	A	203	MES	C5-N4-C3	2.10	113.37	108.84
4	A	204	HEM	O2D-CGD-CBD	2.09	120.60	114.00
2	A	205	GOL	C3-C2-C1	-2.08	104.17	111.80
4	B	703	HEM	C4D-C3D-C2D	2.07	109.90	106.89
2	A	202	GOL	C3-C2-C1	-2.04	104.31	111.80
4	B	703	HEM	O1D-CGD-CBD	-2.02	116.70	123.09

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	GOL	O1-C1-C2-C3
2	B	704	GOL	O1-C1-C2-C3
2	A	201	GOL	O1-C1-C2-O2
2	B	704	GOL	O1-C1-C2-O2
5	B	705	PEG	O1-C1-C2-O2
2	A	201	GOL	C1-C2-C3-O3
2	A	206	GOL	O1-C1-C2-C3
2	B	704	GOL	C1-C2-C3-O3
2	A	201	GOL	O2-C2-C3-O3
5	A	209	PEG	O1-C1-C2-O2
5	B	705	PEG	O2-C3-C4-O4
2	A	206	GOL	O1-C1-C2-O2
2	B	704	GOL	O2-C2-C3-O3
5	B	701	PEG	O1-C1-C2-O2
5	B	705	PEG	C1-C2-O2-C3
5	A	207	PEG	C1-C2-O2-C3
5	A	209	PEG	C1-C2-O2-C3
5	B	701	PEG	C4-C3-O2-C2
5	A	209	PEG	C4-C3-O2-C2
2	B	702	GOL	O1-C1-C2-O2
5	A	207	PEG	C4-C3-O2-C2
4	B	703	HEM	CAA-CBA-CGA-O2A
4	A	204	HEM	CAA-CBA-CGA-O2A
4	A	204	HEM	CAD-CBD-CGD-O2D
4	B	703	HEM	CAA-CBA-CGA-O1A
4	A	204	HEM	CAD-CBD-CGD-O1D
4	A	204	HEM	CAA-CBA-CGA-O1A

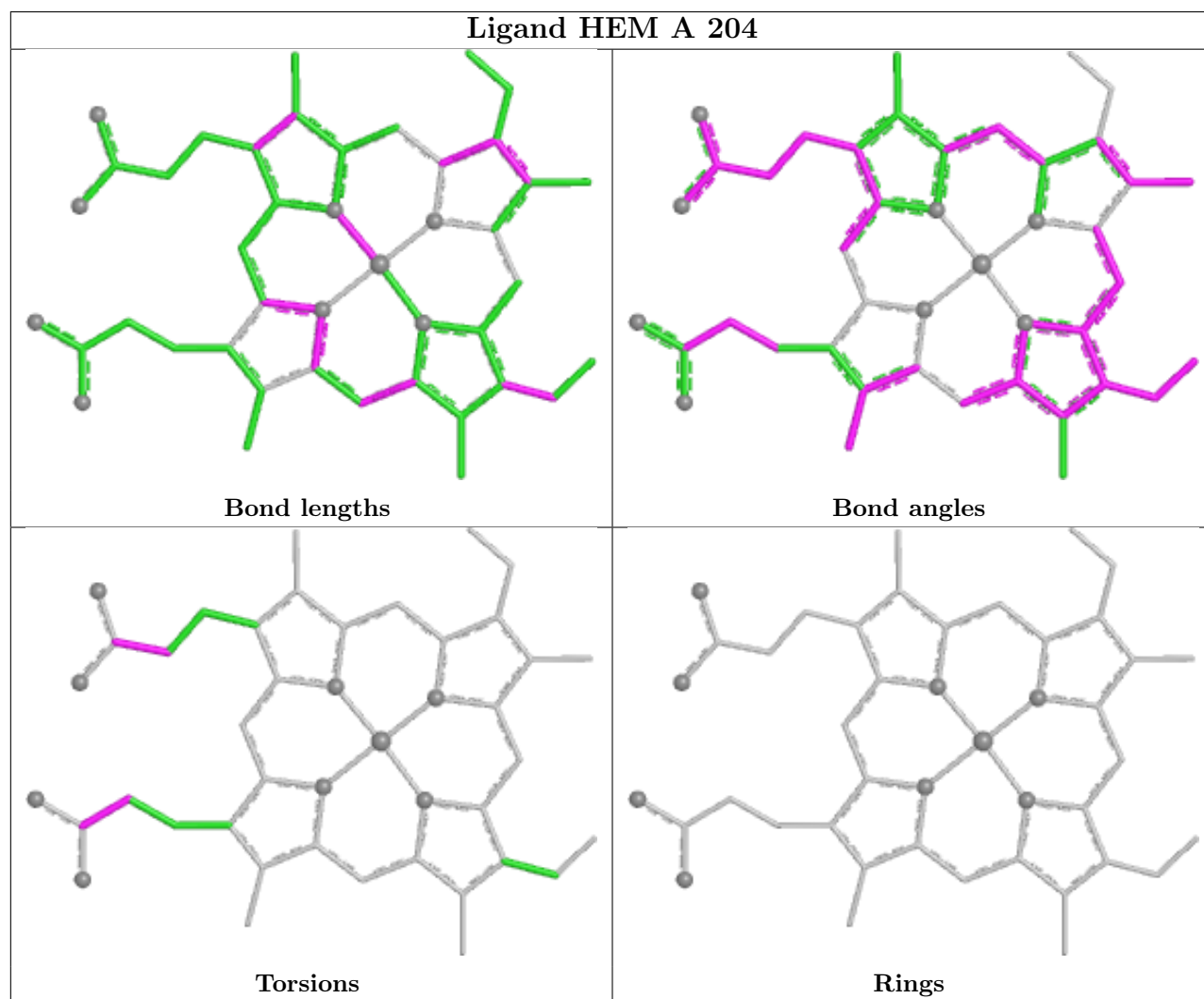
There are no ring outliers.

