



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 03:48 AM EDT

PDB ID : 1LY8
Title : The crystal structure of a mutant enzyme of Coprinus cinereus peroxidase provides an understanding of its increased thermostability and insight into modelling of protein structures
Authors : Houborg, K.; Harris, P.; Poulsen, J.-C.N.; Svendsen, A.; Schneider, P.; Larsen, S.
Deposited on : 2002-06-07
Resolution : 2.05 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 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 : 2.23.2
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) : 2.23.2

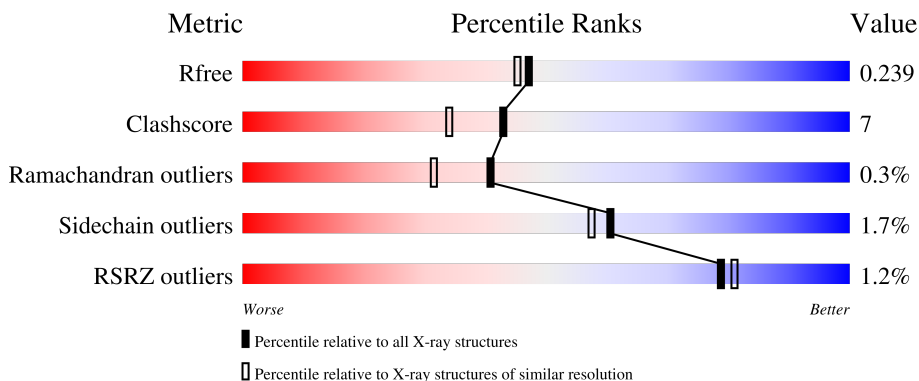
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	343	 85% 13% ..
1	B	343	 86% 12% ..

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
7	GOL	A	811	-	-	-	X
7	GOL	B	802	-	-	-	X
7	GOL	B	803	-	-	-	X
7	GOL	B	805	-	-	-	X
7	GOL	B	808	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5874 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 Peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	339	2504	1559	430	501	14	0	5	0
1	B	338	2499	1555	429	501	14	0	5	0

There are 14 discrepancies between the modelled and reference sequences:

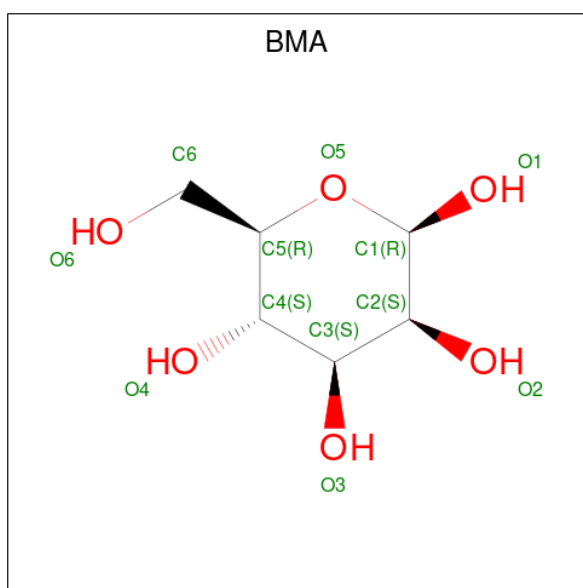
Chain	Residue	Modelled	Actual	Comment	Reference
A	49	SER	ILE	engineered mutation	UNP P28314
A	53	ALA	VAL	engineered mutation	UNP P28314
A	121	ALA	THR	engineered mutation	UNP P28314
A	166	PHE	MET	engineered mutation	UNP P28314
A	239	GLY	GLU	engineered mutation	UNP P28314
A	242	ILE	MET	engineered mutation	UNP P28314
A	272	PHE	TYR	engineered mutation	UNP P28314
B	49	SER	ILE	engineered mutation	UNP P28314
B	53	ALA	VAL	engineered mutation	UNP P28314
B	121	ALA	THR	engineered mutation	UNP P28314
B	166	PHE	MET	engineered mutation	UNP P28314
B	239	GLY	GLU	engineered mutation	UNP P28314
B	242	ILE	MET	engineered mutation	UNP P28314
B	272	PHE	TYR	engineered mutation	UNP P28314

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



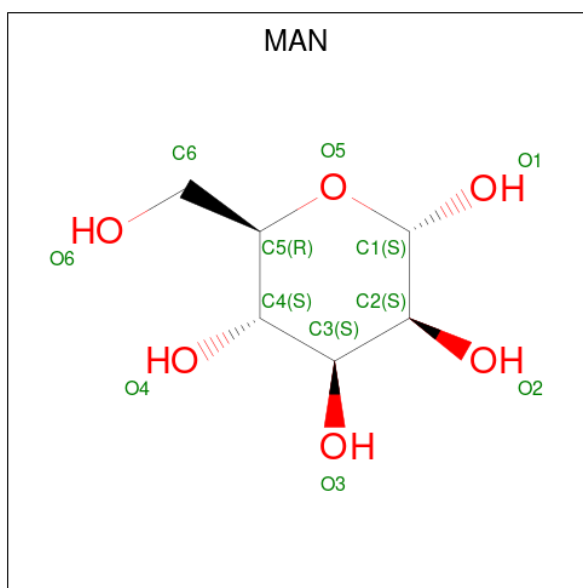
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is beta-D-mannopyranose (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf		
4	A	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
5	A	2	Total	Ca	0	0
			2	2		
5	B	2	Total	Ca	0	0
			2	2		

