Full wwPDB X-ray Structure Validation Report ⓘ

Feb 20, 2024 – 08:03 AM EST

PDB ID	:	4M09
Title	:	Crystal Structure of Mutant Chlorite Dismutase from Candidatus Nitrospira defluvii W146Y R173Q
Authors	:	Gysel, K.; Hagmueller, A.; Djinovic-Carugo, K.
Deposited on	:	2013-08-01
Resolution	:	2.45 Å(reported)

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

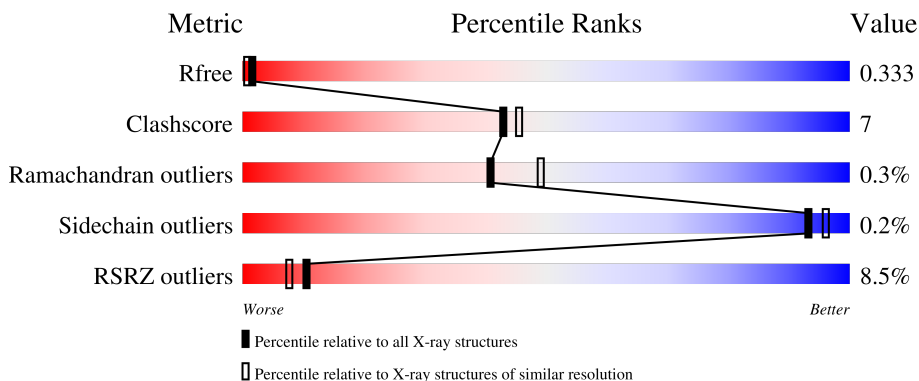|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.45 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		0.333
Clashscore		7
Ramachandran outliers		0.3%
Sidechain outliers		0.2%
RSRZ outliers		8.5%

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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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	241	10% / 83% / 16% / ·
1	B	241	8% / 79% / 20% / ·
1	C	241	8% / 83% / 15% / ·
1	D	241	8% / 85% / 13% / ·
1	E	241	7% / 80% / 18% / ·

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 10015 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 Chlorite dismutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total 1915	C 1220	N 332	O 357	S 6	0	0	0
1	B	238	Total 1915	C 1220	N 332	O 357	S 6	0	0	0
1	C	236	Total 1902	C 1213	N 330	O 353	S 6	0	0	0
1	D	236	Total 1902	C 1213	N 330	O 353	S 6	0	0	0
1	E	237	Total 1910	C 1217	N 331	O 356	S 6	0	0	0

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP B3U4H7
A	-1	ALA	-	expression tag	UNP B3U4H7
A	0	MET	-	expression tag	UNP B3U4H7
A	146	TYR	TRP	engineered mutation	UNP B3U4H7
A	173	GLN	ARG	engineered mutation	UNP B3U4H7
B	-2	GLY	-	expression tag	UNP B3U4H7
B	-1	ALA	-	expression tag	UNP B3U4H7
B	0	MET	-	expression tag	UNP B3U4H7
B	146	TYR	TRP	engineered mutation	UNP B3U4H7
B	173	GLN	ARG	engineered mutation	UNP B3U4H7
C	-2	GLY	-	expression tag	UNP B3U4H7
C	-1	ALA	-	expression tag	UNP B3U4H7
C	0	MET	-	expression tag	UNP B3U4H7
C	146	TYR	TRP	engineered mutation	UNP B3U4H7
C	173	GLN	ARG	engineered mutation	UNP B3U4H7
D	-2	GLY	-	expression tag	UNP B3U4H7
D	-1	ALA	-	expression tag	UNP B3U4H7
D	0	MET	-	expression tag	UNP B3U4H7
D	146	TYR	TRP	engineered mutation	UNP B3U4H7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	173	GLN	ARG	engineered mutation	UNP B3U4H7
E	-2	GLY	-	expression tag	UNP B3U4H7
E	-1	ALA	-	expression tag	UNP B3U4H7
E	0	MET	-	expression tag	UNP B3U4H7
E	146	TYR	TRP	engineered mutation	UNP B3U4H7
E	173	GLN	ARG	engineered mutation	UNP B3U4H7

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
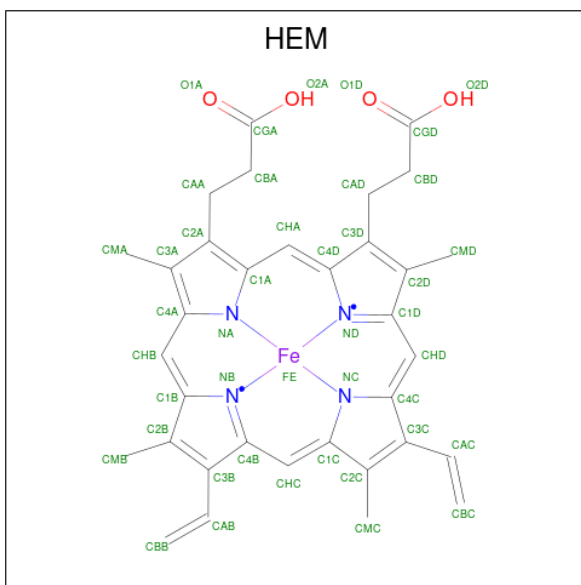
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 4	C 2	O 2	0	0
4	B	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	D	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0

- Molecule 5 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).
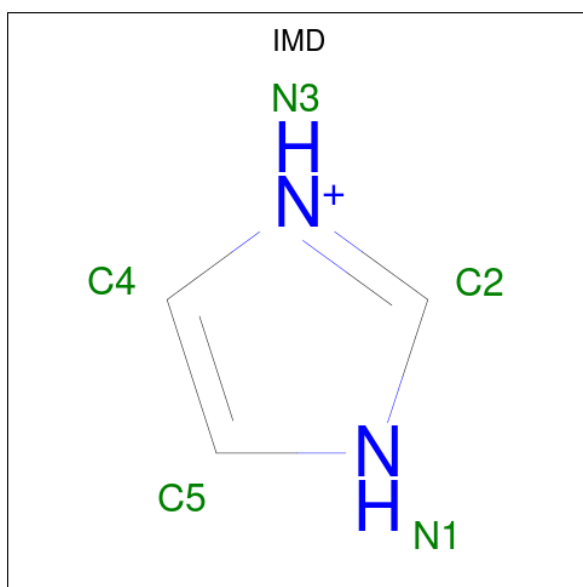
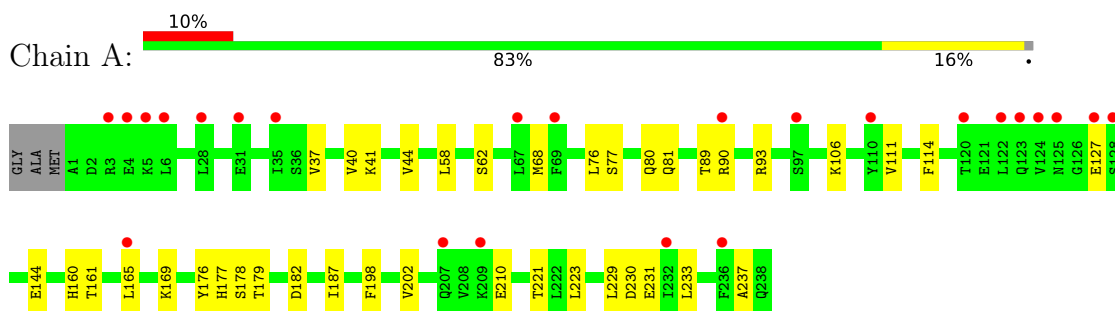| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 5	C 3	N 2	0	0
5	D	1	Total 5	C 3	N 2	0	0

• Molecule 6 is water.

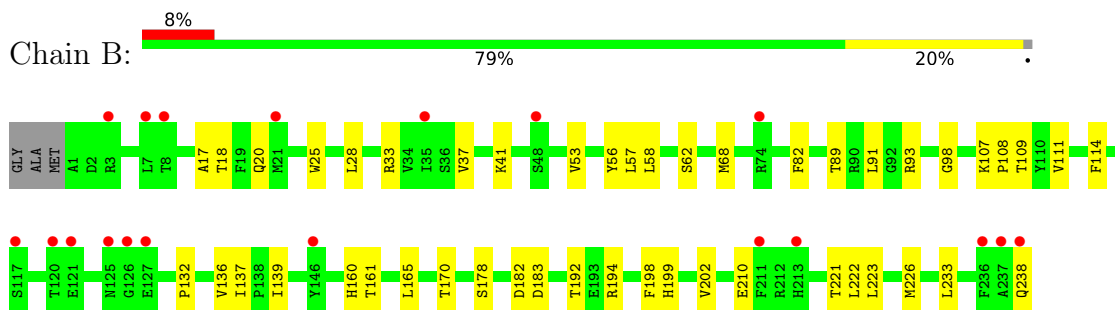| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	38	Total 38	O 38	0	0
6	B	38	Total 38	O 38	0	0
6	C	36	Total 36	O 36	0	0
6	D	27	Total 27	O 27	0	0
6	E	26	Total 26	O 26	0	0