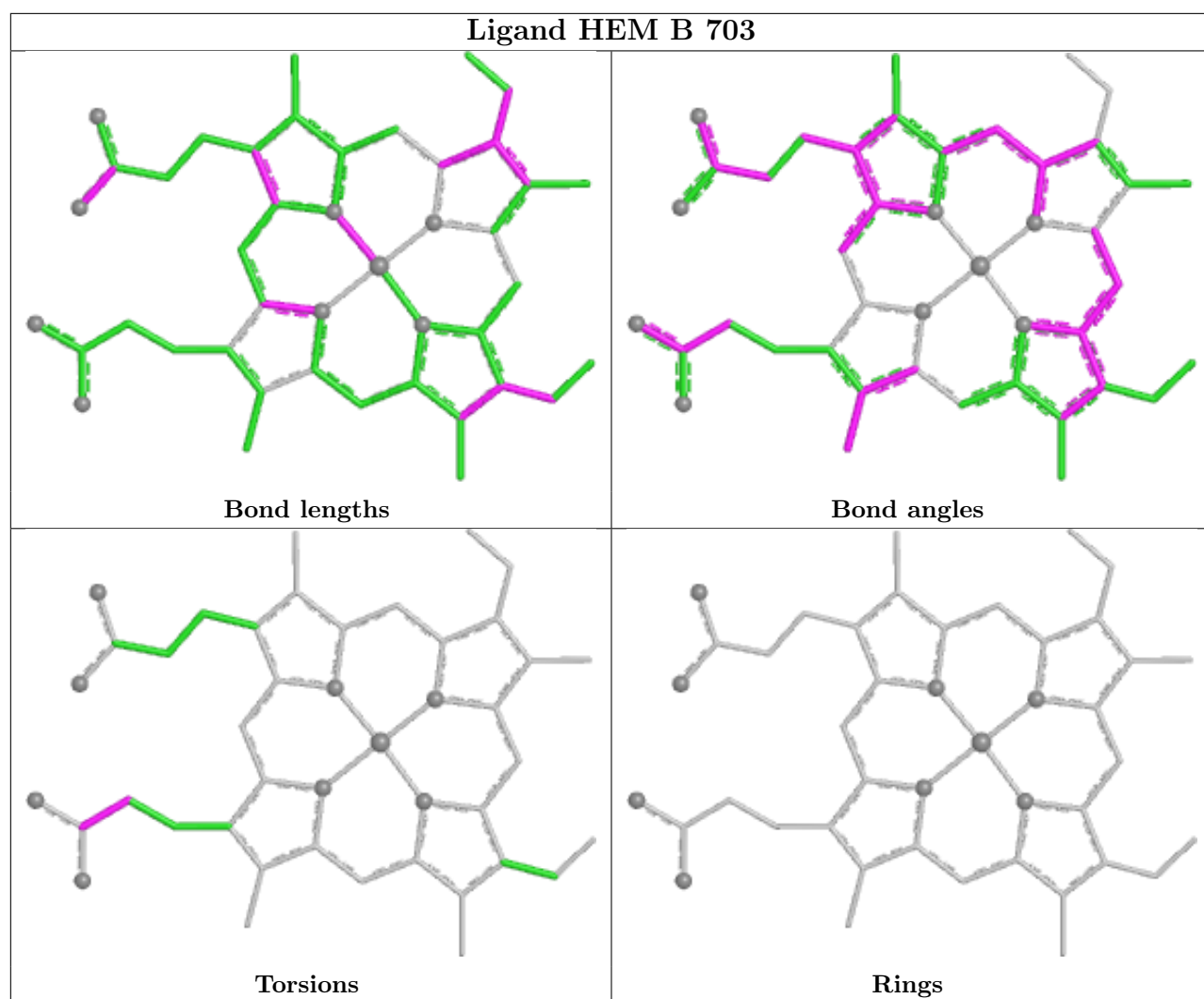
6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	205	GOL	2	0
2	A	202	GOL	1	0
2	B	704	GOL	3	0
5	A	207	PEG	3	0
5	B	705	PEG	5	0
5	B	701	PEG	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.





