



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 07:19 PM BST

PDB ID : 3EJ6  
Title : Neurospora Crassa Catalase-3 Crystal Structure  
Authors : Diaz, A.; Valdes, V.-J.; Rudino-Pinera, E.; Horjales, E.; Hansberg, W.  
Deposited on : 2008-09-17  
Resolution : 2.30 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](mailto: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 : 2.13.1  
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) : 2.13.1

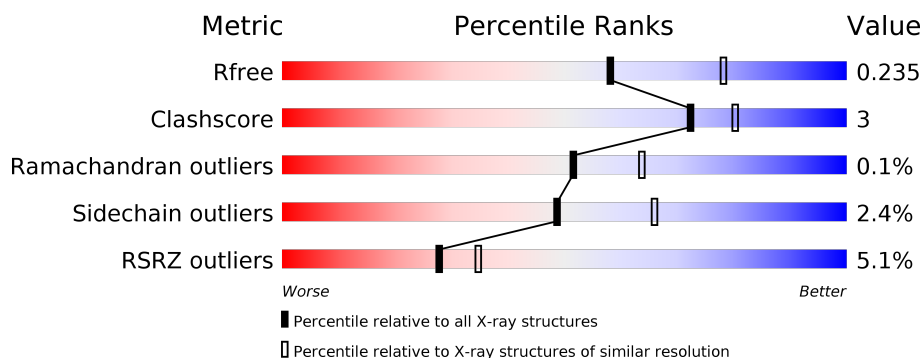
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	688	<div> <div>7%</div> <div> <div></div> <div>88%</div> <div>11%</div> </div> </div>
1	B	688	<div> <div>5%</div> <div> <div></div> <div>89%</div> <div>10%</div> </div> </div>
1	C	688	<div> <div>4%</div> <div> <div></div> <div>90%</div> <div>9%</div> </div> </div>
1	D	688	<div> <div>5%</div> <div> <div></div> <div>89%</div> <div>10%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	5002	-	-	-	X
2	NAG	B	5006	-	-	-	X
2	NAG	B	5007	-	-	-	X

## 2 Entry composition [i](#)

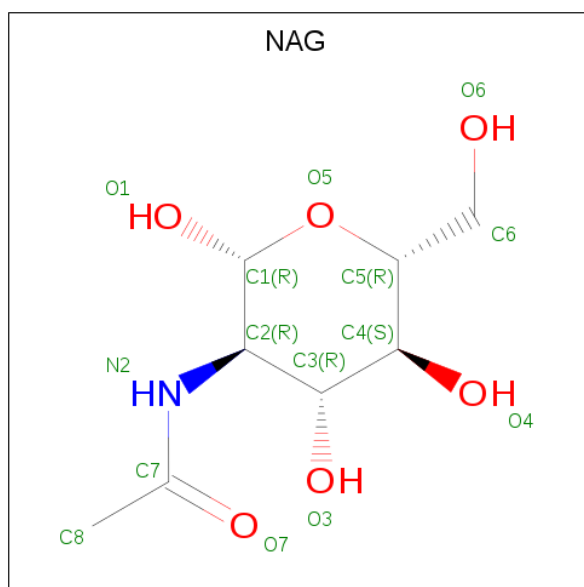
There are 4 unique types of molecules in this entry. The entry contains 23009 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Catalase-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	681	Total	C	N	O	S	47	0	0
			5340	3381	941	1012	6			
1	B	681	Total	C	N	O	S	72	0	0
			5340	3381	941	1012	6			
1	C	681	Total	C	N	O	S	83	0	0
			5340	3381	941	1012	6			
1	D	681	Total	C	N	O	S	64	0	0
			5340	3381	941	1012	6			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



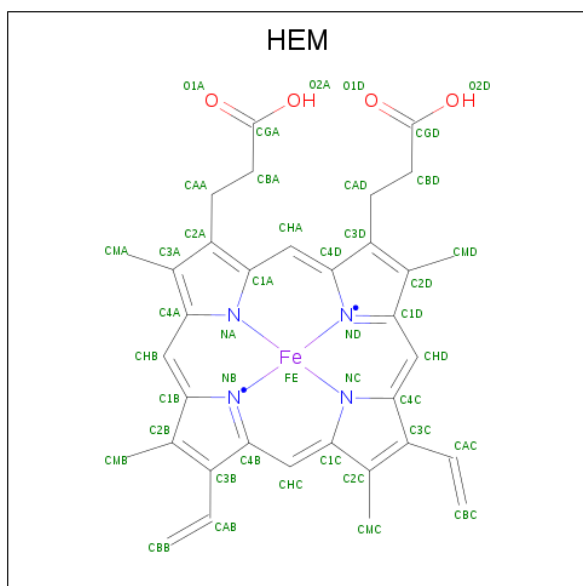
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

*Continued on next page...*

Continued from previous page...

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

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

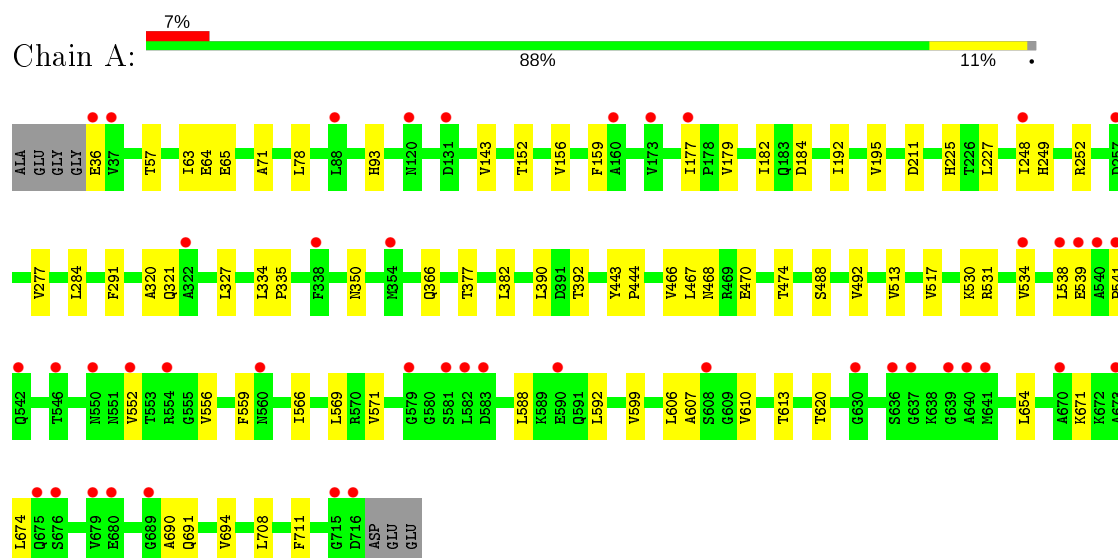
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	319	Total 319	O 319	0	0
4	B	336	Total 336	O 336	0	0
4	C	362	Total 362	O 362	0	0
4	D	348	Total 348	O 348	0	0

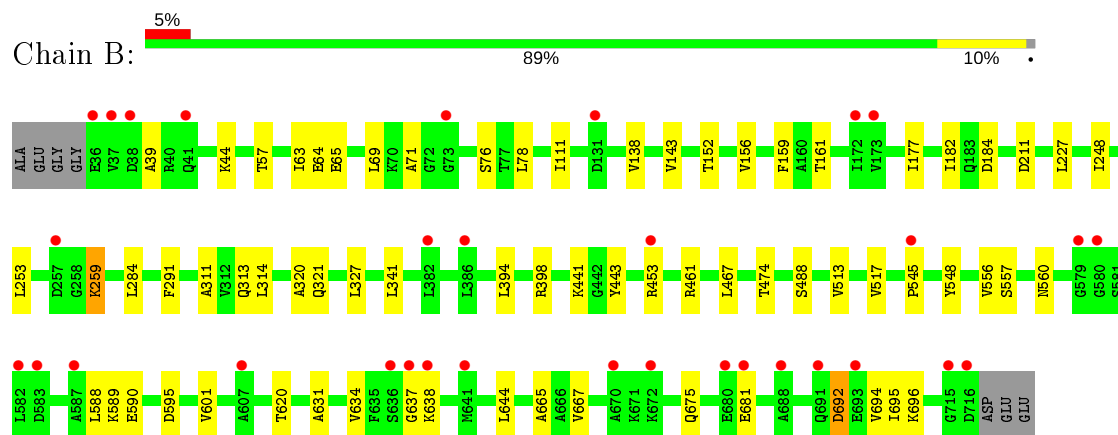
### 3 Residue-property plots

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.

