



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 13, 2023 – 07:41 pm GMT

PDB ID : 4AJ9  
Title : Catalase 3 from Neurospora crassa  
Authors : Zarate-Romero, A.; Rudino-Pinera, E.  
Deposited on : 2012-02-16  
Resolution : 1.85 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, 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

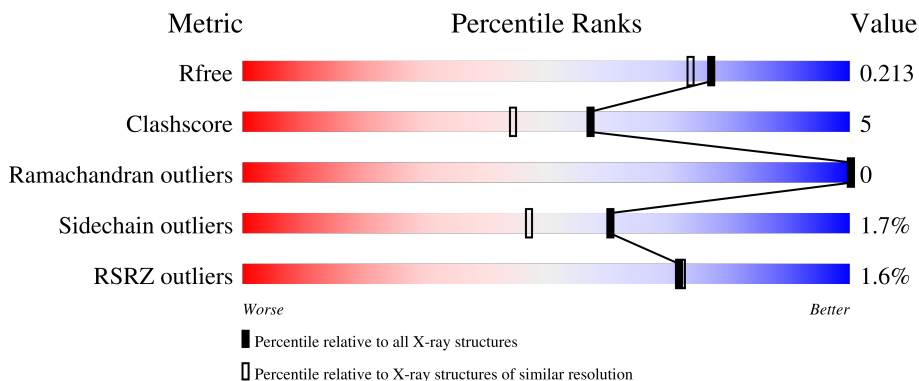
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.85 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	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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  $\geq 3$ , 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	682	2% 88% 11% ..
1	B	682	2% 88% 11% .
1	C	682	2% 90% 10%
1	D	682	2% 90% 9% ..

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 24066 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
			Total	C	N	O	S			
1	A	677	Total	C	N	O	S	0	9	0
			5383	3406	957	1014	6			
1	B	679	Total	C	N	O	S	0	12	0
			5419	3424	963	1026	6			
1	C	682	Total	C	N	O	S	0	10	0
			5427	3431	961	1029	6			
1	D	678	Total	C	N	O	S	0	9	0
			5385	3408	956	1015	6			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



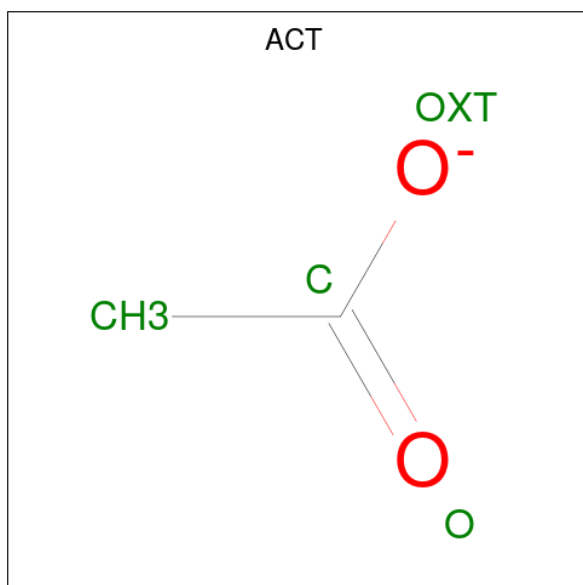
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
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		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula:  $C_2H_3O_2$ ).



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

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 3 2 1	0	0
4	A	1	Total C O 3 2 1	0	0
4	A	1	Total C O 3 2 1	0	0
4	A	1	Total C O 3 2 1	0	0
4	A	1	Total C O 6 4 2	0	0
4	A	1	Total C O 6 4 2	0	0
4	A	1	Total C O 9 6 3	0	0
4	B	1	Total C O 3 2 1	0	0
4	B	1	Total C O 3 2 1	0	0
4	B	1	Total C O 6 4 2	0	0
4	B	1	Total C O 6 4 2	0	0
4	B	1	Total C O 6 4 2	0	0
4	B	1	Total C O 12 8 4	0	0
4	B	1	Total C O 12 8 4	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 3 2 1	0	0
4	C	1	Total C O 3 2 1	0	0
4	C	1	Total C O 6 4 2	0	0
4	C	1	Total C O 6 4 2	0	0
4	C	1	Total C O 9 6 3	0	0
4	D	1	Total C O 3 2 1	0	0
4	D	1	Total C O 3 2 1	0	0
4	D	1	Total C O 3 2 1	0	0
4	D	1	Total C O 6 4 2	0	0
4	D	1	Total C O 9 6 3	0	0