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	181/188 (96%)	-0.27	8 (4%) 34 34	14, 24, 52, 80	0
1	B	181/188 (96%)	-0.30	8 (4%) 34 34	14, 23, 49, 73	0
All	All	362/376 (96%)	-0.28	16 (4%) 34 34	14, 23, 52, 80	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	46	LEU	11.1
1	A	44	ILE	9.7
1	B	44	ILE	9.3
1	A	42	ALA	9.0
1	A	46	LEU	8.3
1	A	43	GLU	6.8
1	B	43	GLU	6.3
1	B	42	ALA	6.1
1	B	40	ALA	3.9
1	A	41	VAL	3.5
1	B	41	VAL	3.5
1	A	40	ALA	3.2
1	A	47	ASP	3.1
1	B	47	ASP	3.0
1	B	45	PRO	2.9
1	A	45	PRO	2.5

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

There are no monosaccharides in this entry.

6.4 Ligands

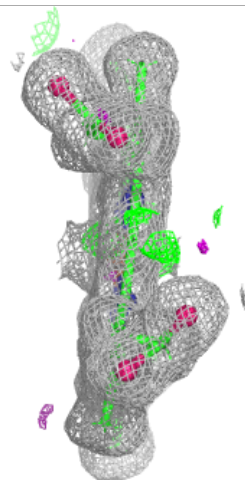
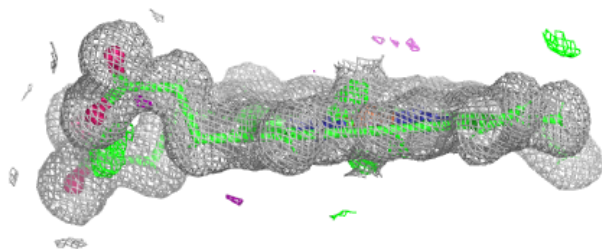
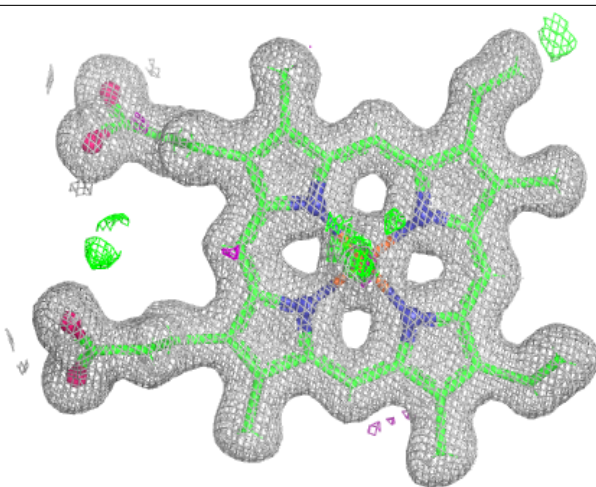
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