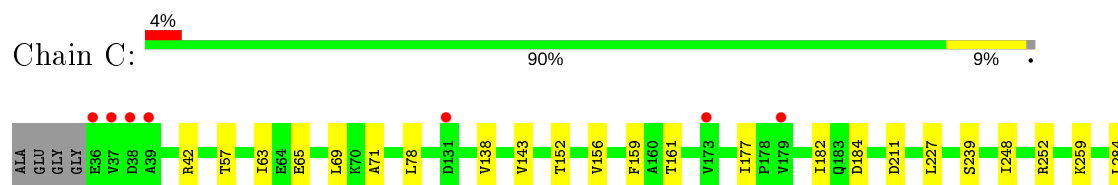
#### • Molecule 1: Catalase-3

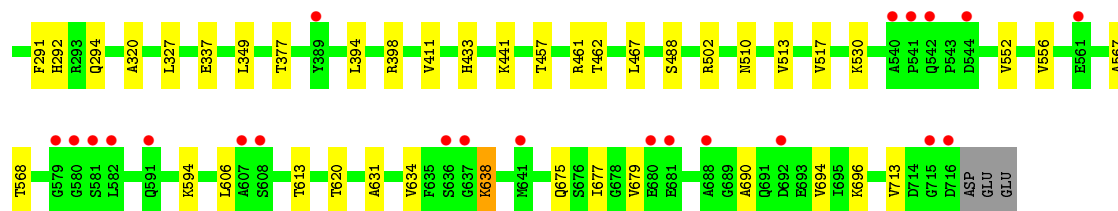


#### • Molecule 1: Catalase-3

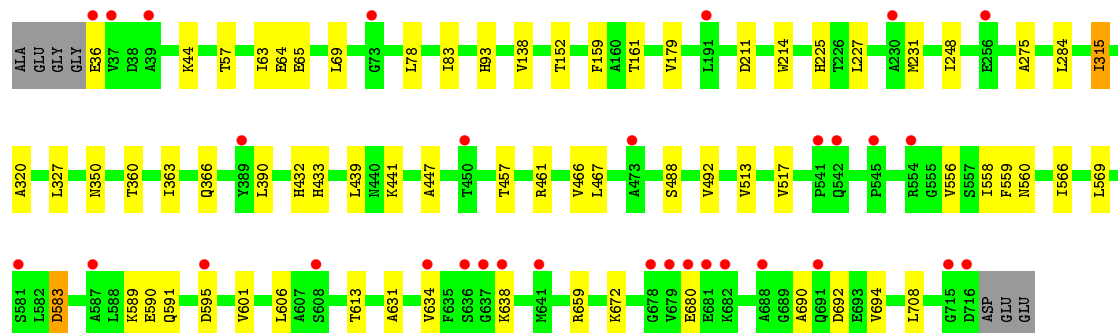
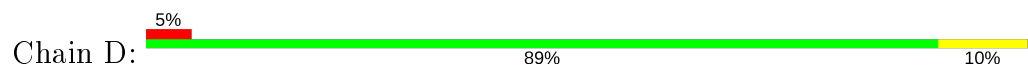


#### • Molecule 1: Catalase-3





● Molecule 1: Catalase-3





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.84Å 154.51Å 162.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.67 – 2.30 34.68 – 2.30	Depositor EDS
% Data completeness (in resolution range)	92.8 (34.67-2.30) 93.0 (34.68-2.30)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.50 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.193 , 0.242 0.235 , 0.235	Depositor DCC
$R_{free}$ test set	13611 reflections (9.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.9	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 34.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	23009	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, NAG

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	0.30	0/5473	0.45	0/7424
1	B	0.34	2/5473 (0.0%)	0.47	3/7424 (0.0%)
1	C	0.34	2/5473 (0.0%)	0.48	2/7424 (0.0%)
1	D	0.34	3/5473 (0.1%)	0.47	2/7424 (0.0%)
All	All	0.33	7/21892 (0.0%)	0.47	7/29696 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	680	GLU	CB-CG	5.82	1.63	1.52
1	C	259	LYS	CG-CD	-5.71	1.33	1.52
1	B	259	LYS	CB-CG	5.64	1.67	1.52
1	C	638	LYS	CA-CB	5.53	1.66	1.53
1	B	638	LYS	CA-CB	-5.52	1.41	1.53
1	D	590	GLU	CA-CB	5.28	1.65	1.53
1	D	44	LYS	CG-CD	-5.10	1.35	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	638	LYS	N-CA-CB	5.55	120.59	110.60
1	C	713	VAL	CA-CB-CG1	5.50	119.15	110.90
1	D	692	ASP	CB-CG-OD2	5.42	123.18	118.30
1	C	675	GLN	CB-CA-C	-5.42	99.56	110.40
1	B	692	ASP	N-CA-CB	-5.39	100.90	110.60
1	B	259	LYS	CA-CB-CG	-5.29	101.76	113.40
1	D	583	ASP	CA-CB-CG	-5.27	101.81	113.40

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	5340	0	5155	43	0
1	B	5340	0	5153	37	0
1	C	5340	0	5154	35	0
1	D	5340	0	5154	37	0
2	A	14	0	13	0	0
2	B	42	0	39	0	0
2	C	28	0	26	0	0
2	D	28	0	26	0	0
3	A	43	0	30	2	0
3	B	43	0	30	1	0
3	C	43	0	30	2	0
3	D	43	0	30	1	0
4	A	319	0	0	0	0
4	B	336	0	0	0	0
4	C	362	0	0	0	0
4	D	348	0	0	0	0
All	All	23009	0	20840	141	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 3.