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.
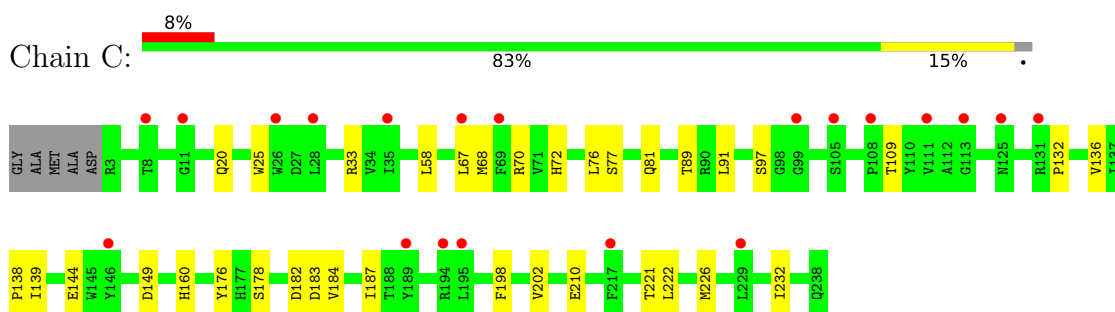
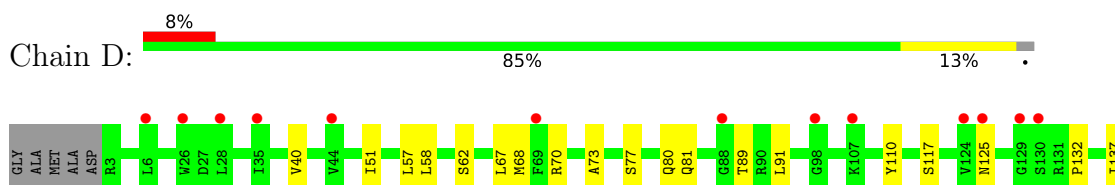- Molecule 1: Chlorite dismutase
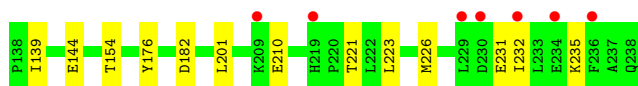
Chain A:

- Molecule 1: Chlorite dismutase

Chain B:

- Molecule 1: Chlorite dismutase

Chain C:

- Molecule 1: Chlorite dismutase

Chain D:

P138 I139 E144 T154 Y176 D182 L201 K209 E210 H219 P220 T221 L222 L223 M226 L229 D230 E231 I232 L233 E234 K235 F236 A237 Q238

• Molecule 1: Chlorite dismutase

Chain E:

7%

80%

18%

GLY ALA MET ALA D2 R3 L7 V12 T18 M21 W25 L28 P29 G30 R33 V34 I35 S36 V37 K41 E45 S48 L58 S62 L67 M68 F69 R74 T75 L76 S77 Q81 R90 R93 G98 T109 F114 K119

V124 N125 G126 E127 P132 V136 I137 T161 L165 P166 Y167 L168 K169 K174 D183 R194 Q207 R216 H219 P220 T221 L222 L223 G224 T225 M226 I232 L233 E234 K235 F236 A237 Q238
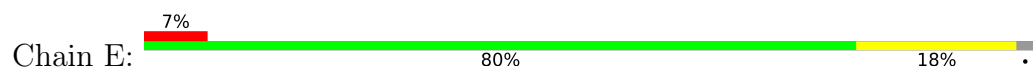
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	138.10Å 114.98Å 118.87Å 90.00° 118.08° 90.00°	Depositor
Resolution (Å)	44.38 – 2.45 44.38 – 2.45	Depositor EDS
% Data completeness (in resolution range)	97.7 (44.38-2.45) 98.3 (44.38-2.45)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 2.45Å)	Xtriage
Refinement program	PHENIX dev_1388	Depositor
R, R_{free}	0.277 , 0.333 0.277 , 0.333	Depositor DCC
R_{free} test set	2975 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	34.3	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 61.7	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	10015	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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: IMD, SO4, HEM, EDO

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	0.23	0/1960	0.45	0/2650
1	B	0.22	0/1960	0.41	0/2650
1	C	0.22	0/1947	0.40	0/2632
1	D	0.21	0/1947	0.37	0/2632
1	E	0.22	0/1955	0.41	0/2643
All	All	0.22	0/9769	0.41	0/13207