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0
7	B	1	Total C O 6 3 3	0	0

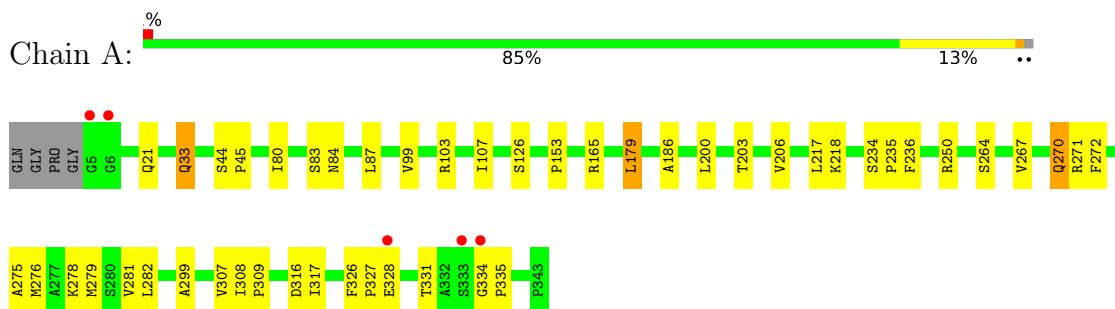
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	332	Total O 332 332	0	0
8	B	305	Total O 305 305	0	0

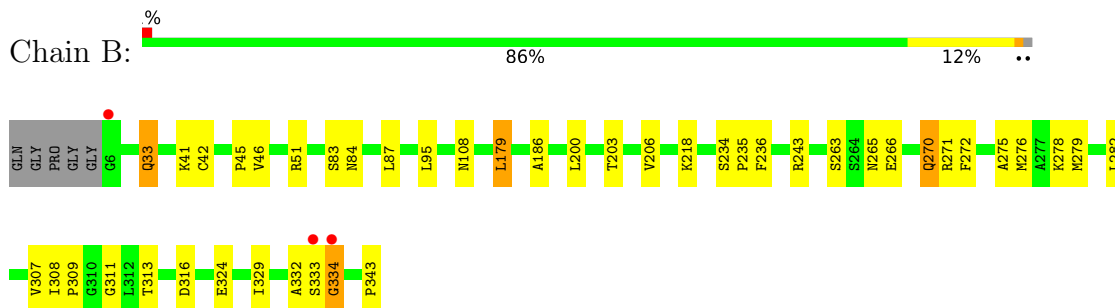
3 Residue-property plots [i](#)

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: Peroxidase



- Molecule 1: Peroxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	74.49Å 114.86Å 73.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.91 – 2.05 19.91 – 2.05	Depositor EDS
% Data completeness (in resolution range)	84.6 (19.91-2.05) 84.8 (19.91-2.05)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.39 (at 2.06Å)	Xtrriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.202 , 0.249 0.193 , 0.239	Depositor DCC
R_{free} test set	1687 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	13.3	Xtrriage
Anisotropy	0.869	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 61.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtrriage
Estimated twinning fraction	0.000 for l,-k,h	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5874	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.86 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9183e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, HEM, CA, GOL, NAG, BMA

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	0.31	0/2561	0.58	0/3489
1	B	0.31	0/2556	0.57	0/3483
All	All	0.31	0/5117	0.57	0/6972