All (141) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:ILE:HD12	3:C:4002:HEM:HMB1	1.64	0.79
1:A:654:LEU:HD21	1:A:674:LEU:HD23	1.65	0.78
1:B:248:ILE:HD12	3:B:4001:HEM:HMB1	1.66	0.76
1:A:248:ILE:HD12	3:A:4000:HEM:HMB1	1.66	0.76
1:C:71:ALA:HB2	1:C:78:LEU:HD21	1.72	0.72
1:A:467:LEU:HD22	1:D:78:LEU:HD11	1.73	0.70
1:C:152:THR:HG21	1:C:284:LEU:HD23	1.74	0.69
1:B:78:LEU:HD11	1:C:467:LEU:HD22	1.73	0.69
1:D:606:LEU:CD1	1:D:613:THR:HG23	2.24	0.68
1:B:467:LEU:HD22	1:C:78:LEU:HD11	1.74	0.67
1:D:152:THR:HG21	1:D:284:LEU:HD23	1.77	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:ALA:HB3	1:A:610:VAL:HG23	1.80	0.64
1:A:152:THR:HG21	1:A:284:LEU:HD23	1.81	0.62
1:A:320:ALA:HA	1:A:327:LEU:HD12	1.82	0.62
1:B:320:ALA:HA	1:B:327:LEU:HD12	1.84	0.60
1:A:571:VAL:HG11	1:A:592:LEU:HD21	1.84	0.59
1:B:71:ALA:HB2	1:B:78:LEU:HD21	1.84	0.58
1:A:531:ARG:O	1:A:534:VAL:HG12	2.03	0.58
1:C:606:LEU:CD1	1:C:613:THR:HG23	2.34	0.57
1:C:152:THR:HG21	1:C:284:LEU:CD2	2.33	0.57
1:B:138:VAL:HG22	1:B:161:THR:HG23	1.85	0.57
1:B:152:THR:HG21	1:B:284:LEU:HD23	1.86	0.57
1:B:57:THR:HG22	1:B:63:ILE:HD13	1.87	0.57
1:B:665:ALA:HB1	1:B:694:VAL:HG13	1.87	0.56
1:A:488:SER:HB2	1:A:556:VAL:HG21	1.90	0.54
1:C:320:ALA:HA	1:C:327:LEU:HD12	1.88	0.54
1:A:143:VAL:HG23	1:A:156:VAL:O	2.08	0.54
1:A:592:LEU:HD23	1:A:599:VAL:HG22	1.90	0.54
1:A:249:HIS:CD2	1:A:382:LEU:HD13	2.43	0.53
1:C:488:SER:HA	1:C:552:VAL:HG13	1.90	0.53
1:D:57:THR:CG2	1:D:63:ILE:HD13	2.39	0.53
1:D:152:THR:HG21	1:D:284:LEU:CD2	2.39	0.53
1:A:559:PHE:HB3	1:A:708:LEU:HD11	1.91	0.53
1:A:606:LEU:CD1	1:A:613:THR:HG23	2.39	0.52
1:D:138:VAL:HG22	1:D:161:THR:HG23	1.90	0.52
1:C:143:VAL:HG23	1:C:156:VAL:O	2.09	0.52
1:C:462:THR:HG22	1:D:466:VAL:HA	1.90	0.52
1:A:78:LEU:HD11	1:D:467:LEU:HD22	1.91	0.52
1:B:488:SER:HB2	1:B:556:VAL:HG21	1.92	0.52
1:D:320:ALA:HA	1:D:327:LEU:HD12	1.90	0.52
1:D:57:THR:HG22	1:D:63:ILE:HD13	1.92	0.52
1:A:57:THR:HG23	1:A:63:ILE:HD13	1.91	0.52
1:D:64:GLU:O	1:D:83:ILE:HG21	2.09	0.52
1:B:152:THR:HG21	1:B:284:LEU:CD2	2.40	0.51
1:B:57:THR:CG2	1:B:63:ILE:HD13	2.41	0.51
1:D:606:LEU:HD13	1:D:613:THR:HG23	1.92	0.51
1:B:667:VAL:HG22	1:B:694:VAL:HG21	1.93	0.51
1:B:284:LEU:HD21	1:B:291:PHE:CD2	2.46	0.50
1:A:492:VAL:HG11	1:A:708:LEU:HB3	1.93	0.50
1:A:57:THR:CG2	1:A:63:ILE:HD13	2.42	0.50
1:A:152:THR:HG21	1:A:284:LEU:CD2	2.42	0.50
1:A:592:LEU:HD23	1:A:599:VAL:CG2	2.42	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:VAL:HG23	1:B:156:VAL:O	2.12	0.49
1:C:42:ARG:HD2	1:C:411:VAL:HG12	1.95	0.49
1:D:366:GLN:HE22	1:D:390:LEU:HD13	1.78	0.49
1:A:71:ALA:HB2	1:A:78:LEU:HD21	1.93	0.49
1:D:513:VAL:O	1:D:517:VAL:HG23	2.13	0.49
1:A:284:LEU:HD21	1:A:291:PHE:CD2	2.48	0.48
1:A:179:VAL:HG11	1:A:225:HIS:CE1	2.49	0.47
1:A:321:GLN:NE2	1:A:474:THR:HG21	2.29	0.47
1:A:513:VAL:O	1:A:517:VAL:HG23	2.14	0.47
1:A:690:ALA:O	1:A:694:VAL:HG23	2.14	0.47
1:B:513:VAL:O	1:B:517:VAL:HG23	2.15	0.47
1:D:492:VAL:HG11	1:D:708:LEU:HB3	1.97	0.47
1:B:39:ALA:HB2	1:B:111:ILE:HD11	1.97	0.47
1:D:488:SER:HB2	1:D:556:VAL:HG21	1.97	0.47
1:C:631:ALA:O	1:C:634:VAL:HG22	2.15	0.46
1:D:566:ILE:HB	1:D:569:LEU:HD12	1.97	0.46
1:D:315:ILE:HD13	1:D:315:ILE:N	2.31	0.46
1:A:588:LEU:HD13	1:A:691:GLN:HG3	1.97	0.46
1:C:252:ARG:NH1	1:C:377:THR:HG22	2.31	0.46
1:C:69:LEU:HG	1:C:78:LEU:HD12	1.97	0.46
1:B:321:GLN:NE2	1:B:474:THR:HG21	2.30	0.46
1:B:69:LEU:HG	1:B:78:LEU:HD12	1.97	0.46
1:D:69:LEU:HG	1:D:78:LEU:HD12	1.97	0.46
1:A:607:ALA:HB3	1:A:610:VAL:CG2	2.45	0.46
1:B:156:VAL:HG22	1:B:177:ILE:HD12	1.97	0.46
1:B:589:LYS:HD2	1:B:601:VAL:HG23	1.98	0.46
1:A:466:VAL:HG23	1:B:461:ARG:O	2.16	0.46
1:D:360:THR:O	1:D:363:ILE:HG22	2.15	0.45
1:C:284:LEU:HD21	1:C:291:PHE:CD2	2.52	0.45
1:A:392:THR:HG21	3:A:4000:HEM:HBD1	1.99	0.45
1:A:566:ILE:HB	1:A:569:LEU:HD12	1.98	0.45
1:C:57:THR:CG2	1:C:63:ILE:HD13	2.47	0.45
1:D:492:VAL:HG11	1:D:708:LEU:HD22	1.98	0.45
1:D:214:TRP:CZ2	1:D:231:MET:HE3	2.51	0.45
1:B:39:ALA:HB2	1:B:111:ILE:CD1	2.48	0.44
1:C:57:THR:HG22	1:C:63:ILE:HD13	1.99	0.44
1:D:248:ILE:HD12	3:D:4003:HEM:HBB2	1.99	0.44
1:D:566:ILE:HD11	1:D:595:ASP:OD1	2.17	0.44
1:C:248:ILE:CD1	3:C:4002:HEM:HMB1	2.43	0.44
1:A:366:GLN:HE22	1:A:390:LEU:HD13	1.83	0.44
1:B:588:LEU:HD12	1:B:695:ILE:HD11	1.98	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:510:ASN:OD1	1:C:513:VAL:HG23	2.17	0.43
1:D:558:ILE:C	1:D:560:ASN:H	2.20	0.43
1:A:93:HIS:CE1	1:C:394:LEU:HD13	2.53	0.43
1:D:432:HIS:CE1	1:D:439:LEU:HB3	2.53	0.43
1:D:690:ALA:O	1:D:694:VAL:HG23	2.19	0.43
1:B:557:SER:HB3	1:B:560:ASN:HB2	1.99	0.43
1:A:192:ILE:HA	1:A:195:VAL:HG22	2.00	0.43
1:C:138:VAL:HG22	1:C:161:THR:HG23	1.99	0.43
1:B:441:LYS:O	1:B:443:TYR:CD1	2.71	0.43
1:C:567:ALA:C	1:C:568:THR:HG23	2.39	0.43
1:A:284:LEU:HD13	1:A:620:THR:HB	2.01	0.43
1:D:63:ILE:HD12	1:D:83:ILE:HG23	2.00	0.43
1:C:138:VAL:CG2	1:C:349:LEU:HD21	2.48	0.43
1:B:644:LEU:HD23	1:C:502:ARG:NH1	2.34	0.43
1:A:182:ILE:HD12	1:A:184:ASP:O	2.18	0.42
1:B:631:ALA:O	1:B:634:VAL:HG22	2.19	0.42
1:C:457:THR:HG23	1:C:461:ARG:HH21	1.84	0.42
1:A:443:TYR:HA	1:A:444:PRO:C	2.40	0.42
1:D:589:LYS:HD2	1:D:601:VAL:HG23	2.01	0.42
1:B:182:ILE:HD12	1:B:184:ASP:O	2.19	0.42
1:D:631:ALA:O	1:D:634:VAL:HG22	2.20	0.42
1:B:394:LEU:HD13	1:D:93:HIS:CE1	2.55	0.42
1:A:277:VAL:HG11	1:A:711:PHE:CZ	2.55	0.42
1:B:313:GLN:HG3	1:B:341:LEU:HD23	2.02	0.41
1:D:275:ALA:HB3	1:D:559:PHE:CZ	2.56	0.41
1:C:156:VAL:HG22	1:C:177:ILE:HD12	2.02	0.41
1:B:64:GLU:HG2	1:D:447:ALA:O	2.21	0.41
1:B:253:LEU:HD12	1:B:314:LEU:HD21	2.02	0.41
1:A:78:LEU:HD22	1:B:76:SER:HB2	2.02	0.41
1:C:284:LEU:HD13	1:C:620:THR:HB	2.02	0.41
1:D:179:VAL:HG21	1:D:225:HIS:ND1	2.36	0.41
1:C:182:ILE:HD12	1:C:184:ASP:O	2.21	0.41
1:C:488:SER:HB2	1:C:556:VAL:HG21	2.02	0.41
1:C:677:ILE:HG13	1:C:679:VAL:HG23	2.03	0.41
1:B:284:LEU:HD13	1:B:620:THR:HB	2.03	0.41
1:C:239:SER:HA	1:C:292:HIS:CD2	2.56	0.41
1:C:513:VAL:O	1:C:517:VAL:HG23	2.21	0.41
1:D:492:VAL:HG21	1:D:708:LEU:HB3	2.03	0.41
1:B:311:ALA:HB1	1:B:341:LEU:HB3	2.03	0.40
1:B:545:PRO:HA	1:B:548:TYR:CD1	2.56	0.40
1:C:138:VAL:HG23	1:C:349:LEU:HD21	2.04	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:SER:HA	1:A:552:VAL:HG13	2.03	0.40
1:D:457:THR:HG23	1:D:461:ARG:HH21	1.85	0.40
1:A:156:VAL:HG22	1:A:177:ILE:HD12	2.04	0.40
1:A:252:ARG:NH1	1:A:377:THR:HG22	2.36	0.40
1:C:690:ALA:O	1:C:694:VAL:HG23	2.22	0.40
1:D:214:TRP:HZ2	1:D:231:MET:HE3	1.87	0.40
1:A:334:LEU:HD12	1:A:335:PRO:HD2	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	679/688 (99%)	652 (96%)	26 (4%)	1 (0%)	51	64
1	B	679/688 (99%)	657 (97%)	21 (3%)	1 (0%)	51	64
1	C	679/688 (99%)	659 (97%)	20 (3%)	0	100	100
1	D	679/688 (99%)	645 (95%)	34 (5%)	0	100	100
All	All	2716/2752 (99%)	2613 (96%)	101 (4%)	2 (0%)	51	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	637	GLY
1	A	541	PRO