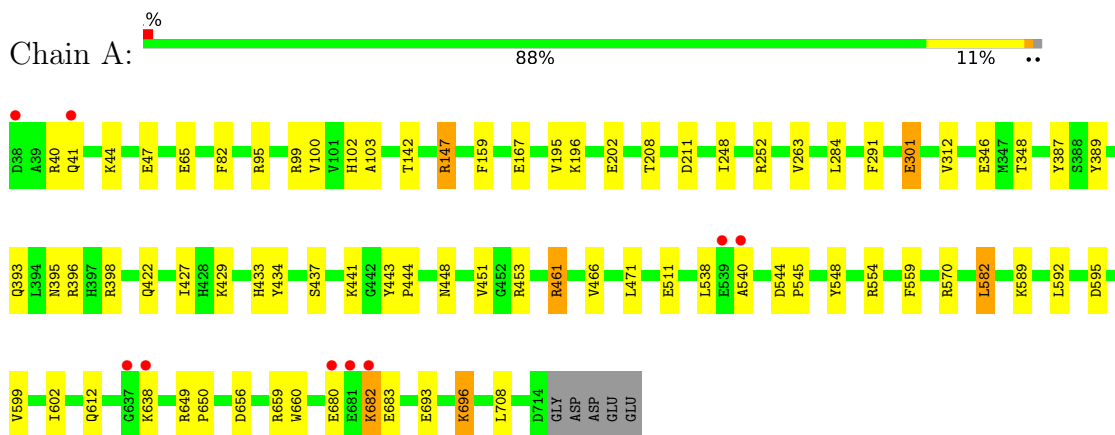
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	630	Total O 630 630	0	0
5	B	553	Total O 553 553	0	0
5	C	487	Total O 488 488	0	1
5	D	445	Total O 445 445	0	0

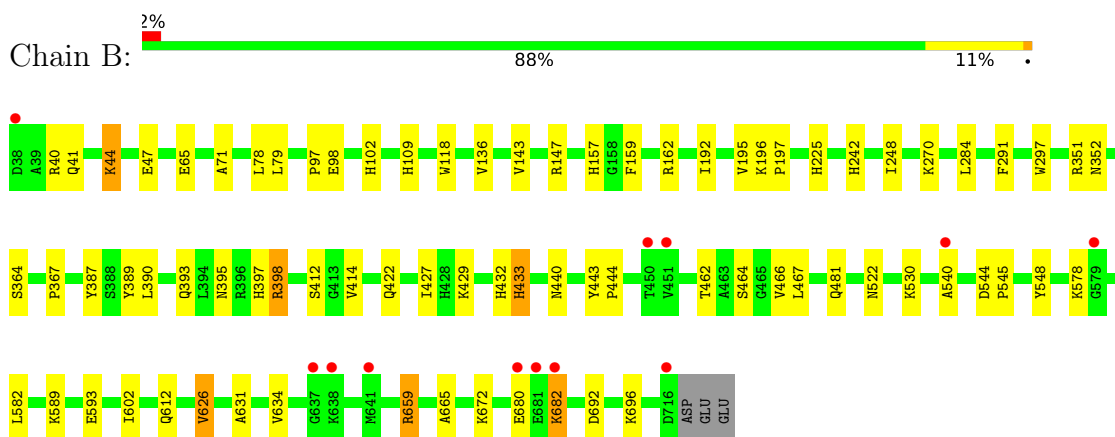
### 3 Residue-property plots

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.