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	335	PRO	Mainchain

5.2 Too-close contacts [i](#)

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	2504	0	2395	34	0
1	B	2499	0	2388	35	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
3	A	11	0	10	1	0
3	B	11	0	10	1	0
4	A	11	0	10	1	0
4	B	11	0	10	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	43	0	30	0	0
6	B	43	0	30	0	0
7	A	24	0	28	0	0
7	B	48	0	56	3	0
8	A	332	0	0	3	0
8	B	305	0	0	3	0
All	All	5874	0	4993	70	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 (70) 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:33:GLN:HE21	1:A:33:GLN:HA	1.39	0.87
1:B:33:GLN:HA	1:B:33:GLN:HE21	1.44	0.83
1:B:265:ASN:H	7:B:808:GOL:H2	1.56	0.70
1:A:179:LEU:HD13	1:A:275:ALA:HB1	1.77	0.67
1:B:236:PHE:CZ	1:B:309:PRO:HG2	2.32	0.64
1:B:311:GLY:HA2	1:B:332:ALA:O	1.98	0.64
1:B:179:LEU:HD13	1:B:275:ALA:HB1	1.79	0.63
1:B:83:SER:HB2	1:B:87:LEU:HD22	1.85	0.58
1:B:279[B]:MET:HE3	1:B:282:LEU:HD12	1.86	0.57
1:A:281[B]:VAL:HG22	1:A:281[B]:VAL:O	2.05	0.56
1:B:45:PRO:HG3	8:B:9269:HOH:O	2.05	0.55
1:A:83:SER:O	1:A:87:LEU:HB2	2.07	0.55
1:A:278:LYS:HZ2	1:A:278:LYS:HB2	1.72	0.54
1:A:179:LEU:HD13	1:A:275:ALA:CB	2.38	0.53
1:A:217:LEU:HD23	1:A:317:ILE:HD13	1.90	0.53
1:A:83:SER:HB2	1:A:87:LEU:HD22	1.92	0.52
1:A:234:SER:HB2	1:A:235:PRO:HD2	1.92	0.52
1:B:218:LYS:HG3	1:B:316:ASP:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:PRO:HD3	8:B:9243:HOH:O	2.09	0.51
1:B:83:SER:O	1:B:87:LEU:HB2	2.11	0.51
1:A:278:LYS:HB2	1:A:278:LYS:NZ	2.26	0.50
1:A:278:LYS:NZ	1:A:278:LYS:CB	2.74	0.50
1:B:270:GLN:HG2	1:B:271:ARG:N	2.26	0.50
1:B:333:SER:O	1:B:334:GLY:O	2.30	0.50
1:A:21:GLN:HG2	8:A:9307:HOH:O	2.10	0.49
1:B:186:ALA:C	1:B:200:LEU:HD13	2.33	0.49
1:B:307:VAL:HG22	1:B:308:ILE:N	2.28	0.49
1:B:243:ARG:HH11	1:B:243:ARG:HG3	1.78	0.48
1:B:108[B]:ASN:ND2	8:B:9025:HOH:O	2.47	0.48
1:A:250:ARG:HH11	1:A:250:ARG:HG3	1.79	0.48
1:B:266:GLU:HB2	7:B:808:GOL:O3	2.14	0.47
1:A:33:GLN:HA	1:A:33:GLN:NE2	2.18	0.47
1:B:236:PHE:HZ	1:B:309:PRO:HG2	1.79	0.47
1:B:179:LEU:HD13	1:B:275:ALA:CB	2.42	0.47
1:A:44:SER:HB3	1:A:45:PRO:HD3	1.96	0.47
1:B:278:LYS:HB3	1:B:278:LYS:NZ	2.30	0.46
1:A:270:GLN:HE21	1:A:270:GLN:HB3	1.49	0.46
1:A:307:VAL:HG22	1:A:308:ILE:N	2.30	0.46
1:A:331:THR:HG21	3:A:600:BMA:H2	1.98	0.46
4:A:700:MAN:H4	8:A:9305:HOH:O	2.15	0.46
1:B:263:SER:HB3	1:B:329:ILE:HD11	1.98	0.46
1:A:264:SER:OG	1:A:267:VAL:HG23	2.15	0.46
1:B:324:GLU:HA	1:B:324:GLU:OE1	2.16	0.46
1:A:80:ILE:HG12	1:A:99:VAL:HG13	1.98	0.46
1:B:33:GLN:HA	1:B:33:GLN:NE2	2.23	0.46
1:B:234:SER:HB2	1:B:235:PRO:HD2	1.96	0.46
1:A:203:THR:HB	1:A:206:VAL:HB	1.97	0.46
1:B:313:THR:HG22	3:B:600:BMA:H3	1.97	0.45
1:A:236:PHE:CZ	1:A:309:PRO:HG2	2.51	0.45
1:A:103:ARG:O	1:A:107:ILE:HG13	2.17	0.44
1:A:186:ALA:HB3	1:A:200:LEU:HD22	1.99	0.44
1:B:42:CYS:HA	1:B:46:VAL:HG21	2.00	0.44
1:B:279[B]:MET:CE	1:B:282:LEU:HD12	2.47	0.44
1:B:203:THR:HB	1:B:206:VAL:HB	2.00	0.43
1:A:218:LYS:HG3	1:A:316:ASP:O	2.19	0.42
1:A:326:PHE:CD1	1:A:327:PRO:HD2	2.54	0.42
1:B:51:ARG:HD3	1:B:95:LEU:HD21	2.02	0.42
1:A:235:PRO:HG2	1:A:236:PHE:CD2	2.55	0.42
1:B:186:ALA:HB3	1:B:200:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:PHE:CZ	1:B:276:MET:HG3	2.55	0.41
1:A:186:ALA:C	1:A:200:LEU:HD13	2.40	0.41
1:A:281[A]:VAL:HG23	8:A:9045:HOH:O	2.19	0.41
1:B:108[A]:ASN:O	1:B:108[A]:ASN:ND2	2.53	0.41
1:A:272:PHE:CE1	1:A:276:MET:HG3	2.55	0.41
1:A:126:SER:HA	1:A:299:ALA:HB2	2.02	0.41
1:A:153:PRO:HG3	1:A:165:ARG:HG2	2.02	0.41
1:A:270:GLN:HG2	1:A:271:ARG:N	2.35	0.41
1:B:278:LYS:HB3	1:B:278:LYS:HZ3	1.86	0.41
1:B:41:LYS:HA	7:B:805:GOL:H2	2.03	0.40
1:A:279[B]:MET:HE3	1:A:282:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	342/343 (100%)	328 (96%)	13 (4%)	1 (0%)	41	31
1	B	341/343 (99%)	332 (97%)	8 (2%)	1 (0%)	41	31
All	All	683/686 (100%)	660 (97%)	21 (3%)	2 (0%)	41	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	334	GLY
1	A	334	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	273/270 (101%)	268 (98%)	5 (2%)	59	55
1	B	273/270 (101%)	269 (98%)	4 (2%)	65	62
All	All	546/540 (101%)	537 (98%)	9 (2%)	60	59