### 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	559/563 (99%)	546 (98%)	13 (2%)	50	67
1	B	559/563 (99%)	545 (98%)	14 (2%)	47	65
1	C	559/563 (99%)	546 (98%)	13 (2%)	50	67
1	D	559/563 (99%)	545 (98%)	14 (2%)	47	65
All	All	2236/2252 (99%)	2182 (98%)	54 (2%)	49	66

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	GLU
1	A	64	GLU
1	A	65	GLU
1	A	159	PHE
1	A	211	ASP
1	A	227	LEU
1	A	350	ASN
1	A	468	ASN
1	A	470	GLU
1	A	530	LYS
1	A	538	LEU
1	A	539	GLU
1	A	671	LYS
1	B	44	LYS
1	B	65	GLU
1	B	159	PHE
1	B	211	ASP
1	B	227	LEU
1	B	259	LYS
1	B	398	ARG
1	B	453	ARG
1	B	590	GLU
1	B	595	ASP
1	B	675	GLN
1	B	681	GLU
1	B	692	ASP
1	B	696	LYS
1	C	65	GLU
1	C	159	PHE
1	C	211	ASP

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	227	LEU
1	C	294	GLN
1	C	337	GLU
1	C	398	ARG
1	C	433	HIS
1	C	441	LYS
1	C	530	LYS
1	C	594	LYS
1	C	638	LYS
1	C	696	LYS
1	D	36	GLU
1	D	65	GLU
1	D	159	PHE
1	D	211	ASP
1	D	227	LEU
1	D	315	ILE
1	D	350	ASN
1	D	433	HIS
1	D	441	LYS
1	D	583	ASP
1	D	591	GLN
1	D	638	LYS
1	D	659	ARG
1	D	672	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	53	GLN
1	A	89	GLN
1	A	133	GLN
1	A	321	GLN
1	A	350	ASN
1	A	362	GLN
1	A	366	GLN
1	A	393	GLN
1	A	417	ASN
1	A	449	GLN
1	A	510	ASN
1	A	512	GLN
1	A	516	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	612	GLN
1	B	51	ASN
1	B	53	GLN
1	B	89	GLN
1	B	304	ASN
1	B	321	GLN
1	B	366	GLN
1	B	393	GLN
1	B	417	ASN
1	B	449	GLN
1	B	512	GLN
1	B	516	ASN
1	B	550	ASN
1	B	691	GLN
1	C	51	ASN
1	C	53	GLN
1	C	66	GLN
1	C	89	GLN
1	C	362	GLN
1	C	366	GLN
1	C	449	GLN
1	C	512	GLN
1	C	516	ASN
1	C	612	GLN
1	D	51	ASN
1	D	53	GLN
1	D	89	GLN
1	D	133	GLN
1	D	294	GLN
1	D	342	GLN
1	D	350	ASN
1	D	366	GLN
1	D	417	ASN
1	D	449	GLN
1	D	512	GLN
1	D	516	ASN
1	D	520	GLN
1	D	550	ASN
1	D	612	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

12 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$
2	NAG	B	5005	1	14,14,15	0.56	0	17,19,21	0.82	0
3	HEM	A	4000	1,4	27,50,50	2.18	5 (18%)	17,82,82	1.51	3 (17%)
2	NAG	C	5008	1	14,14,15	0.54	0	17,19,21	0.75	0
2	NAG	B	5006	1	14,14,15	0.51	0	17,19,21	0.75	0
2	NAG	A	5002	1	14,14,15	0.53	0	17,19,21	0.61	0
3	HEM	B	4001	1	27,50,50	2.17	5 (18%)	17,82,82	1.45	3 (17%)
2	NAG	C	5009	1	14,14,15	0.61	0	17,19,21	0.72	0
3	HEM	D	4003	1	27,50,50	2.16	5 (18%)	17,82,82	1.47	2 (11%)
2	NAG	B	5007	1	14,14,15	0.42	0	17,19,21	1.32	2 (11%)
3	HEM	C	4002	1	27,50,50	2.17	5 (18%)	17,82,82	1.49	3 (17%)
2	NAG	D	5014	1	14,14,15	0.49	0	17,19,21	0.86	0
2	NAG	D	5013	1	14,14,15	0.59	0	17,19,21	0.66	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	NAG	B	5005	1	-	1/6/23/26	0/1/1/1
3	HEM	A	4000	1,4	-	0/6/54/54	-
2	NAG	C	5008	1	-	1/6/23/26	0/1/1/1
2	NAG	B	5006	1	-	3/6/23/26	0/1/1/1
2	NAG	A	5002	1	-	4/6/23/26	0/1/1/1
3	HEM	B	4001	1	-	0/6/54/54	-
2	NAG	C	5009	1	-	0/6/23/26	0/1/1/1
3	HEM	D	4003	1	-	0/6/54/54	-
2	NAG	B	5007	1	-	0/6/23/26	0/1/1/1
3	HEM	C	4002	1	-	0/6/54/54	-
2	NAG	D	5014	1	-	4/6/23/26	0/1/1/1
2	NAG	D	5013	1	-	0/6/23/26	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	4001	HEM	C3D-C2D	5.43	1.53	1.37
3	D	4003	HEM	C3D-C2D	5.41	1.53	1.37
3	A	4000	HEM	C3D-C2D	5.40	1.53	1.37
3	C	4002	HEM	C3D-C2D	5.40	1.53	1.37
3	A	4000	HEM	C3B-C2B	-4.74	1.33	1.40
3	C	4002	HEM	C3B-C2B	-4.70	1.33	1.40
3	D	4003	HEM	C3C-C2C	-4.69	1.33	1.40
3	B	4001	HEM	C3C-C2C	-4.66	1.33	1.40
3	A	4000	HEM	C3C-C2C	-4.63	1.33	1.40
3	C	4002	HEM	C3C-C2C	-4.59	1.34	1.40
3	B	4001	HEM	C3B-C2B	-4.49	1.34	1.40
3	D	4003	HEM	C3B-C2B	-4.42	1.34	1.40
3	B	4001	HEM	C3B-CAB	3.51	1.55	1.47
3	C	4002	HEM	C3C-CAC	3.51	1.55	1.47
3	B	4001	HEM	C3C-CAC	3.47	1.54	1.47
3	A	4000	HEM	C3C-CAC	3.46	1.54	1.47
3	D	4003	HEM	C3C-CAC	3.43	1.54	1.47
3	C	4002	HEM	C3B-CAB	3.38	1.54	1.47
3	D	4003	HEM	C3B-CAB	3.37	1.54	1.47
3	A	4000	HEM	C3B-CAB	3.36	1.54	1.47