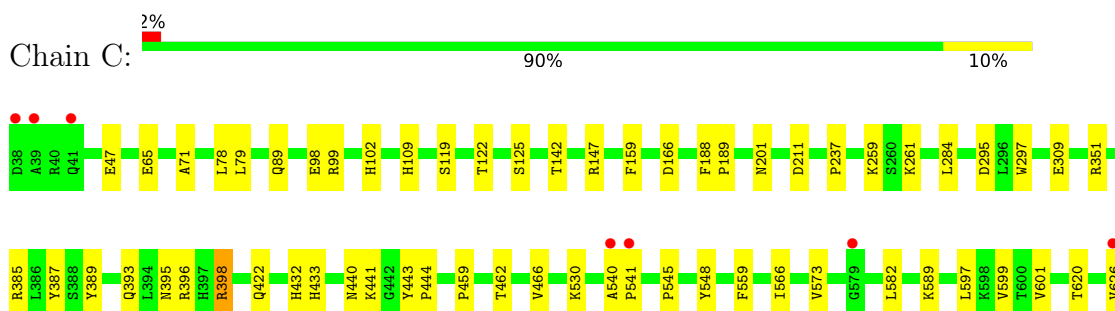
- Molecule 1: CATALASE-3



- Molecule 1: CATALASE-3

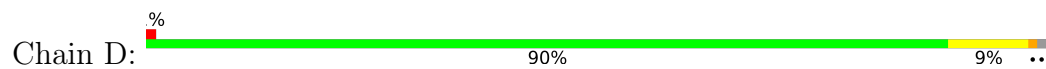


- Molecule 1: CATALASE-3





● Molecule 1: CATALASE-3





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.75Å 154.19Å 160.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.70 – 1.85 29.70 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.8 (29.70-1.85) 97.8 (29.70-1.85)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 1.85Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.177 , 0.218 0.173 , 0.213	Depositor DCC
$R_{free}$ test set	13547 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	10.1	Xtrriage
Anisotropy	0.046	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 48.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.019 for -h,l,k	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	24066	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	11.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE, ACT, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.37	0/5519	0.55	1/7484 (0.0%)
1	B	0.36	0/5552	0.54	0/7529
1	C	0.35	0/5561	0.51	0/7542
1	D	0.36	0/5521	0.53	0/7485
All	All	0.36	0/22153	0.53	1/30040 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	461	ARG	NE-CZ-NH2	-6.10	117.25	120.30

There are no chirality outliers.

There are no planarity outliers.

### 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	5383	0	5211	66	0
1	B	5419	0	5231	65	0
1	C	5427	0	5235	58	0
1	D	5385	0	5213	49	0
2	A	43	0	30	2	0
2	B	43	0	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	43	0	30	1	0
2	D	43	0	30	3	0
3	A	8	0	6	1	0
3	B	8	0	6	1	0
3	C	8	0	6	1	0
3	D	8	0	6	1	0
4	A	33	0	35	4	0
4	B	48	0	56	2	0
4	C	27	0	30	1	0
4	D	24	0	25	1	0
5	A	630	0	0	13	0
5	B	553	0	0	4	0
5	C	488	0	0	8	0
5	D	445	0	0	6	0
All	All	24066	0	21180	210	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 5.