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	84	ASN
1	A	179	LEU
1	A	270	GLN
1	A	328	GLU
1	B	33	GLN
1	B	84	ASN
1	B	179	LEU
1	B	270	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	84	ASN
1	A	127	ASN
1	A	270	GLN
1	A	302	ASN
1	B	21	GLN
1	B	33	GLN
1	B	69	GLN
1	B	127	ASN
1	B	270	GLN
1	B	302	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 4 are monoatomic - leaving 20 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
7	GOL	B	802	-	5,5,5	1.12	0	5,5,5	1.75	2 (40%)
2	NAG	A	500	1	14,14,15	0.56	0	17,19,21	0.76	1 (5%)
7	GOL	A	811	-	5,5,5	1.14	0	5,5,5	1.65	1 (20%)
7	GOL	B	803	-	5,5,5	1.15	0	5,5,5	1.80	1 (20%)
7	GOL	B	808	-	5,5,5	1.09	0	5,5,5	1.76	2 (40%)
7	GOL	B	805	-	5,5,5	1.08	0	5,5,5	1.72	1 (20%)
4	MAN	B	700	1	11,11,12	0.46	0	15,15,17	0.43	0
7	GOL	A	810	-	5,5,5	1.19	0	5,5,5	1.78	1 (20%)
7	GOL	B	804	-	5,5,5	1.10	0	5,5,5	1.75	1 (20%)
6	HEM	B	344	1	27,50,50	3.99	13 (48%)	17,82,82	2.82	8 (47%)
3	BMA	A	600	1	11,11,12	0.52	0	15,15,17	0.61	0
4	MAN	A	700	1	11,11,12	0.44	0	15,15,17	0.41	0
2	NAG	B	500	1	14,14,15	0.59	0	17,19,21	0.74	1 (5%)
3	BMA	B	600	1	11,11,12	0.47	0	15,15,17	0.60	0
7	GOL	B	800	-	5,5,5	1.11	0	5,5,5	1.73	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	GOL	A	806	-	5,5,5	1.11	0	5,5,5	1.79	1 (20%)
7	GOL	B	807	-	5,5,5	1.12	0	5,5,5	1.72	1 (20%)
6	HEM	A	344	1	27,50,50	4.36	21 (77%)	17,82,82	3.48	10 (58%)
7	GOL	B	809	-	5,5,5	1.11	0	5,5,5	1.72	1 (20%)
7	GOL	A	801	-	5,5,5	1.08	0	5,5,5	1.79	2 (40%)

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
7	GOL	B	802	-	-	0/4/4/4	-
2	NAG	A	500	1	-	0/6/23/26	0/1/1/1
7	GOL	A	811	-	-	0/4/4/4	-
7	GOL	B	803	-	-	0/4/4/4	-
7	GOL	B	808	-	-	0/4/4/4	-
7	GOL	B	805	-	-	0/4/4/4	-
4	MAN	B	700	1	-	0/2/19/22	0/1/1/1
7	GOL	A	810	-	-	0/4/4/4	-
7	GOL	B	804	-	-	0/4/4/4	-
6	HEM	B	344	1	-	0/6/54/54	-
3	BMA	A	600	1	-	2/2/19/22	0/1/1/1
4	MAN	A	700	1	-	0/2/19/22	0/1/1/1
2	NAG	B	500	1	-	0/6/23/26	0/1/1/1
3	BMA	B	600	1	-	2/2/19/22	0/1/1/1
7	GOL	B	800	-	-	0/4/4/4	-
7	GOL	A	806	-	-	0/4/4/4	-
7	GOL	B	807	-	-	0/4/4/4	-
6	HEM	A	344	1	-	0/6/54/54	-
7	GOL	B	809	-	-	0/4/4/4	-
7	GOL	A	801	-	-	0/4/4/4	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	344	HEM	CMA-C3A	10.84	1.74	1.51
6	B	344	HEM	CMB-C2B	9.43	1.74	1.51
6	A	344	HEM	CMB-C2B	8.80	1.72	1.51
6	A	344	HEM	C1C-C2C	8.75	1.62	1.42
6	B	344	HEM	CMD-C2D	8.63	1.69	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	344	HEM	C4A-NA	6.84	1.50	1.36
6	B	344	HEM	C1C-C2C	6.54	1.57	1.42
6	A	344	HEM	CMA-C3A	6.38	1.64	1.51
6	A	344	HEM	C3B-C2B	6.34	1.49	1.40
6	A	344	HEM	CAD-C3D	-6.27	1.41	1.52
6	A	344	HEM	CAA-C2A	5.57	1.60	1.52
6	A	344	HEM	C1A-NA	-5.45	1.24	1.36
6	B	344	HEM	C3B-C2B	5.35	1.47	1.40
6	A	344	HEM	C3D-C2D	4.92	1.52	1.37
6	A	344	HEM	CMD-C2D	4.13	1.60	1.51
6	B	344	HEM	C4A-CHB	-3.83	1.30	1.41
6	B	344	HEM	C1A-NA	-3.66	1.28	1.36
6	A	344	HEM	C4A-CHB	-3.51	1.31	1.41
6	A	344	HEM	C1D-ND	3.33	1.43	1.36
6	A	344	HEM	C2A-C3A	3.32	1.47	1.37
6	B	344	HEM	C3C-CAC	3.05	1.54	1.47
6	A	344	HEM	CMC-C2C	2.89	1.58	1.51
6	A	344	HEM	CBB-CAB	-2.89	1.09	1.29
6	A	344	HEM	CBC-CAC	2.79	1.47	1.29
6	A	344	HEM	C4D-C3D	2.69	1.48	1.42
6	A	344	HEM	C3B-CAB	-2.66	1.42	1.47
6	B	344	HEM	CAD-C3D	-2.57	1.47	1.52
6	B	344	HEM	C4D-C3D	2.50	1.48	1.42
6	B	344	HEM	CAA-C2A	-2.41	1.48	1.52
6	A	344	HEM	C3C-C2C	2.40	1.43	1.40
6	A	344	HEM	C4B-NB	-2.27	1.31	1.36
6	B	344	HEM	C1D-CHD	2.24	1.47	1.41
6	A	344	HEM	C4B-CHC	-2.04	1.35	1.41
6	B	344	HEM	C4B-NB	-2.01	1.32	1.36