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5007	NAG	C1-O5-C5	3.87	117.43	112.19

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4000	HEM	CBD-CAD-C3D	-2.83	107.27	112.48
3	C	4002	HEM	CBD-CAD-C3D	-2.82	107.29	112.48
2	B	5007	NAG	O5-C5-C6	2.80	111.59	107.20
3	D	4003	HEM	C1D-C2D-C3D	-2.71	105.11	107.00
3	A	4000	HEM	C1D-C2D-C3D	-2.61	105.18	107.00
3	C	4002	HEM	C1D-C2D-C3D	-2.51	105.25	107.00
3	B	4001	HEM	CBD-CAD-C3D	-2.51	107.85	112.48
3	D	4003	HEM	CBD-CAD-C3D	-2.49	107.88	112.48
3	B	4001	HEM	C1D-C2D-C3D	-2.41	105.32	107.00
3	C	4002	HEM	CBA-CAA-C2A	-2.12	108.58	112.49
3	B	4001	HEM	CAA-CBA-CGA	-2.06	109.22	112.67
3	A	4000	HEM	CBA-CAA-C2A	-2.01	108.79	112.49

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5002	NAG	C8-C7-N2-C2
2	A	5002	NAG	O7-C7-N2-C2
2	A	5002	NAG	O5-C5-C6-O6
2	D	5014	NAG	O5-C5-C6-O6
2	A	5002	NAG	C4-C5-C6-O6
2	B	5006	NAG	C8-C7-N2-C2
2	B	5006	NAG	O7-C7-N2-C2
2	D	5014	NAG	C4-C5-C6-O6
2	B	5006	NAG	C1-C2-N2-C7
2	D	5014	NAG	C1-C2-N2-C7
2	B	5005	NAG	C3-C2-N2-C7
2	D	5014	NAG	C3-C2-N2-C7
2	C	5008	NAG	C8-C7-N2-C2

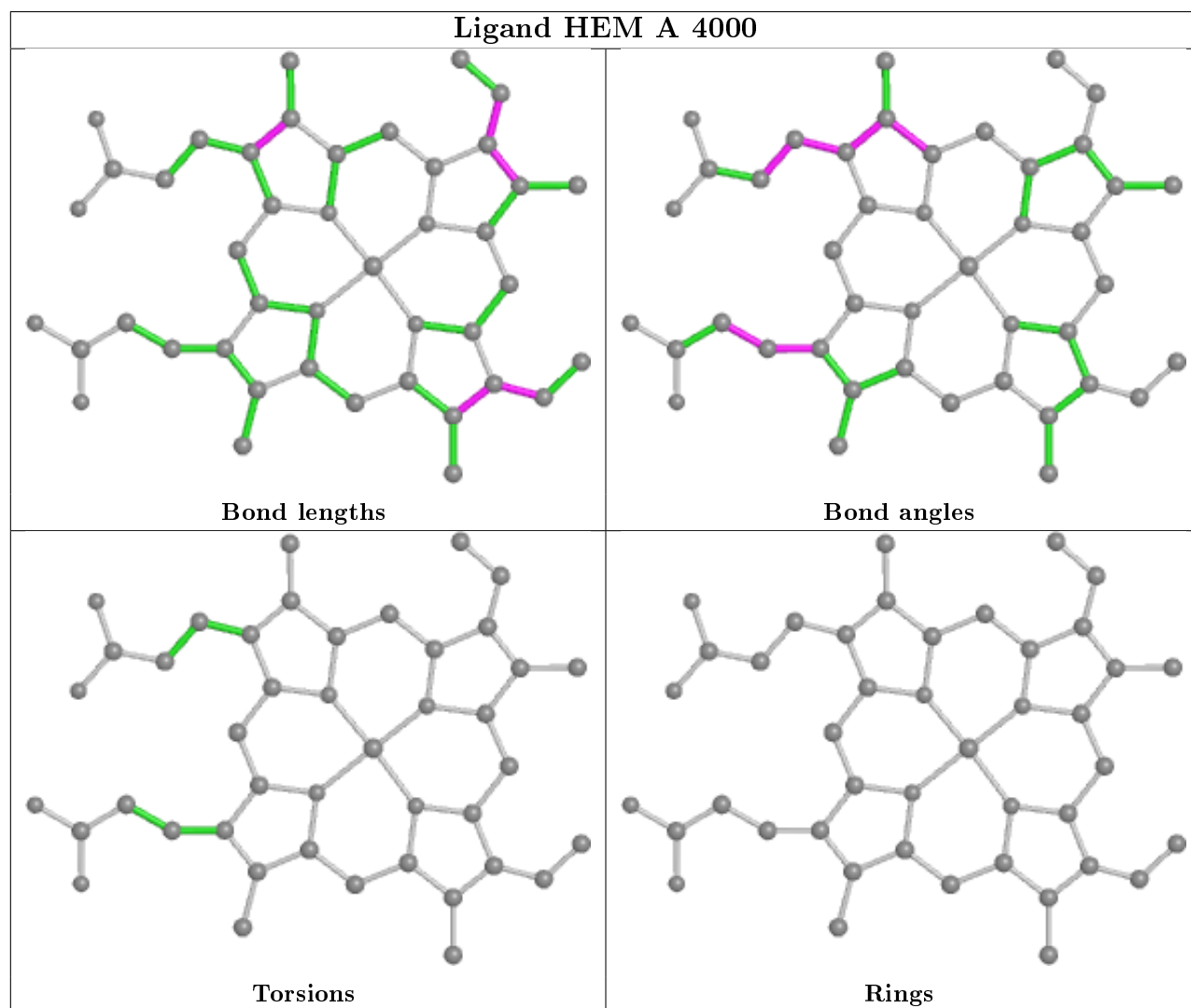
There are no ring outliers.