All (210) 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)
5:C:2154:HOH:O	1:D:147[B]:ARG:O	1.56	1.21
5:A:2227:HOH:O	1:B:147[A]:ARG:O	1.69	1.09
1:A:147[A]:ARG:O	5:A:2112:HOH:O	1.71	1.08
5:A:2426:HOH:O	1:C:398:ARG:NH2	1.93	1.02
1:C:147[A]:ARG:O	1:D:147[A]:ARG:O	1.79	1.01
1:A:398:ARG:HG2	1:B:398:ARG:HH11	1.34	0.93
1:C:147[B]:ARG:O	5:C:2060:HOH:O	1.87	0.91
1:B:40:ARG:NH2	1:B:47:GLU:OE2	2.03	0.90
1:C:398:ARG:NE	1:D:398:ARG:HE	1.71	0.89
1:C:441:LYS:HG2	4:C:1726:1PE:H122	1.53	0.88
1:A:40:ARG:NH2	1:A:47:GLU:OE2	2.08	0.85
1:A:147[B]:ARG:O	1:B:147[B]:ARG:O	2.00	0.80
1:B:530:LYS:HG2	1:B:540:ALA:HB1	1.63	0.79
1:C:626[A]:VAL:HG12	1:C:665:ALA:HB3	1.64	0.79
1:C:633:ARG:HH21	1:C:638:LYS:NZ	1.80	0.79
1:A:398:ARG:HD3	1:D:422:GLN:NE2	1.98	0.78
1:D:544:ASP:OD2	5:D:2353:HOH:O	2.03	0.76
1:C:398:ARG:HE	1:D:398:ARG:HE	1.29	0.76
1:A:398:ARG:CZ	1:B:398:ARG:HD3	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ARG:HG2	1:B:398:ARG:NH1	2.00	0.74
1:C:398:ARG:NE	1:D:398:ARG:NE	2.37	0.72
1:A:511:GLU:OE2	1:A:538:LEU:HD21	1.88	0.72
1:A:422:GLN:NE2	1:D:398:ARG:HG3	2.05	0.70
1:A:544:ASP:OD2	5:A:2521:HOH:O	2.10	0.70
1:C:633:ARG:HH21	1:C:638:LYS:HZ1	1.40	0.70
1:A:545:PRO:HA	1:A:548:TYR:CD2	2.28	0.68
1:B:589:LYS:O	1:B:593:GLU:HG3	1.94	0.68
1:C:530:LYS:HG2	1:C:540:ALA:HB1	1.75	0.68
1:D:38:ASP:OD2	1:D:44:LYS:NZ	2.25	0.68
1:A:659:ARG:HD2	5:A:2608:HOH:O	1.95	0.67
1:A:395:ASN:O	1:A:398:ARG:HD2	1.96	0.66
1:B:118:TRP:CZ3	4:B:1726:1PE:H141	2.30	0.66
4:A:1724:1PE:H241	5:A:2146:HOH:O	1.95	0.65
1:B:412:SER:O	5:B:2331:HOH:O	2.14	0.65
1:A:195[A]:VAL:HG21	3:A:1716:ACT:H1	1.79	0.65
1:D:692:ASP:OD2	5:D:2438:HOH:O	2.15	0.64
1:D:195[A]:VAL:HG21	3:D:1717:ACT:H1	1.80	0.63
1:A:638:LYS:HB3	1:A:638:LYS:NZ	2.15	0.61
1:A:41:GLN:O	1:A:44:LYS:HG2	2.01	0.61
1:B:522:ASN:ND2	1:B:544[B]:ASP:OD1	2.34	0.60
1:C:309:GLU:OE1	5:C:2257:HOH:O	2.17	0.60
1:A:346:GLU:OE2	1:A:348:THR:OG1	2.10	0.59
1:B:692:ASP:O	1:B:696:LYS:HG3	2.03	0.59
1:B:422:GLN:NE2	1:C:398:ARG:HD3	2.18	0.58
1:B:414:VAL:H	4:B:1720:1PE:C12	2.17	0.58
1:A:167:GLU:OE2	1:A:453:ARG:NE	2.37	0.57
1:C:566:ILE:HD12	1:C:597:LEU:HD21	1.86	0.57