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	1915	0	1887	25	0
1	B	1915	0	1887	34	0
1	C	1902	0	1875	22	0
1	D	1902	0	1875	18	0
1	E	1910	0	1879	29	0
2	A	43	0	30	2	0
2	B	43	0	30	5	0
2	C	43	0	30	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	43	0	30	4	0
2	E	43	0	30	3	0
3	A	10	0	0	1	0
3	B	10	0	0	1	0
3	C	10	0	0	0	0
3	D	10	0	0	1	0
3	E	5	0	0	1	0
4	A	4	0	6	2	0
4	B	4	0	6	0	0
4	C	12	0	18	0	0
4	D	4	0	6	0	0
4	E	12	0	18	1	0
5	A	5	0	5	0	0
5	D	5	0	5	0	0
6	A	38	0	0	0	0
6	B	38	0	0	2	0
6	C	36	0	0	3	0
6	D	27	0	0	0	0
6	E	26	0	0	0	0
All	All	10015	0	9617	133	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 (133) 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:93:ARG:NH1	4:A:303:EDO:O1	2.14	0.81
1:E:233:LEU:HA	1:E:236:PHE:HD2	1.51	0.76
1:E:28:LEU:O	1:E:33:ARG:NH1	2.21	0.73
1:B:28:LEU:O	1:B:33:ARG:NH1	2.22	0.73
1:B:33:ARG:NH2	1:B:238:GLN:O	2.22	0.72
2:E:301:HEM:HHC	2:E:301:HEM:HBB2	1.72	0.70
2:A:301:HEM:HHC	2:A:301:HEM:HBB2	1.75	0.68
1:E:232:ILE:HG22	1:E:236:PHE:HE2	1.61	0.66
1:A:179:THR:O	1:B:199:HIS:ND1	2.22	0.66
1:E:7:LEU:O	1:E:174:LYS:NZ	2.29	0.66
1:D:139:ILE:HD11	2:D:301:HEM:HAC	1.79	0.65
1:D:201:LEU:HD21	2:D:301:HEM:HAB	1.80	0.62
1:B:139:ILE:HD11	2:B:301:HEM:HAC	1.80	0.61
1:C:58:LEU:HD11	1:C:68:MET:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:SER:OG	6:C:413:HOH:O	2.16	0.61
1:B:58:LEU:HD11	1:B:68:MET:HB2	1.82	0.60
1:A:58:LEU:HD11	1:A:68:MET:HB2	1.84	0.60
1:B:192:THR:HG22	1:B:194:ARG:H	1.66	0.59
1:E:30:GLY:H	4:E:302:EDO:H12	1.66	0.59
1:A:160:HIS:ND1	1:A:210:GLU:OE1	2.36	0.58
1:D:132:PRO:HD2	1:D:226:MET:HB3	1.85	0.58
1:B:136:VAL:HB	1:B:222:LEU:HB2	1.86	0.57
1:E:137:ILE:HG12	1:E:221:THR:HG23	1.85	0.57
2:D:301:HEM:HMC2	2:D:301:HEM:HBC2	1.87	0.56
1:A:80:GLN:NE2	1:B:57:LEU:O	2.38	0.55
1:A:90:ARG:HG3	1:A:93:ARG:HE	1.71	0.55
2:D:301:HEM:HMB1	2:D:301:HEM:HBB2	1.88	0.55
1:C:20:GLN:NE2	6:C:431:HOH:O	2.31	0.55
2:C:301:HEM:HBB2	2:C:301:HEM:HMB2	1.89	0.54
1:B:37:VAL:HG12	1:B:41:LYS:HE3	1.90	0.54
1:B:25:TRP:CE2	1:B:33:ARG:HD2	2.43	0.54
1:D:144:GLU:N	1:D:144:GLU:OE2	2.40	0.54
2:A:301:HEM:HMC1	2:A:301:HEM:HBC2	1.89	0.54
1:E:62:SER:OG	1:E:223:LEU:O	2.25	0.54
1:D:58:LEU:HB3	1:D:62:SER:HB2	1.90	0.53
2:E:301:HEM:HMC1	2:E:301:HEM:HBC2	1.90	0.53
1:B:160:HIS:ND1	1:B:210:GLU:OE1	2.33	0.53
1:C:132:PRO:HD2	1:C:226:MET:HB3	1.90	0.53
1:C:25:TRP:CE2	1:C:33:ARG:HD3	2.43	0.53
1:B:132:PRO:HD2	1:B:226:MET:HB3	1.89	0.53
1:C:160:HIS:ND1	1:C:210:GLU:OE1	2.38	0.53
1:D:117:SER:N	3:D:304:SO4:O4	2.37	0.52
1:B:62:SER:OG	1:B:223:LEU:O	2.26	0.52
1:B:137:ILE:HG12	1:B:221:THR:HG23	1.92	0.52
1:A:62:SER:OG	1:A:223:LEU:O	2.25	0.52
1:B:89:THR:HG22	1:B:91:LEU:H	1.74	0.52
1:E:18:THR:OG1	1:E:98:GLY:O	2.27	0.52
1:C:77:SER:O	1:C:81:GLN:HG2	2.10	0.51
1:C:144:GLU:OE1	1:C:144:GLU:N	2.42	0.51
1:E:233:LEU:HA	1:E:236:PHE:CD2	2.39	0.51
3:A:302:SO4:O1	1:B:20:GLN:NE2	2.44	0.51
1:A:37:VAL:HG12	1:A:41:LYS:HE3	1.92	0.50
1:E:58:LEU:HD11	1:E:68:MET:HB2	1.94	0.50
1:E:232:ILE:HG22	1:E:236:PHE:CE2	2.44	0.50
1:B:170:THR:O	1:B:192:THR:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:TRP:O	1:B:33:ARG:HD3	2.12	0.50
1:E:2:ASP:O	1:E:3:ARG:HB2	2.11	0.49
1:B:18:THR:OG1	1:B:98:GLY:O	2.27	0.49
1:E:37:VAL:HG12	1:E:41:LYS:HE3	1.95	0.49
2:B:301:HEM:HMB2	2:B:301:HEM:HBB2	1.94	0.48
1:C:139:ILE:HD11	2:C:301:HEM:HAC	1.94	0.48
1:D:57:LEU:HD13	1:D:232:ILE:HG23	1.96	0.48
1:D:40:VAL:HG21	1:D:91:LEU:HD23	1.96	0.48
1:E:90:ARG:O	1:E:93:ARG:HG2	2.13	0.48
1:C:221:THR:OG1	1:E:183:ASP:OD1	2.25	0.48
1:A:230:ASP:OD2	1:A:231:GLU:N	2.46	0.48
2:E:301:HEM:HBA1	2:E:301:HEM:HHA	1.96	0.47
1:A:179:THR:HB	1:B:199:HIS:CE1	2.49	0.47
1:B:139:ILE:CD1	2:B:301:HEM:HAC	2.45	0.47
1:D:110:TYR:HB3	1:D:154:THR:HG23	1.97	0.47
1:E:132:PRO:HD2	1:E:226:MET:HB3	1.97	0.47
1:E:219:HIS:NE2	3:E:305:SO4:O4	2.48	0.47
1:E:127:GLU:HB2	1:E:169:LYS:O	2.14	0.46
1:E:30:GLY:O	1:E:34:VAL:HG23	2.16	0.46
1:E:77:SER:O	1:E:81:GLN:HG2	2.15	0.46
2:B:301:HEM:HMC1	2:B:301:HEM:HBC2	1.97	0.46
1:B:37:VAL:HG22	1:B:233:LEU:HB3	1.98	0.46
1:C:109:THR:N	2:C:301:HEM:O1A	2.48	0.46
1:A:127:GLU:HB2	1:A:169:LYS:O	2.16	0.46
1:C:89:THR:HG22	1:C:91:LEU:H	1.81	0.46
1:D:80:GLN:NE2	1:E:225:THR:OG1	2.42	0.45
1:A:144:GLU:OE1	1:A:144:GLU:N	2.47	0.45
1:E:161:THR:O	1:E:165:LEU:HG	2.17	0.45
1:A:221:THR:OG1	1:C:183:ASP:OD1	2.27	0.45
1:E:216:ARG:NH2	1:E:219:HIS:O	2.30	0.44
1:C:176:TYR:HB2	1:C:187:ILE:HB	1.99	0.44
1:D:137:ILE:HG12	1:D:221:THR:HG23	1.99	0.44
1:C:178:SER:OG	1:C:182:ASP:OD1	2.35	0.44
1:E:90:ARG:HG3	1:E:93:ARG:HE	1.83	0.44
1:C:136:VAL:HB	1:C:222:LEU:HB2	1.98	0.44
1:C:149:ASP:OD1	6:C:427:HOH:O	2.20	0.44
1:B:68:MET:O	6:B:427:HOH:O	2.21	0.43
1:D:77:SER:O	1:D:81:GLN:HG2	2.18	0.43
1:C:67:LEU:HD12	1:C:232:ILE:HG21	1.99	0.43
1:A:106:LYS:HD2	1:A:177:HIS:CG	2.53	0.43
1:A:77:SER:O	1:A:81:GLN:HG2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:THR:O	1:B:165:LEU:HG	2.17	0.43
1:B:198:PHE:O	1:B:202:VAL:HG23	2.17	0.43
1:C:198:PHE:O	1:C:202:VAL:HG23	2.19	0.43
1:E:76:LEU:HD23	1:E:76:LEU:HA	1.86	0.43
1:A:40:VAL:HG22	1:A:89:THR:HG21	1.99	0.43
1:B:111:VAL:HA	1:B:114:PHE:CD2	2.53	0.43
1:D:51:ILE:HG22	1:D:73:ALA:HB2	2.00	0.43
1:A:111:VAL:HA	1:A:114:PHE:CD2	2.54	0.43
1:B:109:THR:N	2:B:301:HEM:O1A	2.44	0.43
1:A:198:PHE:O	1:A:202:VAL:HG23	2.19	0.43
1:B:107:LYS:HA	1:B:108:PRO:HD3	1.92	0.43
1:C:70:ARG:HG2	1:C:72:HIS:CE1	2.53	0.43
1:D:231:GLU:O	1:D:235:LYS:HG2	2.19	0.42
1:D:70:ARG:NH1	1:D:176:TYR:OH	2.52	0.42
1:A:37:VAL:HG13	1:A:233:LEU:HB3	2.01	0.42
1:D:67:LEU:HD23	1:D:68:MET:N	2.34	0.42
1:A:161:THR:O	1:A:165:LEU:HG	2.19	0.42
1:D:62:SER:OG	1:D:223:LEU:O	2.33	0.42
1:B:17:ALA:O	1:B:68:MET:HA	2.20	0.42
1:E:114:PHE:O	1:E:119:LYS:HE3	2.19	0.42
1:B:182:ASP:HB2	1:B:183:ASP:H	1.71	0.42
1:D:89:THR:HG22	1:D:91:LEU:H	1.85	0.42
1:E:25:TRP:CE2	1:E:33:ARG:HD2	2.55	0.42
1:A:93:ARG:NH2	4:A:303:EDO:O2	2.40	0.41
1:B:56:TYR:O	6:B:427:HOH:O	2.22	0.41
1:A:76:LEU:HD23	1:A:76:LEU:HA	1.86	0.41
1:C:138:PRO:HB2	1:C:184:VAL:HG11	2.02	0.41
1:E:45:GLU:HA	1:E:48:SER:HB3	2.02	0.41
1:E:136:VAL:HB	1:E:222:LEU:HB2	2.02	0.41
1:A:178:SER:OG	1:A:182:ASP:OD1	2.38	0.41
1:B:178:SER:OG	1:B:182:ASP:OD1	2.37	0.40
1:C:76:LEU:HD23	1:C:76:LEU:HA	1.81	0.40
1:A:44:VAL:HG21	1:A:229:LEU:CD2	2.51	0.40
1:A:176:TYR:HB2	1:A:187:ILE:HB	2.03	0.40
1:B:53:VAL:HG21	1:B:82:PHE:CZ	2.56	0.40
1:B:93:ARG:NH2	3:B:302:SO4:O2	2.54	0.40
2:C:301:HEM:HMC1	2:C:301:HEM:HBC2	2.04	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	236/241 (98%)	227 (96%)	8 (3%)	1 (0%)	34	41
1	B	236/241 (98%)	228 (97%)	8 (3%)	0	100	100
1	C	234/241 (97%)	227 (97%)	7 (3%)	0	100	100
1	D	234/241 (97%)	221 (94%)	12 (5%)	1 (0%)	34	41
1	E	235/241 (98%)	227 (97%)	7 (3%)	1 (0%)	34	41
All	All	1175/1205 (98%)	1130 (96%)	42 (4%)	3 (0%)	41	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237	ALA
1	E	237	ALA
1	D	125	ASN

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	205/206 (100%)	205 (100%)	0	100	100
1	B	205/206 (100%)	205 (100%)	0	100	100
1	C	204/206 (99%)	204 (100%)	0	100	100
1	D	204/206 (99%)	202 (99%)	2 (1%)	76	84
1	E	205/206 (100%)	205 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1023/1030 (99%)	1021 (100%)	2 (0%)	93 96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	182	ASP
1	D	210	GLU