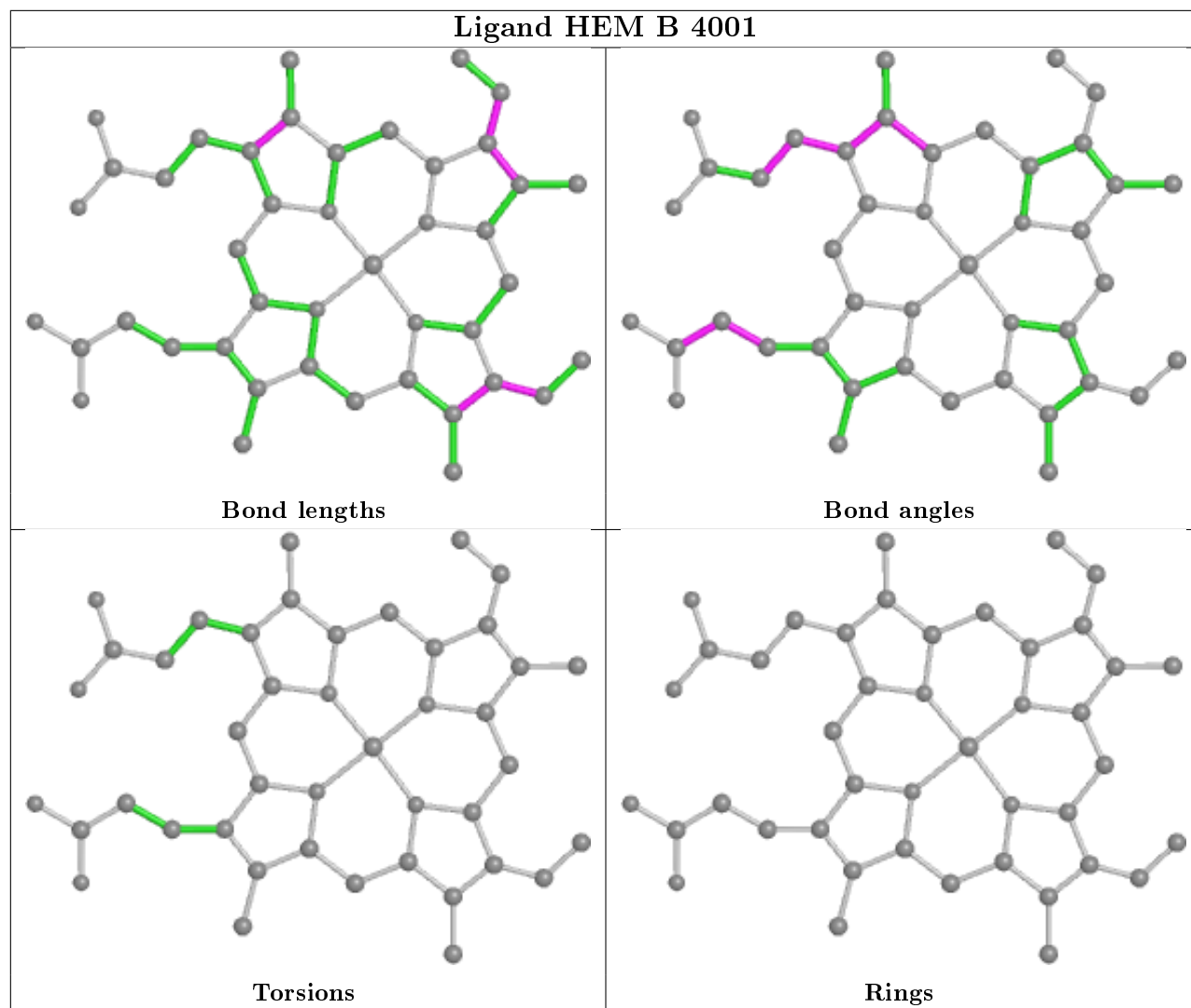
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	4000	HEM	2	0
3	B	4001	HEM	1	0
3	D	4003	HEM	1	0
3	C	4002	HEM	2	0

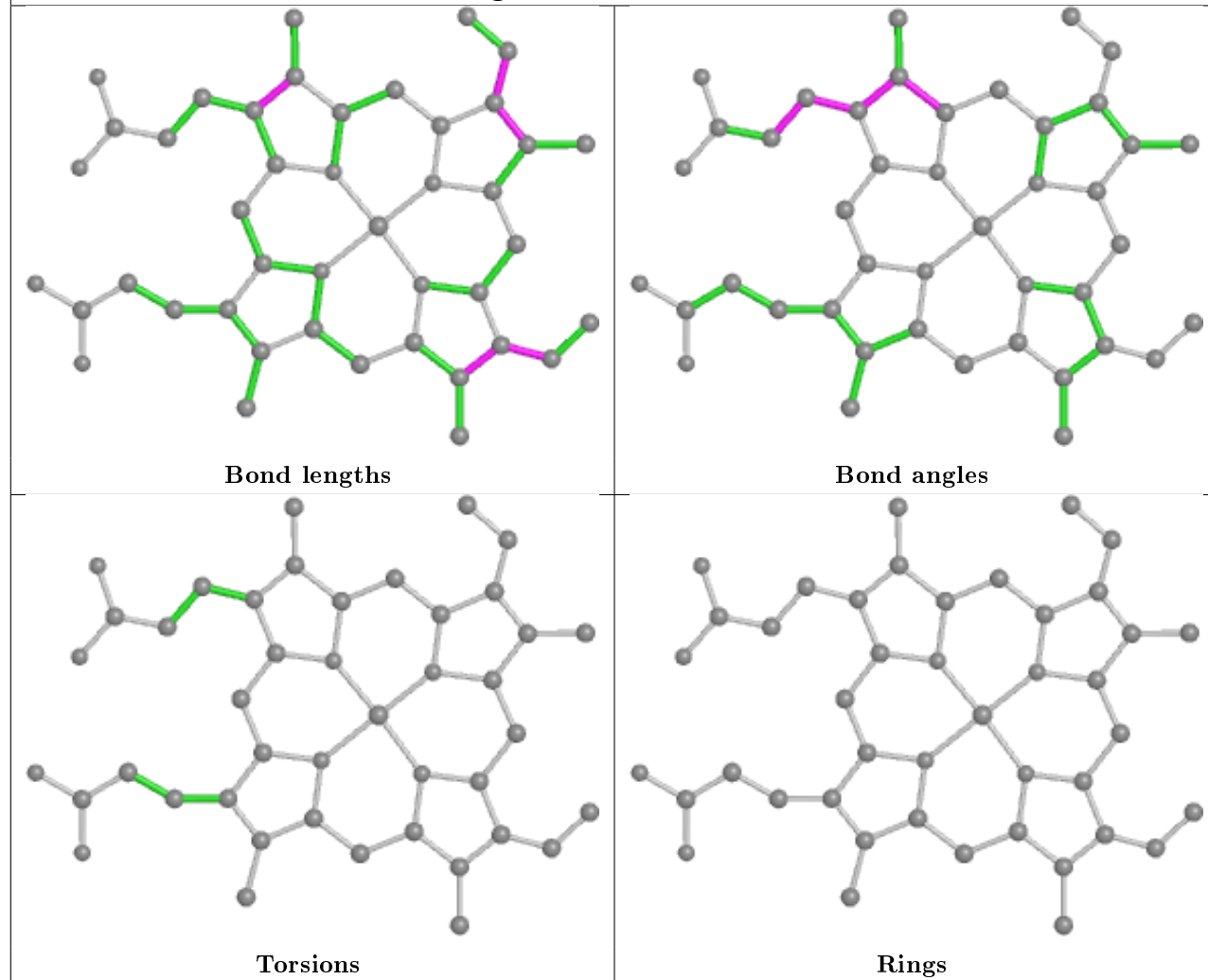
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