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	344	HEM	CAA-CBA-CGA	-7.28	100.46	112.67
6	A	344	HEM	C1D-C2D-C3D	-6.71	102.33	107.00
6	A	344	HEM	C4A-C3A-C2A	-5.64	103.08	107.00
6	A	344	HEM	CMC-C2C-C3C	5.28	134.55	124.68
6	B	344	HEM	C1D-C2D-C3D	-5.07	103.47	107.00
6	B	344	HEM	C4A-C3A-C2A	-4.83	103.63	107.00
6	B	344	HEM	CAA-CBA-CGA	-4.28	105.49	112.67
6	B	344	HEM	C4C-C3C-C2C	-3.91	104.17	106.90
6	B	344	HEM	CMC-C2C-C3C	3.36	130.96	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	344	HEM	C4C-C3C-C2C	-3.35	104.56	106.90
6	B	344	HEM	C3B-C4B-NB	3.13	113.25	109.21
6	B	344	HEM	CMB-C2B-C3B	3.01	130.30	124.68
6	B	344	HEM	CMD-C2D-C3D	2.91	130.44	124.94
6	A	344	HEM	CBA-CAA-C2A	-2.70	107.50	112.49
6	A	344	HEM	CBD-CAD-C3D	2.65	117.37	112.48
7	B	803	GOL	O1-C1-C2	2.59	122.64	110.20
7	B	809	GOL	O1-C1-C2	2.52	122.29	110.20
7	B	802	GOL	O1-C1-C2	2.52	122.26	110.20
7	B	804	GOL	O1-C1-C2	2.50	122.19	110.20
7	A	806	GOL	O1-C1-C2	2.50	122.17	110.20
7	A	810	GOL	O1-C1-C2	2.49	122.16	110.20
7	A	801	GOL	O1-C1-C2	2.49	122.15	110.20
7	B	808	GOL	O1-C1-C2	2.46	121.98	110.20
7	B	800	GOL	O1-C1-C2	2.44	121.92	110.20
6	A	344	HEM	CMB-C2B-C3B	2.44	129.25	124.68
6	A	344	HEM	C3B-C4B-NB	2.44	112.36	109.21
7	B	807	GOL	O1-C1-C2	2.43	121.85	110.20
7	B	805	GOL	O1-C1-C2	2.42	121.82	110.20
7	A	811	GOL	O1-C1-C2	2.28	121.11	110.20
2	A	500	NAG	C2-N2-C7	-2.20	119.77	122.90
2	B	500	NAG	C2-N2-C7	-2.14	119.86	122.90
7	B	802	GOL	O2-C2-C1	2.07	118.25	109.12
6	A	344	HEM	CMA-C3A-C4A	2.03	131.59	128.46
7	B	800	GOL	O2-C2-C1	2.03	118.06	109.12
7	A	801	GOL	O2-C2-C1	2.01	117.98	109.12
7	B	808	GOL	O2-C2-C1	2.01	117.98	109.12

There are no chirality outliers.