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 ⓘ

25 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	$\#|Z| > 2$
3	SO4	C	302	-	4,4,4	0.14	0	6,6,6	0.05	0
4	EDO	E	303	-	3,3,3	0.47	0	2,2,2	0.32	0
4	EDO	D	305	-	3,3,3	0.47	0	2,2,2	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
4	EDO	E	304	-	3,3,3	0.46	0	2,2,2	0.32	0
5	IMD	A	304	-	3,5,5	0.42	0	4,5,5	0.59	0
3	SO4	A	302	-	4,4,4	0.15	0	6,6,6	0.04	0
2	HEM	D	301	5,1	41,50,50	1.97	7 (17%)	45,82,82	1.70	7 (15%)
3	SO4	E	305	-	4,4,4	0.14	0	6,6,6	0.04	0
4	EDO	A	303	-	3,3,3	0.46	0	2,2,2	0.19	0
3	SO4	A	305	-	4,4,4	0.14	0	6,6,6	0.05	0
4	EDO	C	305	-	3,3,3	0.45	0	2,2,2	0.33	0
2	HEM	C	301	1	41,50,50	1.98	8 (19%)	45,82,82	1.65	6 (13%)
3	SO4	C	303	-	4,4,4	0.14	0	6,6,6	0.05	0
4	EDO	B	304	-	3,3,3	0.46	0	2,2,2	0.33	0
3	SO4	B	302	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	B	303	-	4,4,4	0.13	0	6,6,6	0.05	0
2	HEM	B	301	1	41,50,50	1.95	7 (17%)	45,82,82	1.72	7 (15%)
2	HEM	E	301	1	41,50,50	1.96	7 (17%)	45,82,82	1.80	8 (17%)
4	EDO	E	302	-	3,3,3	0.46	0	2,2,2	0.33	0
3	SO4	D	303	-	4,4,4	0.14	0	6,6,6	0.06	0
4	EDO	C	304	-	3,3,3	0.45	0	2,2,2	0.33	0
3	SO4	D	304	-	4,4,4	0.15	0	6,6,6	0.04	0
2	HEM	A	301	1	41,50,50	1.96	7 (17%)	45,82,82	1.86	10 (22%)
4	EDO	C	306	-	3,3,3	0.46	0	2,2,2	0.34	0
5	IMD	D	302	2	3,5,5	0.42	0	4,5,5	0.60	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
2	HEM	A	301	1	-	8/12/54/54	-
2	HEM	B	301	1	-	4/12/54/54	-
2	HEM	D	301	5,1	-	2/12/54/54	-
2	HEM	E	301	1	-	4/12/54/54	-
4	EDO	C	306	-	-	0/1/1/1	-
4	EDO	C	304	-	-	0/1/1/1	-
4	EDO	A	303	-	-	1/1/1/1	-
4	EDO	E	302	-	-	0/1/1/1	-
4	EDO	E	303	-	-	0/1/1/1	-
4	EDO	D	305	-	-	0/1/1/1	-
4	EDO	C	305	-	-	0/1/1/1	-
4	EDO	E	304	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	C	301	1	-	4/12/54/54	-
5	IMD	A	304	-	-	-	0/1/1/1
4	EDO	B	304	-	-	0/1/1/1	-
5	IMD	D	302	2	-	-	0/1/1/1

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	HEM	C3D-C2D	8.22	1.54	1.36
2	D	301	HEM	C3D-C2D	8.19	1.54	1.36
2	B	301	HEM	C3D-C2D	8.03	1.53	1.36
2	E	301	HEM	C3D-C2D	8.03	1.53	1.36
2	A	301	HEM	C3D-C2D	7.91	1.53	1.36
2	A	301	HEM	C3C-CAC	3.93	1.55	1.47
2	D	301	HEM	C3C-CAC	3.88	1.55	1.47
2	E	301	HEM	C3C-CAC	3.87	1.55	1.47
2	B	301	HEM	C3C-C2C	-3.86	1.35	1.40
2	B	301	HEM	C3C-CAC	3.81	1.55	1.47
2	C	301	HEM	C3C-CAC	3.78	1.55	1.47
2	C	301	HEM	C3C-C2C	-3.74	1.35	1.40
2	E	301	HEM	C3C-C2C	-3.73	1.35	1.40
2	D	301	HEM	C3C-C2C	-3.72	1.35	1.40
2	A	301	HEM	C3C-C2C	-3.71	1.35	1.40
2	C	301	HEM	CAB-C3B	3.07	1.55	1.47
2	B	301	HEM	CAB-C3B	3.05	1.55	1.47
2	D	301	HEM	CAB-C3B	3.04	1.55	1.47
2	E	301	HEM	CAB-C3B	2.89	1.55	1.47
2	A	301	HEM	CAB-C3B	2.86	1.55	1.47
2	C	301	HEM	FE-ND	2.65	2.10	1.96
2	A	301	HEM	FE-ND	2.65	2.09	1.96
2	B	301	HEM	FE-NB	2.50	2.09	1.96
2	E	301	HEM	FE-ND	2.45	2.09	1.96
2	D	301	HEM	FE-NB	2.37	2.08	1.96
2	A	301	HEM	FE-NB	2.35	2.08	1.96
2	E	301	HEM	FE-NB	2.34	2.08	1.96
2	D	301	HEM	FE-ND	2.26	2.08	1.96
2	B	301	HEM	FE-ND	2.24	2.07	1.96
2	C	301	HEM	FE-NB	2.19	2.07	1.96
2	E	301	HEM	CAA-C2A	2.16	1.55	1.52
2	C	301	HEM	CMB-C2B	2.03	1.55	1.50
2	A	301	HEM	CAA-C2A	2.03	1.55	1.52
2	B	301	HEM	CMB-C2B	2.02	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	HEM	CMB-C2B	2.01	1.55	1.50
2	C	301	HEM	CMD-C2D	2.01	1.55	1.50

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	HEM	C4D-ND-C1D	6.69	111.99	105.07
2	D	301	HEM	C4D-ND-C1D	6.61	111.90	105.07
2	A	301	HEM	C4D-ND-C1D	6.57	111.86	105.07
2	E	301	HEM	C4D-ND-C1D	6.47	111.75	105.07
2	C	301	HEM	C4D-ND-C1D	6.36	111.64	105.07
2	A	301	HEM	C4C-CHD-C1D	4.15	128.04	122.56
2	D	301	HEM	C4C-CHD-C1D	3.89	127.69	122.56
2	E	301	HEM	C4C-CHD-C1D	3.85	127.64	122.56
2	C	301	HEM	C4C-CHD-C1D	3.40	127.04	122.56
2	B	301	HEM	C4C-CHD-C1D	3.31	126.93	122.56
2	A	301	HEM	C1B-NB-C4B	2.98	108.15	105.07
2	E	301	HEM	C1B-NB-C4B	2.96	108.14	105.07
2	E	301	HEM	C4B-CHC-C1C	2.79	126.25	122.56
2	C	301	HEM	C4B-CHC-C1C	2.79	126.24	122.56
2	B	301	HEM	C4B-CHC-C1C	2.77	126.21	122.56
2	A	301	HEM	CAD-C3D-C4D	2.75	129.46	124.66
2	E	301	HEM	C3B-C2B-C1B	2.73	108.51	106.49
2	A	301	HEM	C4B-CHC-C1C	2.68	126.09	122.56
2	A	301	HEM	C3B-C2B-C1B	2.64	108.45	106.49
2	D	301	HEM	C4B-CHC-C1C	2.55	125.92	122.56
2	C	301	HEM	CAD-CBD-CGD	-2.50	108.22	113.60
2	C	301	HEM	C1B-NB-C4B	2.43	107.58	105.07
2	D	301	HEM	C1B-NB-C4B	2.42	107.57	105.07
2	E	301	HEM	CHC-C4B-C3B	2.32	128.12	124.57
2	A	301	HEM	CHC-C4B-C3B	2.26	128.02	124.57
2	B	301	HEM	CMC-C2C-C3C	2.25	128.90	124.68
2	B	301	HEM	CAD-CBD-CGD	-2.24	108.78	113.60
2	B	301	HEM	C1B-NB-C4B	2.24	107.39	105.07
2	C	301	HEM	CMC-C2C-C3C	2.23	128.85	124.68
2	D	301	HEM	CMC-C2C-C3C	2.15	128.69	124.68
2	D	301	HEM	C3B-C2B-C1B	2.13	108.07	106.49
2	E	301	HEM	C4A-C3A-C2A	2.13	108.47	107.00
2	B	301	HEM	CHA-C4D-ND	2.11	126.99	124.38
2	E	301	HEM	CMA-C3A-C4A	-2.11	125.22	128.46
2	A	301	HEM	CAD-CBD-CGD	-2.06	109.18	113.60
2	A	301	HEM	CMC-C2C-C3C	2.05	128.51	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	301	HEM	CAD-CBD-CGD	-2.04	109.22	113.60
2	A	301	HEM	CHD-C1D-ND	2.00	126.61	124.43

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	301	HEM	C1A-C2A-CAA-CBA
2	E	301	HEM	C3A-C2A-CAA-CBA
2	A	301	HEM	C4D-C3D-CAD-CBD
2	C	301	HEM	C4D-C3D-CAD-CBD
2	A	301	HEM	C2D-C3D-CAD-CBD
2	A	301	HEM	C3D-CAD-CBD-CGD
2	A	301	HEM	C4B-C3B-CAB-CBB
2	E	301	HEM	C4B-C3B-CAB-CBB
2	C	301	HEM	C2D-C3D-CAD-CBD
2	D	301	HEM	C2D-C3D-CAD-CBD
2	A	301	HEM	C1A-C2A-CAA-CBA
2	A	301	HEM	C3A-C2A-CAA-CBA
2	D	301	HEM	C4D-C3D-CAD-CBD
2	C	301	HEM	CAA-CBA-CGA-O2A
2	A	301	HEM	CAD-CBD-CGD-O1D
2	C	301	HEM	CAA-CBA-CGA-O1A
2	A	301	HEM	CAD-CBD-CGD-O2D
2	B	301	HEM	CAD-CBD-CGD-O2D
2	B	301	HEM	CAA-CBA-CGA-O2A
2	B	301	HEM	CAD-CBD-CGD-O1D
2	B	301	HEM	CAA-CBA-CGA-O1A
4	A	303	EDO	O1-C1-C2-O2
2	E	301	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

11 monomers are involved in 25 short contacts:

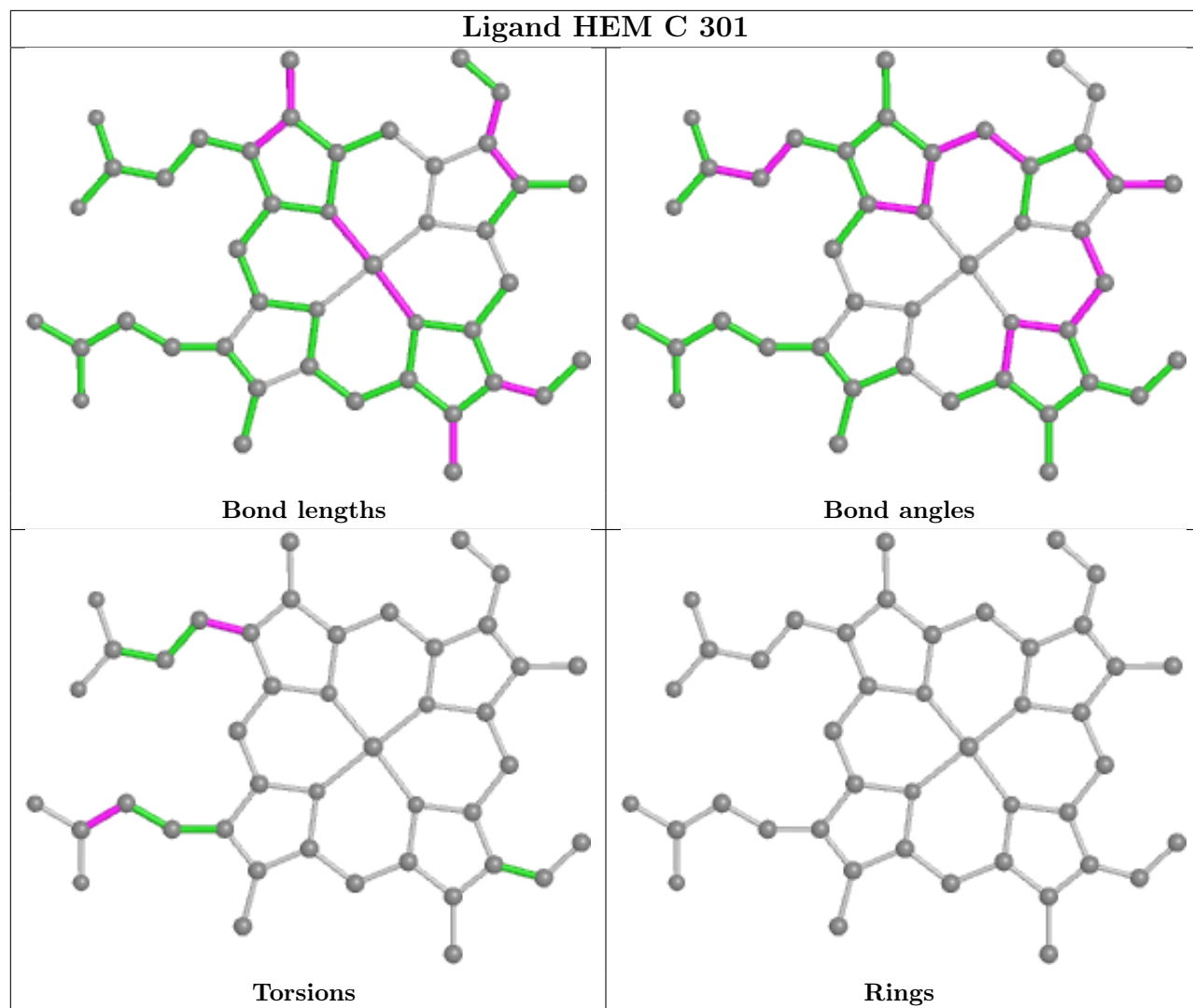| Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	302	SO4	1	0
2	D	301	HEM	4	0
3	E	305	SO4	1	0
4	A	303	EDO	2	0
2	C	301	HEM	4	0
3	B	302	SO4	1	0

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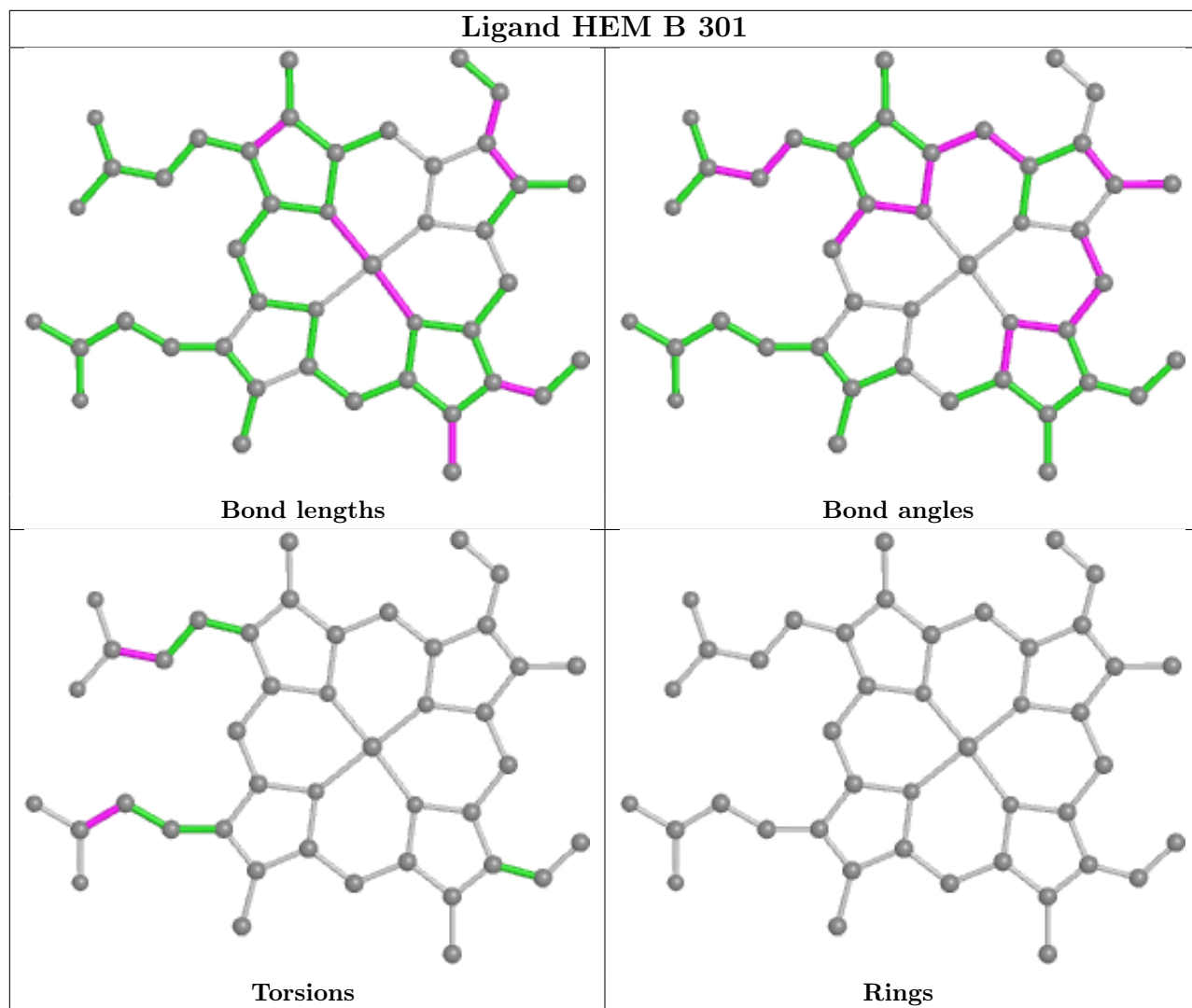
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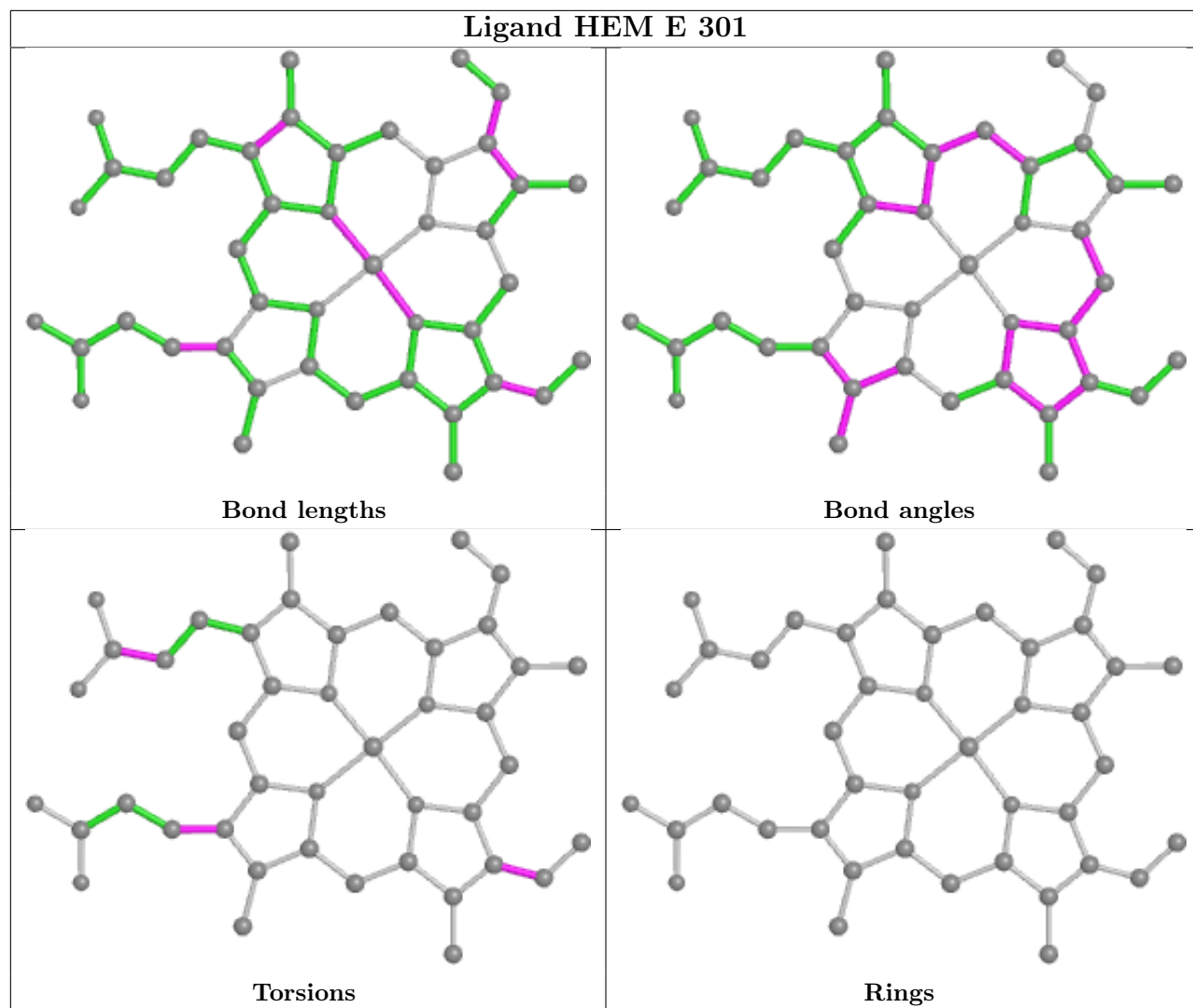| Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	HEM	5	0
2	E	301	HEM	3	0
4	E	302	EDO	1	0
3	D	304	SO4	1	0
2	A	301	HEM	2	0