1:A:252:ARG:NH1	1:A:461:ARG:HD3	2.19	0.57
1:B:41:GLN:HA	1:B:44:LYS:HE3	1.87	0.57
1:D:343[A]:VAL:HG22	5:D:2245:HOH:O	2.05	0.56
1:D:672:LYS:O	1:D:672:LYS:HE3	2.06	0.56
1:A:398:ARG:NH2	5:A:2380:HOH:O	2.03	0.55
1:A:659:ARG:HH22	4:A:1722:1PE:H122	1.71	0.55
1:A:47:GLU:OE1	5:A:2013:HOH:O	2.18	0.55
1:B:545:PRO:HA	1:B:548:TYR:CD2	2.43	0.54
1:D:624:ALA:HB2	1:D:702:LEU:HD21	1.88	0.54
1:B:270:LYS:HA	1:B:270:LYS:HE2	1.90	0.54
1:B:544[B]:ASP:OD1	1:B:544[B]:ASP:N	2.41	0.53
1:A:680:GLU:O	1:A:683:GLU:HG3	2.09	0.53
1:B:157:HIS:HE1	5:B:2121:HOH:O	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:TYR:HB2	1:C:79:LEU:HD11	1.90	0.53
1:C:297:TRP:CE3	1:D:201:ASN:HB3	2.44	0.53
1:D:102:HIS:CE1	1:D:143:VAL:HG22	2.43	0.53
1:B:98:GLU:HB2	1:B:147[A]:ARG:HG3	1.91	0.53
1:B:680:GLU:HB3	1:B:682:LYS:HZ2	1.74	0.53
1:C:545:PRO:HA	1:C:548:TYR:CD2	2.44	0.53
1:C:559:PHE:HB3	1:C:708:LEU:HD11	1.90	0.52
1:D:545:PRO:HA	1:D:548:TYR:CD2	2.45	0.52
1:A:448:ASN:OD1	1:A:451[A]:VAL:HG12	2.10	0.52
1:D:301:GLU:HG2	1:D:352:ASN:ND2	2.25	0.52
1:A:589:LYS:HG3	1:A:599:VAL:HB	1.91	0.52
1:C:201:ASN:HB3	1:D:297:TRP:CE3	2.44	0.52
1:B:466:VAL:HG22	1:B:467:LEU:O	2.09	0.51
1:B:364:SER:HB3	1:B:393:GLN:CD	2.31	0.51
1:B:659:ARG:HD3	5:B:2522:HOH:O	2.11	0.51
1:C:659:ARG:HD2	5:C:2472:HOH:O	2.10	0.51
1:B:578:LYS:HE3	5:B:2473:HOH:O	2.10	0.50
1:A:103:ALA:O	1:A:147[B]:ARG:HG2	2.12	0.50
1:C:237:PRO:HB3	3:C:1722:ACT:H1	1.93	0.50
1:D:239:SER:HA	1:D:292:HIS:CD2	2.46	0.50
1:A:427:ILE:O	1:D:47:GLU:HA	2.11	0.50
1:B:242:HIS:O	3:B:1719:ACT:H2	2.12	0.50
1:A:693:GLU:O	1:A:696:LYS:HD3	2.12	0.50
1:C:261:LYS:HE2	5:C:2071:HOH:O	2.12	0.50
1:C:677:ILE:HG13	1:C:679:VAL:HG23	1.94	0.49
1:D:591:GLN:O	1:D:594:LYS:HB2	2.13	0.49
1:A:301:GLU:HA	1:A:301:GLU:OE1	2.13	0.49
1:A:99:ARG:HA	1:A:396[A]:ARG:HD3	1.94	0.49
1:B:395:ASN:O	1:B:398:ARG:NH2	2.43	0.49
1:B:432:HIS:HB2	1:B:440:ASN:HB3	1.94	0.49
1:D:97:PRO:HG3	1:D:398:ARG:NH2	2.28	0.49
1:A:570[B]:ARG:HB2	1:A:570[B]:ARG:HH11	1.78	0.48
1:A:147[A]:ARG:HD2	5:A:2158:HOH:O	2.13	0.48
5:A:2226:HOH:O	1:B:147[B]:ARG:HD2	2.13	0.48
1:B:225:HIS:CE1	1:B:481:GLN:HB3	2.48	0.48
1:A:680:GLU:HB3	1:A:682:LYS:CE	2.43	0.48