All (4) torsion outliers are listed below:

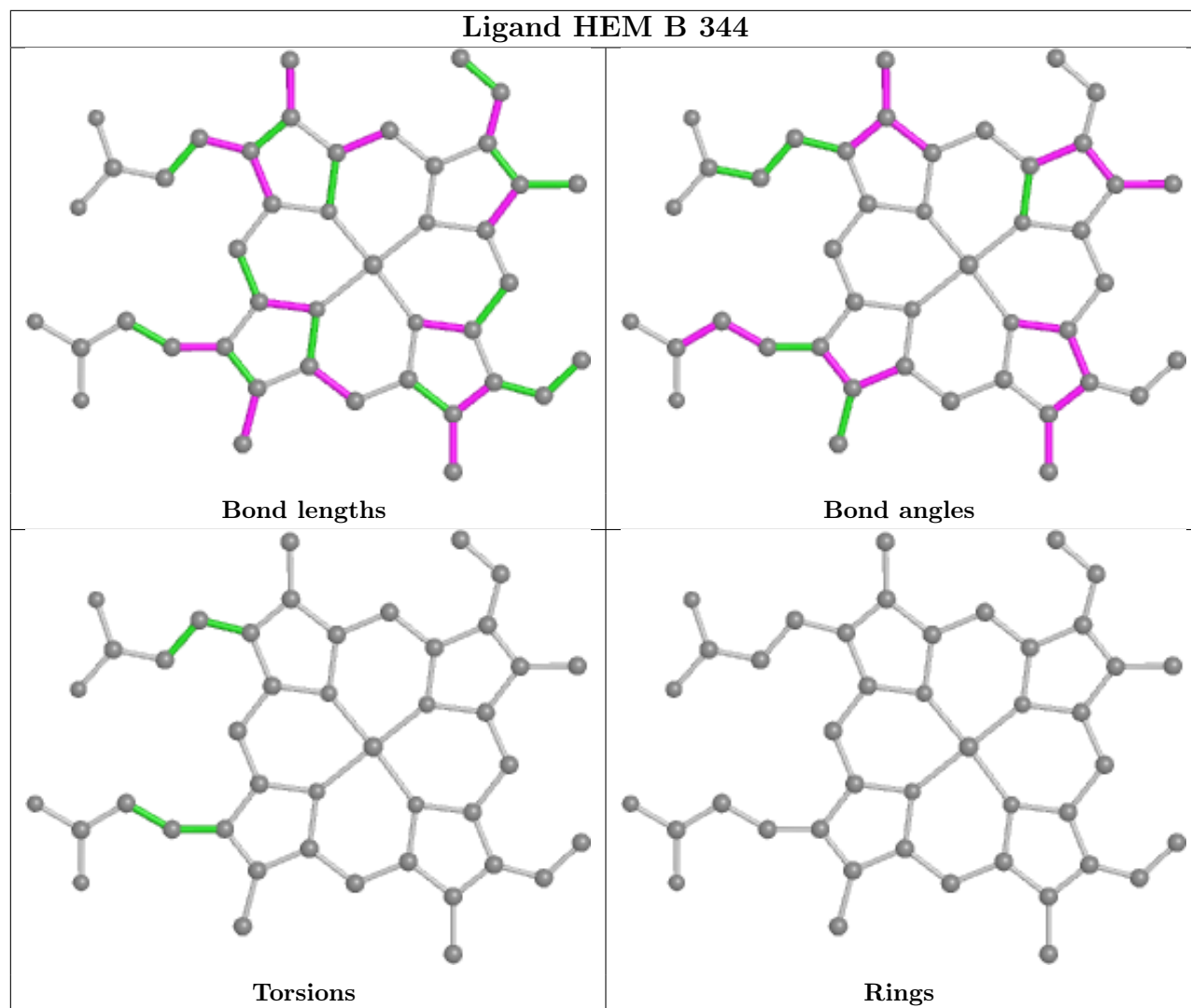
Mol	Chain	Res	Type	Atoms
3	B	600	BMA	O5-C5-C6-O6
3	B	600	BMA	C4-C5-C6-O6
3	A	600	BMA	C4-C5-C6-O6
3	A	600	BMA	O5-C5-C6-O6