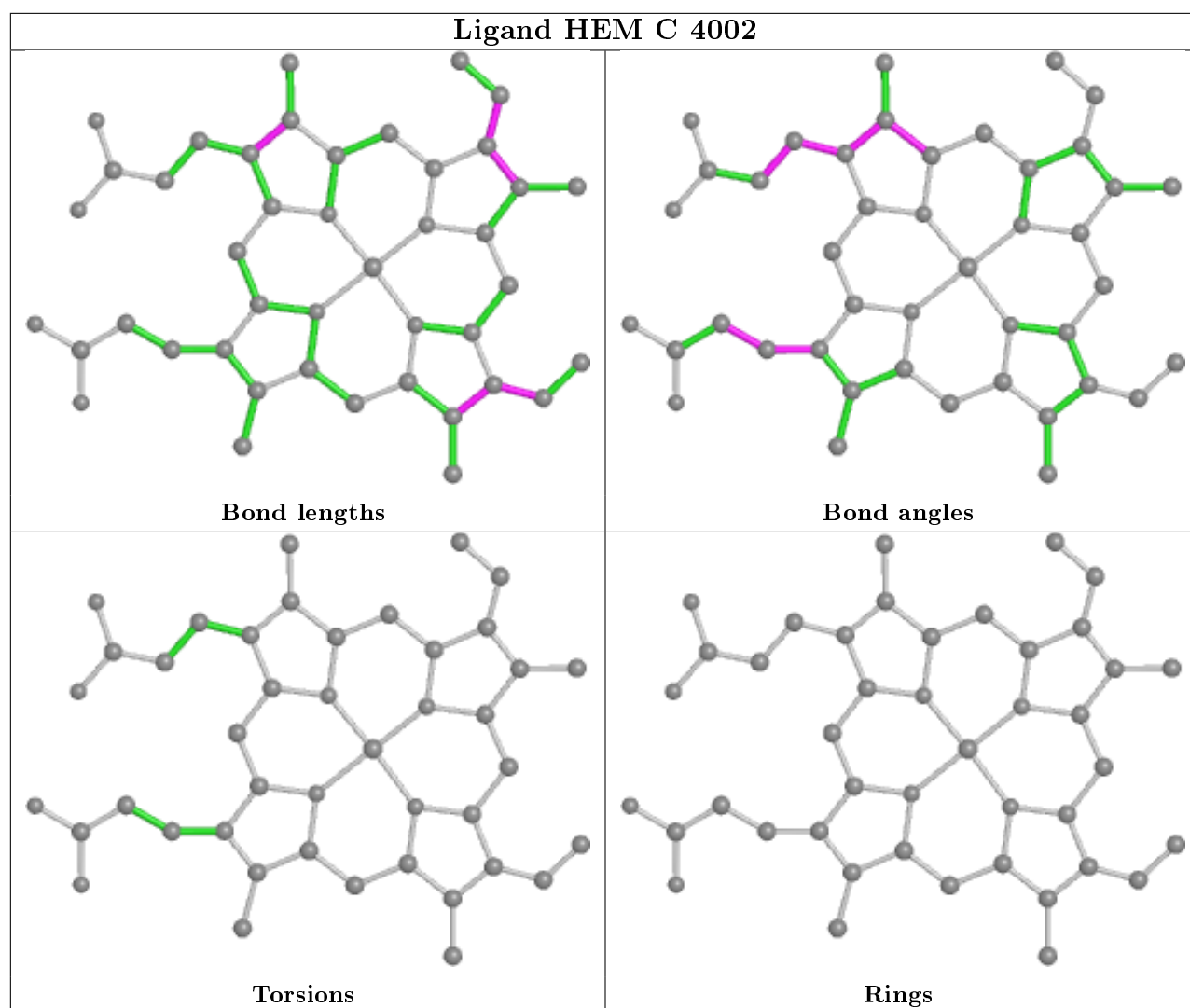




## Ligand HEM D 4003







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	681/688 (98%)	0.59	45 (6%)	18	23	23, 23, 23, 24	13 (1%)
1	B	681/688 (98%)	0.46	32 (4%)	31	38	23, 23, 23, 24	20 (2%)
1	C	681/688 (98%)	0.41	29 (4%)	35	42	23, 23, 23, 24	22 (3%)
1	D	681/688 (98%)	0.45	32 (4%)	31	38	23, 23, 23, 25	16 (2%)
All	All	2724/2752 (98%)	0.48	138 (5%)	28	35	23, 23, 23, 25	71 (2%)

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	37	VAL	8.3
1	D	37	VAL	8.3
1	B	37	VAL	8.1
1	A	36	GLU	7.9
1	C	36	GLU	7.8
1	B	36	GLU	7.7
1	A	541	PRO	7.6
1	D	716	ASP	7.5
1	A	37	VAL	7.3
1	D	36	GLU	6.9
1	B	715	GLY	6.4
1	B	680	GLU	6.2
1	C	715	GLY	5.9
1	A	716	ASP	5.8
1	C	716	ASP	5.7
1	B	716	ASP	5.5
1	A	540	ALA	4.8
1	C	540	ALA	4.6
1	A	641	MET	4.4
1	D	715	GLY	4.3
1	C	641	MET	4.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	579	GLY	4.1
1	D	682	LYS	4.1
1	D	641	MET	4.1
1	B	579	GLY	3.9
1	A	608	SER	3.9
1	A	552	VAL	3.8
1	A	675	GLN	3.7
1	A	542	GLN	3.7
1	D	680	GLU	3.6
1	C	579	GLY	3.6
1	B	636	SER	3.5
1	D	681	GLU	3.5
1	D	636	SER	3.4
1	C	542	GLN	3.4
1	D	638	LYS	3.4
1	B	587	ALA	3.4
1	B	688	ALA	3.3
1	A	582	LEU	3.2
1	C	580	GLY	3.2
1	A	715	GLY	3.1
1	A	554	ARG	3.0
1	C	173	VAL	3.0
1	B	453	ARG	3.0
1	B	641	MET	2.9
1	A	322	ALA	2.9
1	C	681	GLU	2.9
1	A	257	ASP	2.9
1	B	681	GLU	2.9
1	A	636	SER	2.9
1	A	680	GLU	2.9
1	D	39	ALA	2.9
1	D	581	SER	2.8
1	A	637	GLY	2.8
1	B	257	ASP	2.8
1	D	595	ASP	2.8
1	A	177	ILE	2.8
1	A	539	GLU	2.8
1	D	637	GLY	2.8
1	A	673	ALA	2.7
1	A	639	GLY	2.7
1	B	386	LEU	2.7
1	B	637	GLY	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	38	ASP	2.7
1	C	38	ASP	2.7
1	A	88	LEU	2.6
1	A	583	ASP	2.6
1	A	679	VAL	2.6
1	A	630	GLY	2.6
1	D	542	GLN	2.6
1	B	172	ILE	2.6
1	D	554	ARG	2.5
1	D	678	GLY	2.5
1	C	541	PRO	2.5
1	B	41	GLN	2.5
1	D	230	ALA	2.5
1	A	120	ASN	2.5
1	B	693	GLU	2.4
1	D	688	ALA	2.4
1	B	580	GLY	2.4
1	A	676	SER	2.4
1	A	354	MET	2.4
1	C	688	ALA	2.4
1	A	248	ILE	2.4
1	C	39	ALA	2.4
1	A	590	GLU	2.4
1	A	160	ALA	2.3
1	A	670	ALA	2.3
1	D	545	PRO	2.3
1	C	591	GLN	2.3
1	B	638	LYS	2.3
1	B	672	LYS	2.3
1	B	691	GLN	2.3
1	B	173	VAL	2.3
1	C	179	VAL	2.3
1	D	691	GLN	2.3
1	A	581	SER	2.3
1	A	173	VAL	2.3
1	C	131	ASP	2.3
1	A	131	ASP	2.3
1	D	541	PRO	2.3
1	D	608	SER	2.3
1	C	637	GLY	2.2
1	D	679	VAL	2.2
1	A	560	ASN	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	583	ASP	2.2
1	C	692	ASP	2.2
1	B	607	ALA	2.2
1	C	607	ALA	2.2
1	D	450	THR	2.2
1	A	538	LEU	2.2
1	B	582	LEU	2.2
1	C	582	LEU	2.2
1	B	545	PRO	2.2
1	D	389	TYR	2.1
1	B	73	GLY	2.1
1	C	680	GLU	2.1
1	D	634	VAL	2.1
1	C	581	SER	2.1
1	C	608	SER	2.1
1	A	338	PHE	2.1
1	C	544	ASP	2.1
1	A	689	GLY	2.1
1	B	131	ASP	2.1
1	D	473	ALA	2.1
1	B	670	ALA	2.1
1	D	587	ALA	2.1
1	C	636	SER	2.1
1	D	73	GLY	2.1
1	D	191	LEU	2.1
1	B	382	LEU	2.0
1	A	640	ALA	2.0
1	D	256	GLU	2.0
1	C	389	TYR	2.0
1	A	546	THR	2.0
1	A	534	VAL	2.0
1	A	550	ASN	2.0
1	C	561	GLU	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