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 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 D 301

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM C 301

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM B 301

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM E 301

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 301

Bond lengths

Bond angles

Torsions

Rings
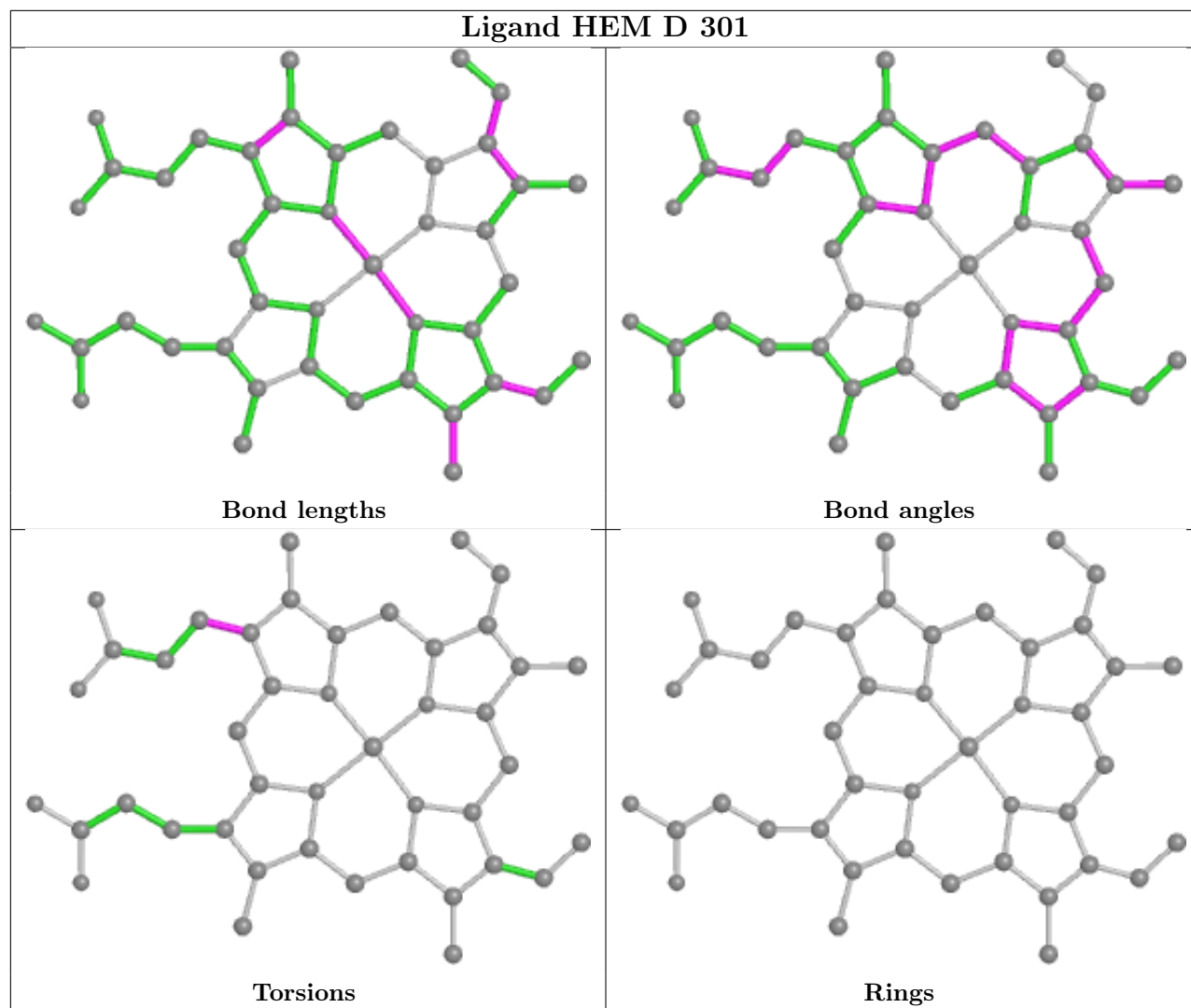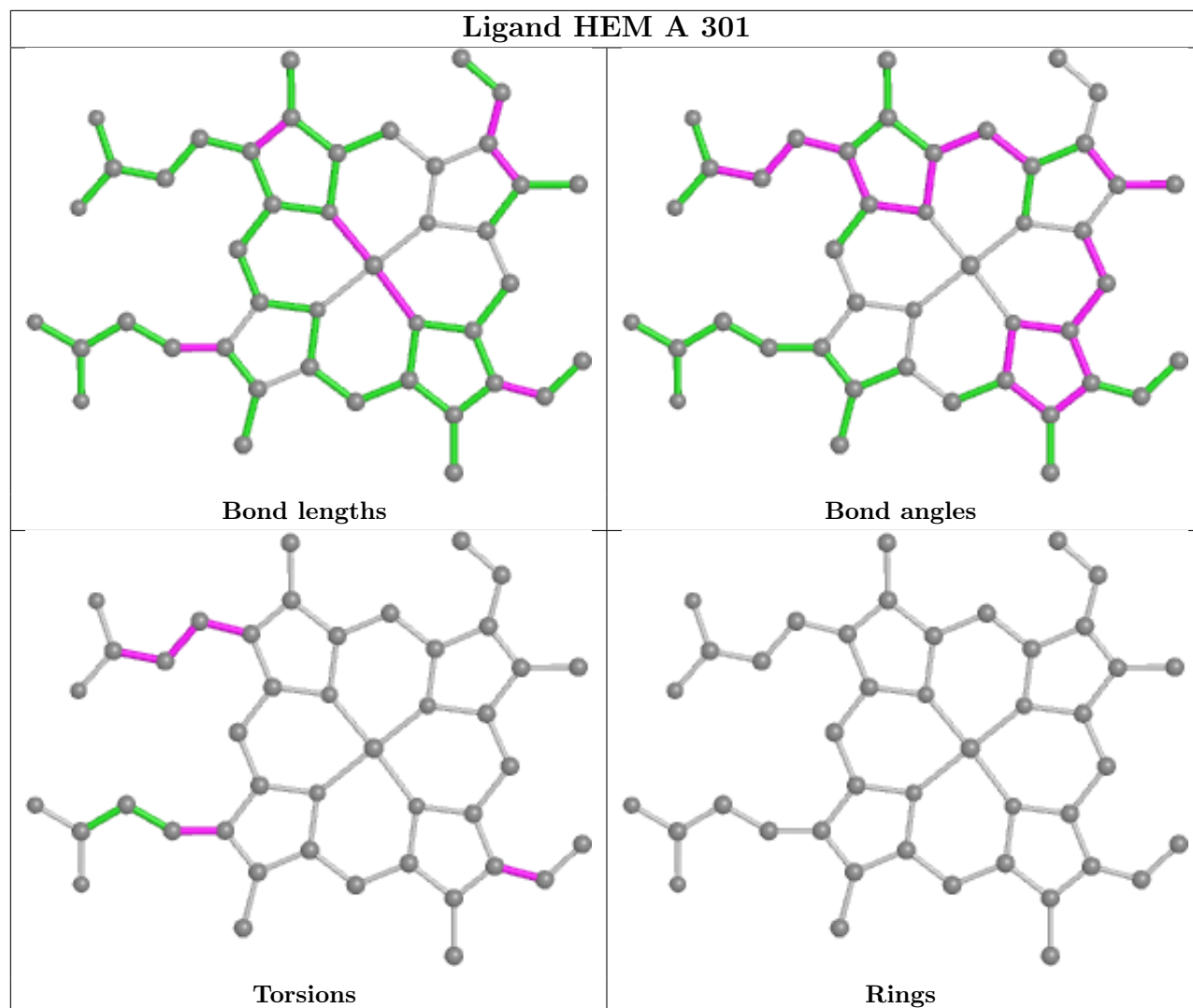
5.7　Other polymers ⓘ