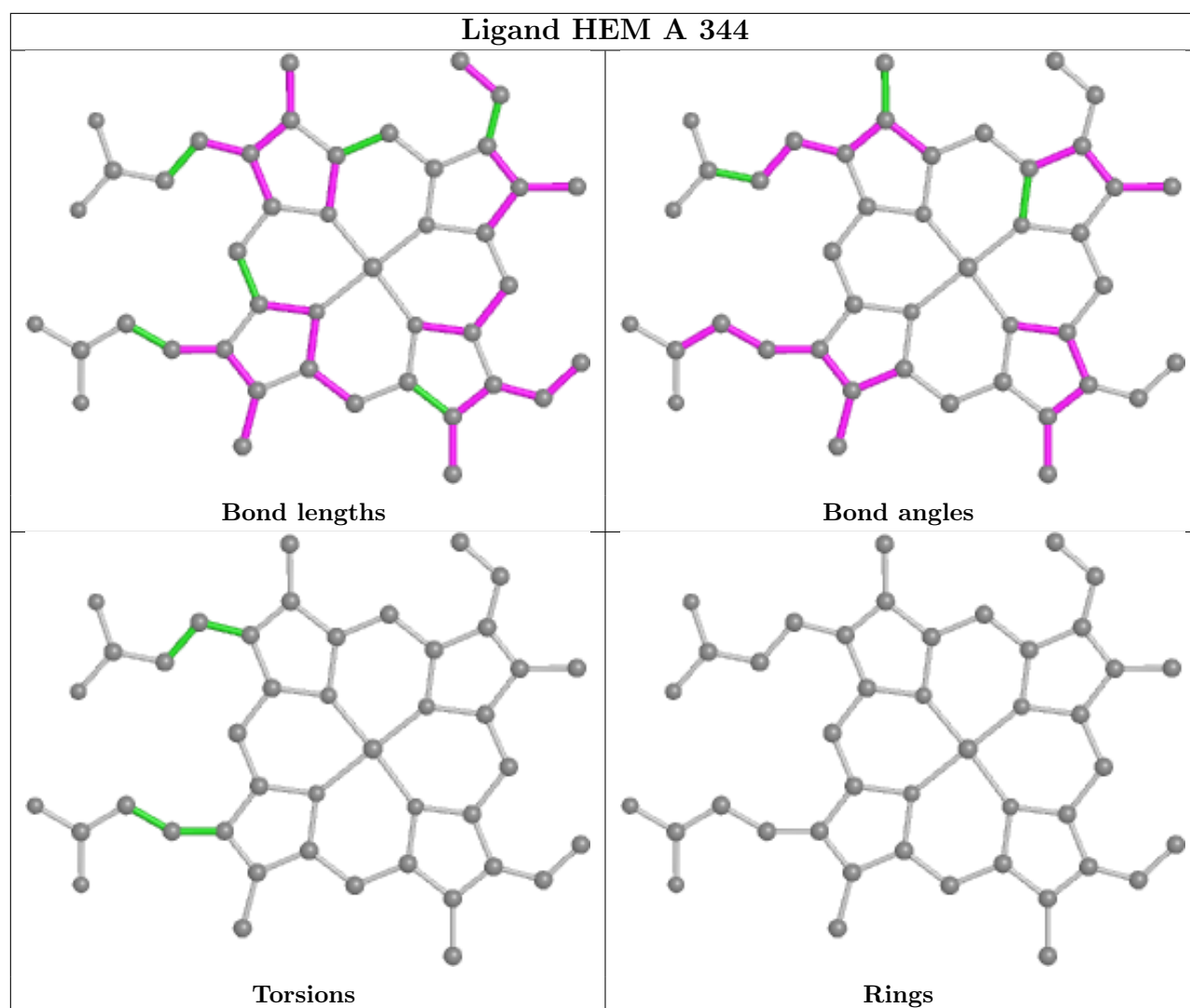
There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	808	GOL	2	0
7	B	805	GOL	1	0
3	A	600	BMA	1	0
4	A	700	MAN	1	0
3	B	600	BMA	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 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	339/343 (98%)	-0.31	5 (1%) 73 76	8, 13, 23, 30	0
1	B	338/343 (98%)	-0.26	3 (0%) 84 86	8, 13, 26, 32	0
All	All	677/686 (98%)	-0.29	8 (1%) 79 81	8, 13, 24, 32	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	334	GLY	5.0
1	A	5	GLY	4.9
1	B	334	GLY	4.6
1	B	6	GLY	3.4
1	A	333	SER	3.3
1	A	6	GLY	3.2
1	B	333	SER	2.9
1	A	328	GLU	2.3

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,

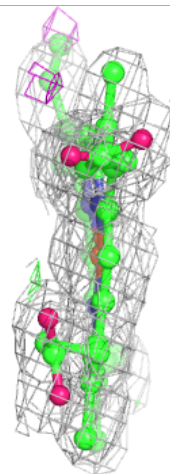
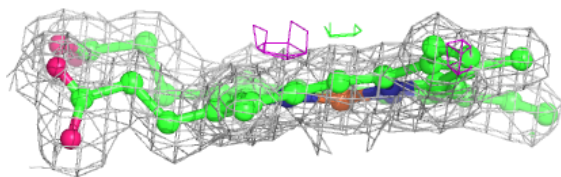
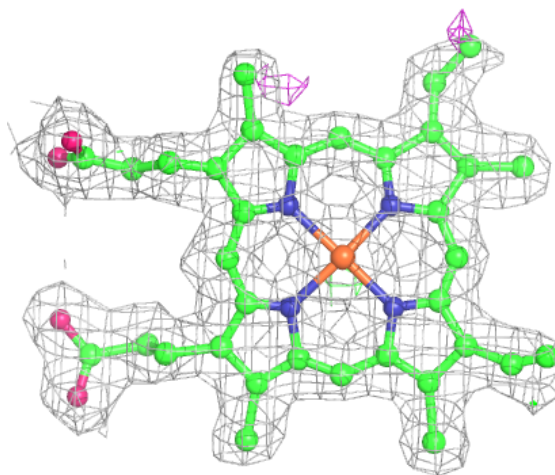
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