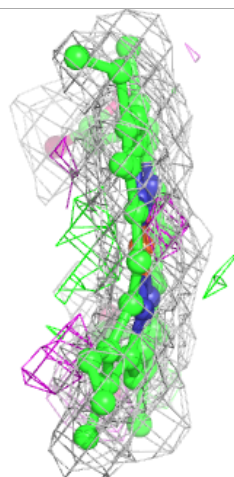
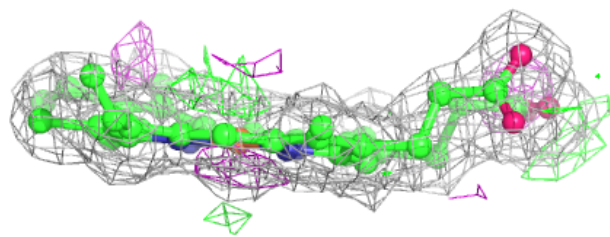
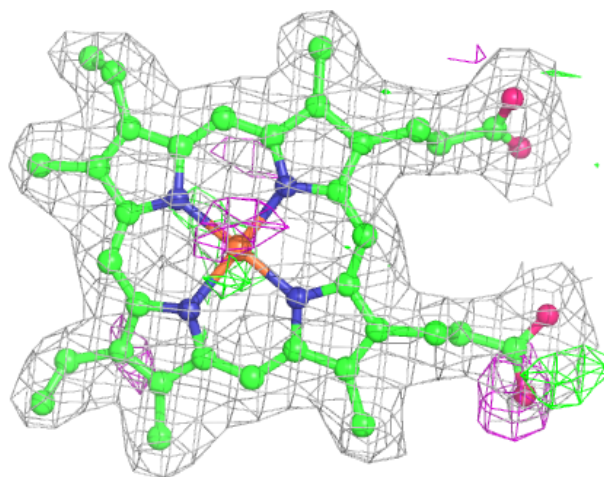
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	B	5007	14/15	0.48	0.47	24,24,24,24	0
2	NAG	A	5002	14/15	0.67	0.48	23,24,24,24	0
2	NAG	D	5014	14/15	0.67	0.32	23,23,23,23	0
2	NAG	C	5009	14/15	0.70	0.39	24,24,24,24	0
2	NAG	D	5013	14/15	0.71	0.37	24,24,25,25	0
2	NAG	B	5006	14/15	0.76	0.40	23,23,23,23	0
2	NAG	C	5008	14/15	0.78	0.24	23,23,23,23	0
2	NAG	B	5005	14/15	0.80	0.41	23,24,24,24	0
3	HEM	D	4003	43/43	0.92	0.20	22,22,22,22	0
3	HEM	A	4000	43/43	0.92	0.14	22,22,22,22	0
3	HEM	B	4001	43/43	0.94	0.16	22,22,22,23	0
3	HEM	C	4002	43/43	0.94	0.19	22,22,23,23	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.

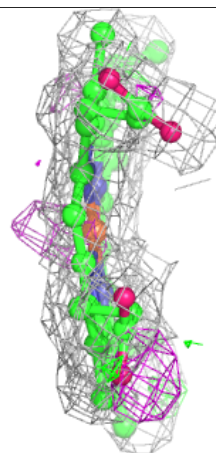
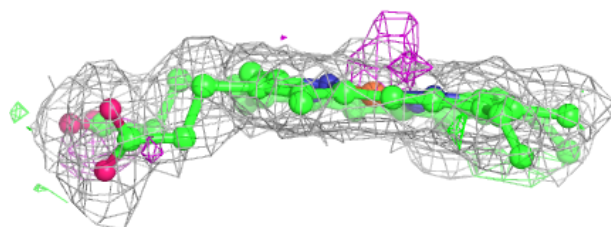
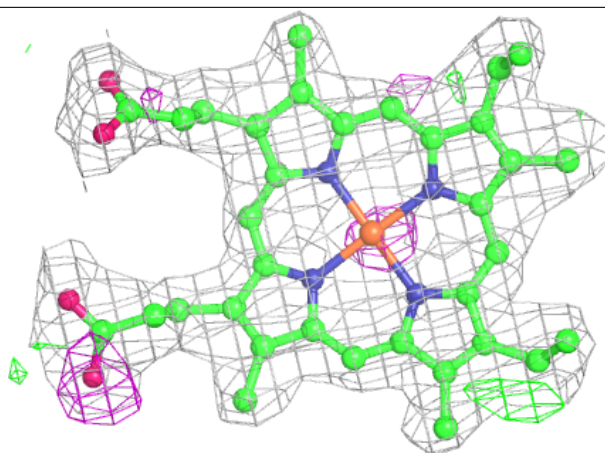
**Electron density around HEM D 4003:**

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



**Electron density around HEM A 4000:**

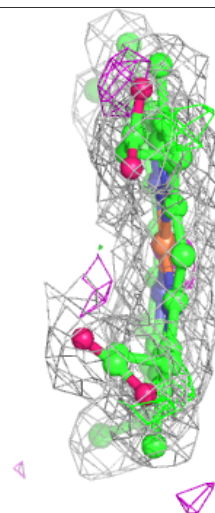
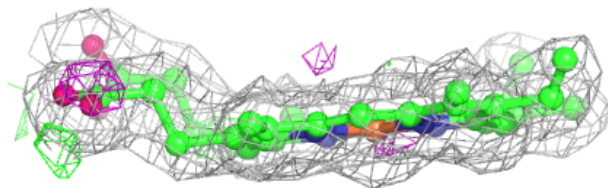
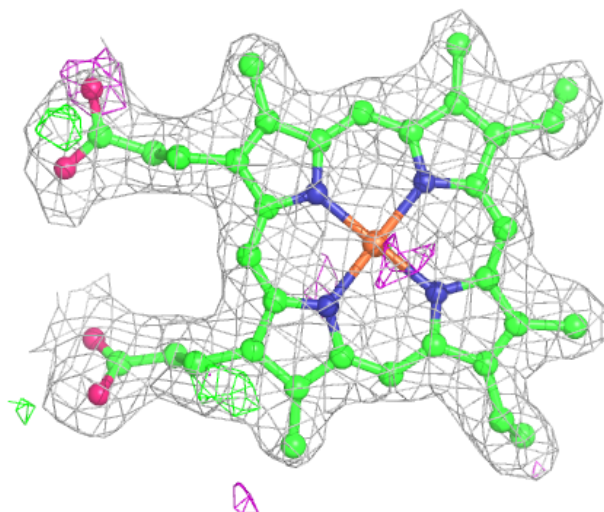
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





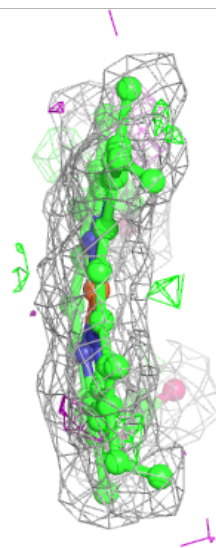
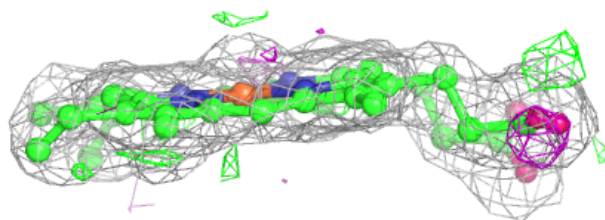
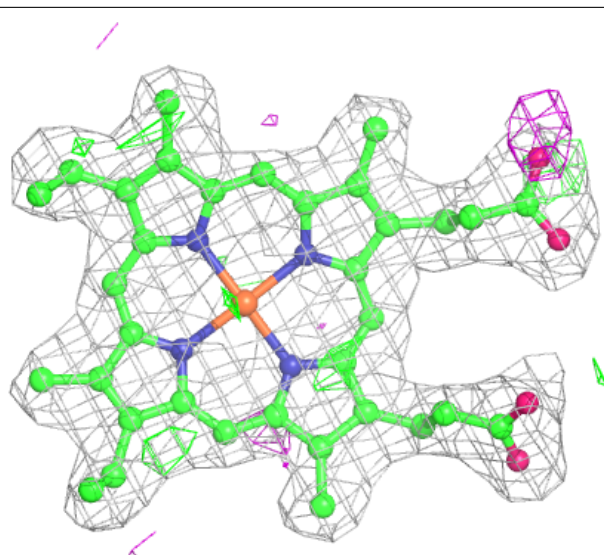
**Electron density around HEM B 4001:**

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



**Electron density around HEM C 4002:**

$2mF_o-DF_c$  (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.