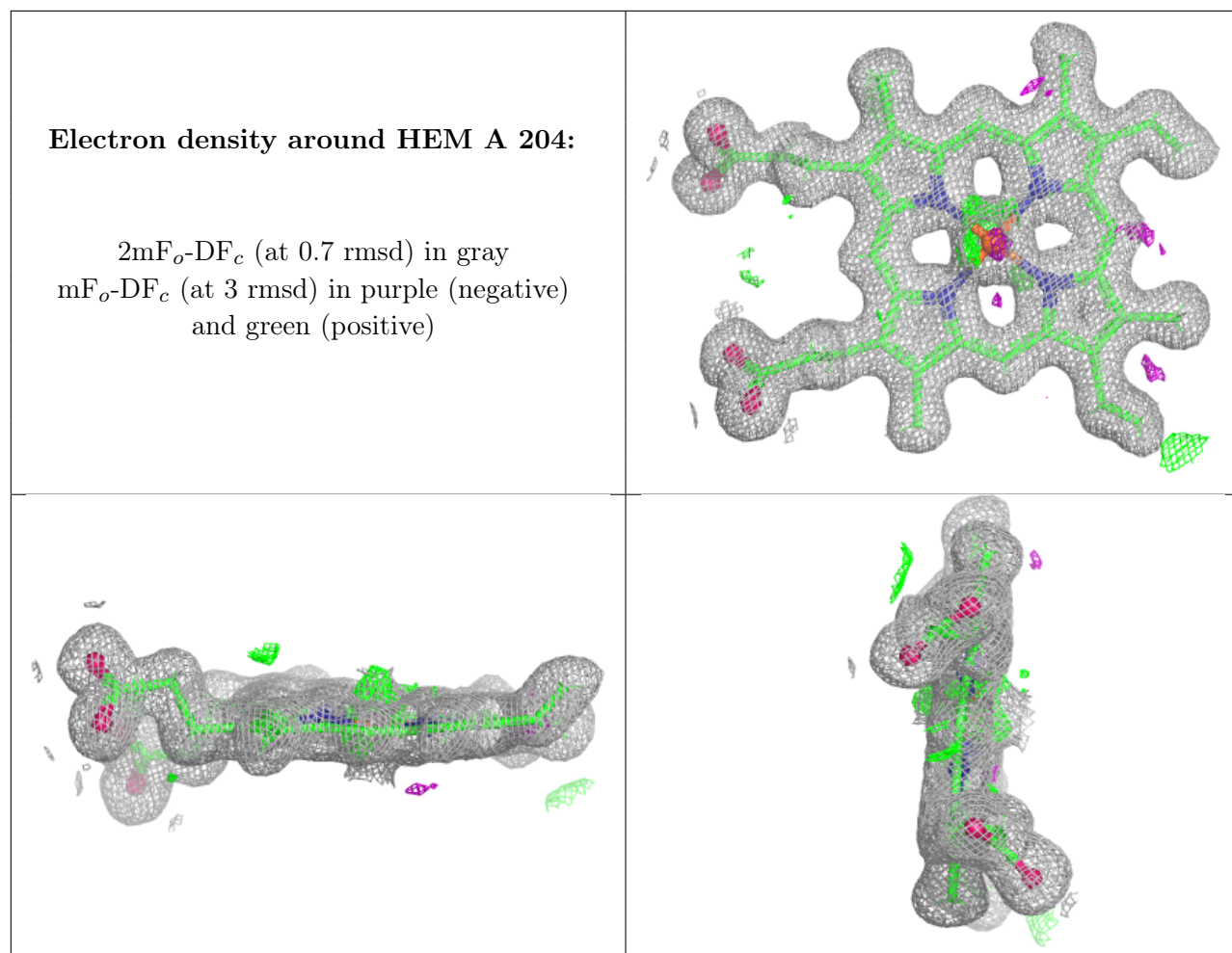
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	PEG	B	705	7/7	0.39	0.28	71,86,86,87	0
5	PEG	A	209	7/7	0.67	0.28	65,78,86,87	0
5	PEG	A	207	7/7	0.70	0.19	57,68,75,75	0
5	PEG	B	701	7/7	0.77	0.14	54,65,74,75	0
2	GOL	A	201	6/6	0.79	0.14	51,57,66,66	0
2	GOL	A	206	6/6	0.80	0.17	49,53,63,63	0
2	GOL	B	702	6/6	0.84	0.19	50,55,63,63	0
2	GOL	A	205	6/6	0.86	0.21	57,59,69,69	0
2	GOL	B	704	6/6	0.88	0.22	26,43,52,52	0
2	GOL	A	202	6/6	0.89	0.15	45,49,56,56	0
6	SO4	A	208	5/5	0.96	0.09	80,80,80,81	0
4	HEM	B	703	43/43	0.99	0.06	13,17,23,25	0
3	MES	A	203	12/12	0.99	0.07	24,31,37,37	0
4	HEM	A	204	43/43	0.99	0.06	13,16,21,23	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 B 703:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.