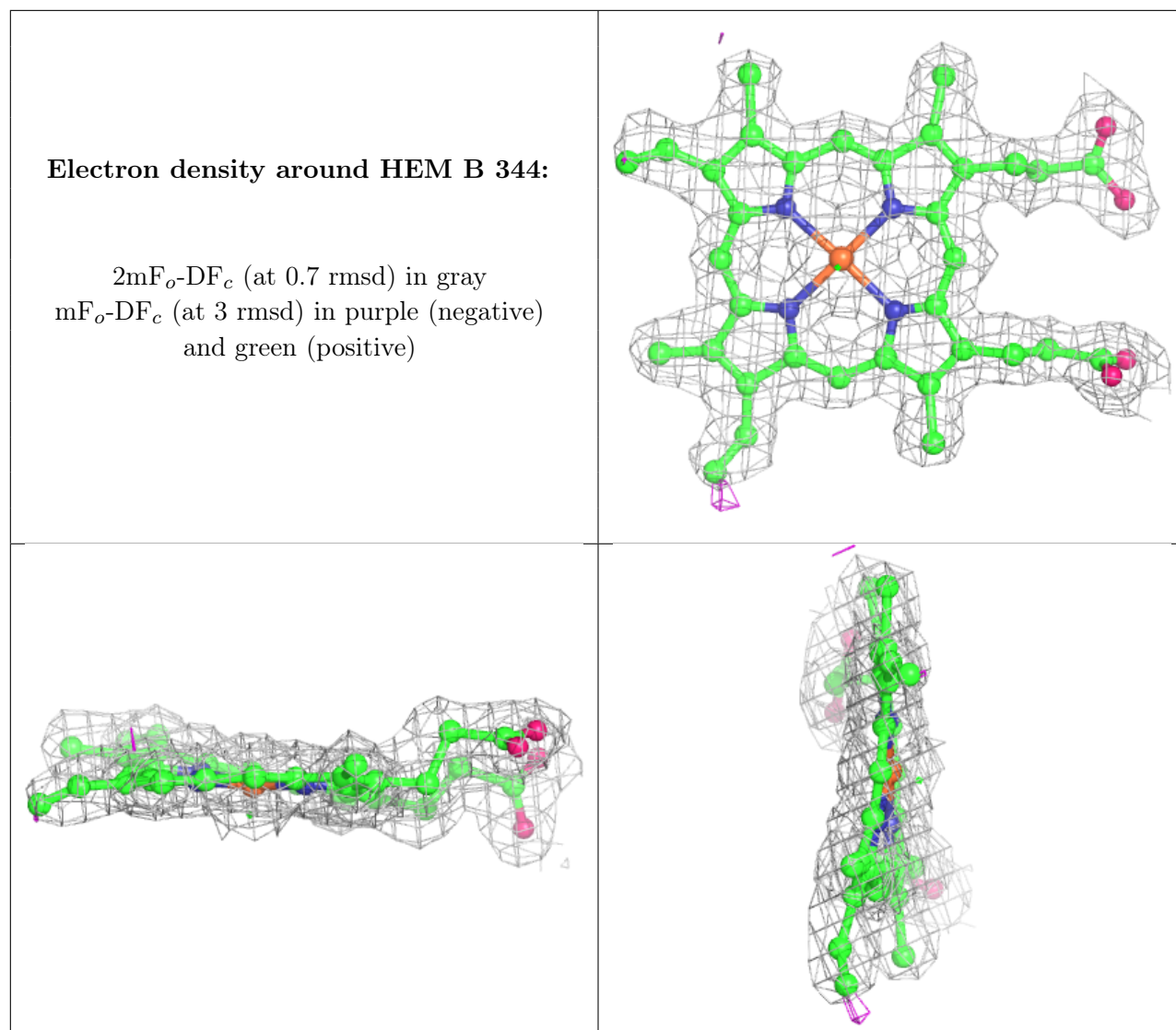
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	GOL	A	801	6/6	0.53	0.32	35,36,37,37	0
7	GOL	B	803	6/6	0.53	0.45	59,59,59,60	0
7	GOL	A	811	6/6	0.54	0.48	53,53,54,54	0
3	BMA	A	600	11/12	0.59	0.28	31,32,33,34	0
7	GOL	B	804	6/6	0.63	0.39	52,52,52,52	0
3	BMA	B	600	11/12	0.64	0.36	35,36,37,38	0
7	GOL	B	808	6/6	0.64	0.51	63,63,63,63	0
7	GOL	B	805	6/6	0.65	0.41	54,54,55,55	0
7	GOL	B	809	6/6	0.65	0.34	56,56,56,56	0
7	GOL	B	802	6/6	0.71	0.41	43,43,43,43	0
7	GOL	A	810	6/6	0.73	0.21	52,53,53,53	0
7	GOL	B	807	6/6	0.75	0.22	50,50,50,51	0
7	GOL	B	800	6/6	0.85	0.13	36,36,37,37	0
4	MAN	A	700	11/12	0.89	0.14	24,24,24,25	0
7	GOL	A	806	6/6	0.89	0.23	40,40,40,40	0
4	MAN	B	700	11/12	0.91	0.13	22,23,24,24	0
2	NAG	B	500	14/15	0.92	0.11	16,17,18,18	0
2	NAG	A	500	14/15	0.94	0.08	13,13,15,16	0
6	HEM	A	344	43/43	0.98	0.08	8,9,10,12	0
6	HEM	B	344	43/43	0.98	0.08	8,10,12,14	0
5	CA	B	9002	1/1	1.00	0.11	11,11,11,11	0
5	CA	B	9003	1/1	1.00	0.06	8,8,8,8	0
5	CA	A	9001	1/1	1.00	0.09	10,10,10,10	0
5	CA	A	9004	1/1	1.00	0.05	9,9,9,9	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 A 344:

$2mF_o-DF_c$ (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.