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(Å^2)	Q<0.9
1	A	238/241 (98%)	0.73	24 (10%)	7	4	31, 63, 114, 150	0
1	B	238/241 (98%)	0.70	19 (7%)	12	9	30, 62, 113, 146	1 (0%)
1	C	236/241 (97%)	0.66	20 (8%)	10	8	32, 65, 114, 136	1 (0%)
1	D	236/241 (97%)	0.64	20 (8%)	10	8	36, 66, 110, 131	1 (0%)
1	E	237/241 (98%)	0.65	18 (7%)	13	10	29, 65, 112, 149	1 (0%)
All	All	1185/1205 (98%)	0.67	101 (8%)	10	8	29, 64, 113, 150	4 (0%)

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	236	PHE	6.7
1	B	3	ARG	6.4
1	A	125	ASN	5.8
1	A	123	GLN	5.4
1	D	232	ILE	5.1
1	D	236	PHE	4.7
1	A	236	PHE	4.7
1	D	229	LEU	4.6
1	D	69	PHE	4.2
1	B	21	MET	4.2
1	E	69	PHE	4.1
1	C	26	TRP	4.1
1	A	124	VAL	3.8
1	C	35	ILE	3.8
1	B	237	ALA	3.7
1	B	120	THR	3.6
1	E	124	VAL	3.6
1	C	125	ASN	3.6
1	E	237	ALA	3.6
1	B	74	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	211	PHE	3.4
1	C	8	THR	3.4
1	B	236	PHE	3.2
1	C	229	LEU	3.2
1	A	207	GLN	3.1
1	D	6	LEU	3.1
1	A	3	ARG	3.0
1	A	35	ILE	3.0
1	A	127	GLU	3.0
1	C	108	PRO	3.0
1	B	125	ASN	2.9
1	A	4	GLU	2.9
1	D	88	GLY	2.8
1	A	122	LEU	2.8
1	C	69	PHE	2.8
1	E	207	GLN	2.7
1	B	7	LEU	2.7
1	B	48	SER	2.6
1	A	6	LEU	2.6
1	E	12	VAL	2.6
1	B	238	GLN	2.6
1	D	125	ASN	2.5
1	D	209	LYS	2.5
1	D	26	TRP	2.5
1	A	232	ILE	2.5
1	D	124	VAL	2.5
1	C	146	TYR	2.5
1	E	167	TYR	2.5
1	E	233	LEU	2.5
1	D	98	GLY	2.5
1	A	128	SER	2.4
1	B	117	SER	2.4
1	B	121	GLU	2.4
1	D	219	HIS	2.4
1	D	230	ASP	2.4
1	C	99	GLY	2.4
1	A	31	GLU	2.4
1	A	90	ARG	2.3
1	D	44	VAL	2.3
1	D	35	ILE	2.3
1	C	113	GLY	2.3
1	B	127	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	234	GLU	2.3
1	A	209	LYS	2.3
1	A	5	LYS	2.3
1	E	234	GLU	2.3
1	D	129	GLY	2.3
1	A	69	PHE	2.3
1	A	67	LEU	2.3
1	C	131	ARG	2.2
1	C	217	PHE	2.2
1	C	189	TYR	2.2
1	D	28	LEU	2.2
1	E	194	ARG	2.2
1	A	28	LEU	2.1
1	C	111	VAL	2.1
1	E	127	GLU	2.1
1	E	35	ILE	2.1
1	C	67	LEU	2.1
1	C	194	ARG	2.1
1	A	120	THR	2.1
1	E	109	THR	2.1
1	B	35	ILE	2.1
1	C	28	LEU	2.1
1	A	97	SER	2.1
1	D	107	LYS	2.1
1	E	67	LEU	2.1
1	E	125	ASN	2.1
1	E	74	ARG	2.1
1	B	146	TYR	2.1
1	A	110	TYR	2.0
1	C	11	GLY	2.0
1	E	21	MET	2.0
1	A	165	LEU	2.0
1	E	232	ILE	2.0
1	B	8	THR	2.0
1	B	213	HIS	2.0
1	B	126	GLY	2.0
1	C	105	SER	2.0
1	D	130	SER	2.0
1	C	195	LEU	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.

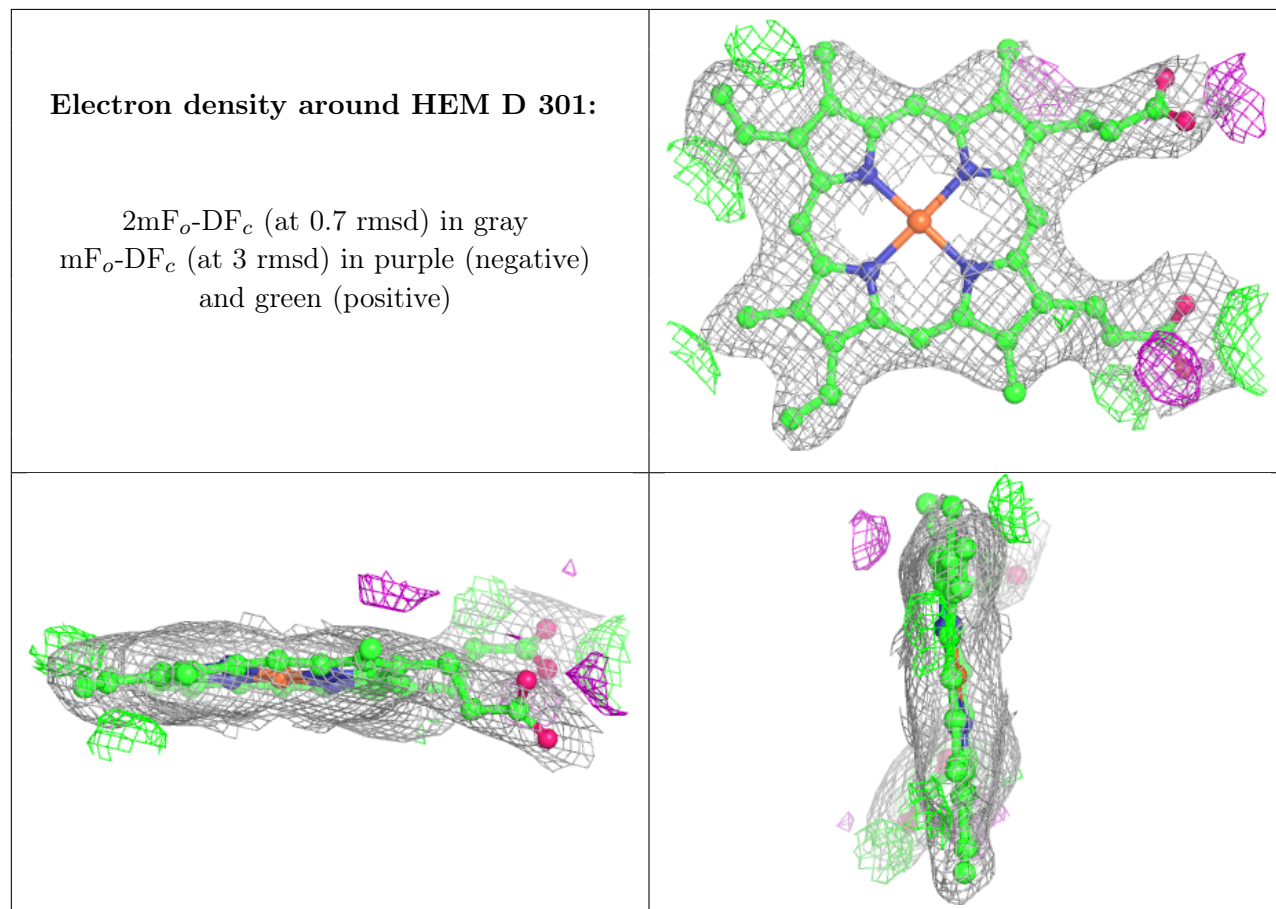## 6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	D	304	5/5	0.65	0.28	115,120,133,138	0
4	EDO	E	303	4/4	0.69	0.34	54,72,77,79	0
3	SO4	C	303	5/5	0.72	0.33	113,114,118,121	0
4	EDO	C	306	4/4	0.80	0.17	56,65,75,88	0
3	SO4	A	305	5/5	0.82	0.40	148,152,156,156	0
4	EDO	A	303	4/4	0.82	0.21	64,74,81,91	0
3	SO4	E	305	5/5	0.83	0.21	96,104,110,115	0
4	EDO	C	305	4/4	0.84	0.15	69,75,79,80	0
3	SO4	B	303	5/5	0.85	0.23	133,134,138,146	0
5	IMD	A	304	5/5	0.85	0.32	35,51,60,62	0
4	EDO	E	302	4/4	0.86	0.12	72,75,83,86	0
4	EDO	C	304	4/4	0.87	0.26	66,74,79,79	0
3	SO4	D	303	5/5	0.88	0.13	110,119,126,130	0
4	EDO	B	304	4/4	0.89	0.35	43,44,50,51	0
4	EDO	D	305	4/4	0.90	0.10	46,49,60,68	0
3	SO4	C	302	5/5	0.91	0.14	84,97,112,117	0
3	SO4	A	302	5/5	0.91	0.24	18,28,51,61	5
2	HEM	D	301	43/43	0.93	0.17	29,57,71,73	0
5	IMD	D	302	5/5	0.93	0.20	67,69,77,79	0
2	HEM	C	301	43/43	0.94	0.17	13,38,56,70	0
3	SO4	B	302	5/5	0.94	0.18	95,108,114,117	0
4	EDO	E	304	4/4	0.95	0.10	59,61,64,67	0
2	HEM	B	301	43/43	0.95	0.17	6,35,59,66	0
2	HEM	A	301	43/43	0.95	0.15	11,31,61,72	0
2	HEM	E	301	43/43	0.96	0.17	10,33,60,77	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.
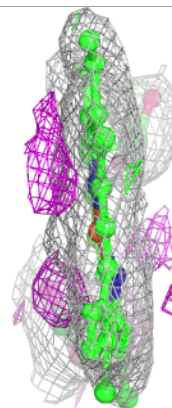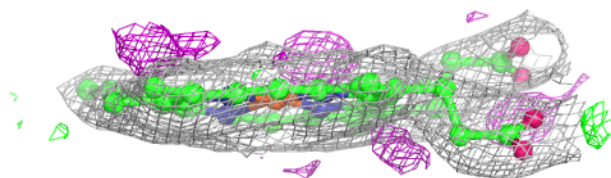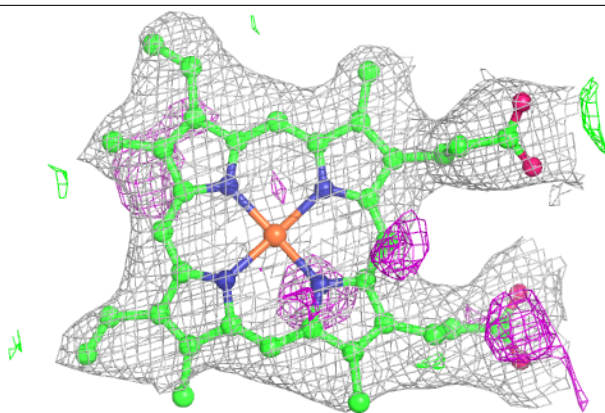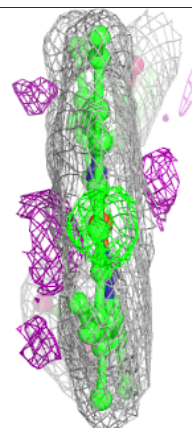
Electron density around HEM D 301:

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

Electron density around HEM C 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
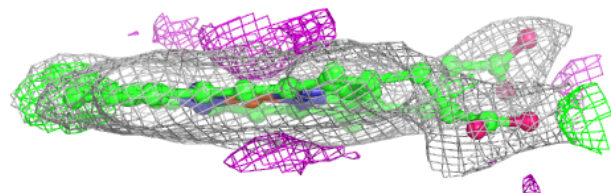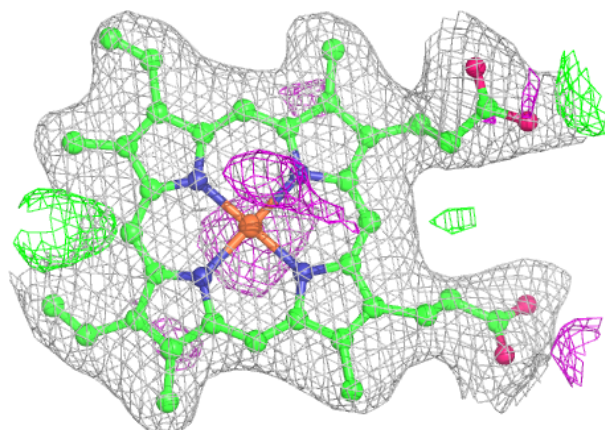and green (positive)
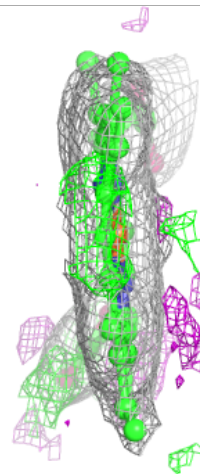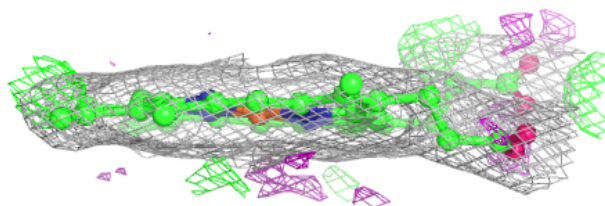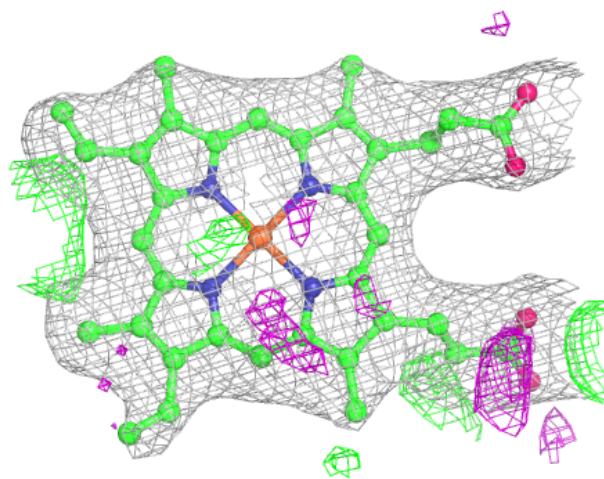
Electron density around HEM B 301:

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

Electron density around HEM A 301:

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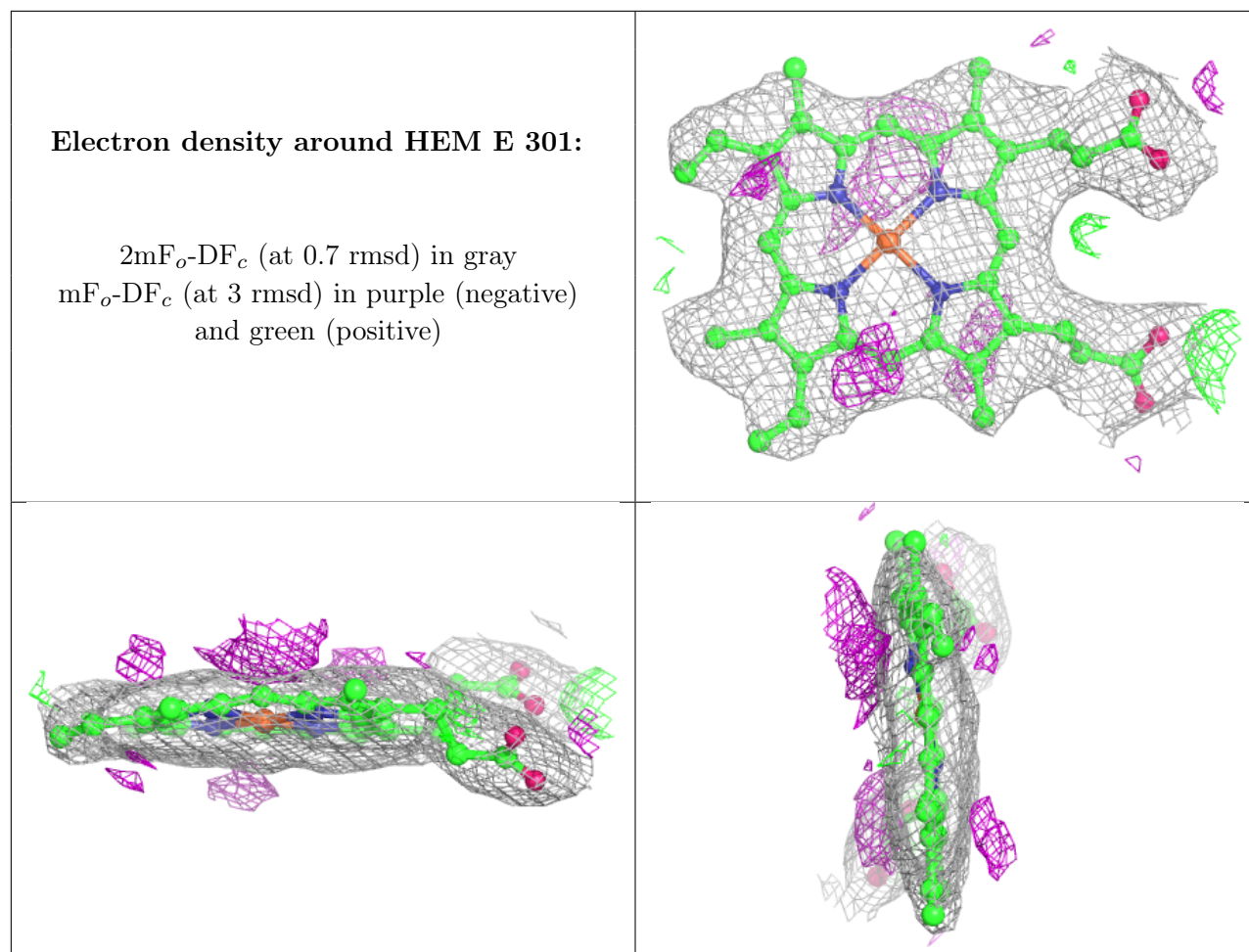mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around HEM E 301:

$2mF_o$-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.