1:C:630:GLY:O	1:C:633:ARG:HG2	2.13	0.48
1:A:248:ILE:HD12	2:A:1715:HEM:HMB1	1.96	0.48
1:A:398:ARG:HH21	1:B:97:PRO:HD3	1.79	0.48
1:C:389:TYR:O	1:C:393:GLN:HG2	2.14	0.47
1:C:432:HIS:HB2	1:C:440:ASN:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:697:GLY:O	1:D:700:GLU:HG2	2.14	0.47
1:B:196:LYS:HB3	1:B:197:PRO:CD	2.44	0.47
2:B:1717:HEM:HMB1	2:B:1717:HEM:HBB2	1.97	0.47
1:A:195[B]:VAL:HG13	1:A:208:THR:HG22	1.96	0.47
1:C:259:LYS:HA	1:C:259:LYS:HD3	1.77	0.47
1:C:541[B]:PRO:HB3	5:C:2170:HOH:O	2.14	0.47
1:A:248:ILE:HD12	2:A:1715:HEM:CBB	2.44	0.47
1:A:389:TYR:O	1:A:393:GLN:HG2	2.15	0.47
1:A:466:VAL:HG12	1:C:462:THR:HG22	1.96	0.47
1:B:433:HIS:ND1	1:B:433:HIS:N	2.60	0.47
1:B:466:VAL:HG23	1:D:461:ARG:O	2.15	0.47
1:A:545:PRO:HA	1:A:548:TYR:CG	2.49	0.46
1:B:367:PRO:HD3	1:B:389:TYR:CD2	2.50	0.46
1:B:397:HIS:HA	1:C:422:GLN:NE2	2.29	0.46
1:C:98:GLU:OE1	1:C:147[B]:ARG:HG3	2.15	0.46
1:B:44:LYS:N	1:B:44:LYS:HD3	2.31	0.46
1:C:395:ASN:O	1:C:398:ARG:HD2	2.15	0.46
1:D:582:LEU:O	1:D:586:LYS:HG3	2.15	0.46
1:A:540:ALA:N	5:A:2537:HOH:O	2.27	0.46
1:A:434:TYR:CE2	1:A:437:SER:HB2	2.51	0.46
1:C:573:VAL:HG22	1:C:626[A]:VAL:CG2	2.45	0.46
1:B:71:ALA:HB2	1:B:78:LEU:HD21	1.98	0.45
1:B:429:LYS:HE3	1:B:429:LYS:HB2	1.73	0.45
1:C:188:PHE:HB3	1:C:189:PRO:HD3	1.98	0.45
1:B:464:SER:HA	1:D:463:ALA:O	2.16	0.45
1:C:443:TYR:HA	1:C:444:PRO:C	2.36	0.45
1:C:589:LYS:HG3	1:C:599:VAL:HB	1.98	0.45
1:A:682:LYS:H	1:A:682:LYS:HZ3	1.64	0.45
1:C:99:ARG:HA	1:C:396[A]:ARG:HD3	1.98	0.45
1:A:659:ARG:NH2	4:A:1722:1PE:H122	2.31	0.45
1:C:582:LEU:HB2	5:C:2427:HOH:O	2.16	0.45
1:B:395:ASN:OD1	1:B:398:ARG:NH2	2.50	0.45
1:C:98:GLU:HB3	1:C:147[B]:ARG:HG3	1.99	0.45
1:B:136:VAL:HA	1:B:162:ARG:O	2.17	0.45
1:B:672:LYS:HA	1:B:672:LYS:HD2	1.88	0.44
1:A:95:ARG:HH21	1:B:196:LYS:HE3	1.82	0.44
1:C:71:ALA:HB2	1:C:78:LEU:HD21	1.98	0.44
1:B:79:LEU:HD11	1:C:387:TYR:HB2	2.00	0.44
1:B:284:LEU:HD21	1:B:291:PHE:CD2	2.53	0.44
1:D:262:LEU:HB2	1:D:315:ILE:HG12	1.99	0.44
1:A:461:ARG:O	1:C:466:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:TYR:O	1:B:393:GLN:HG2	2.18	0.44
1:D:389:TYR:O	1:D:393:GLN:HG2	2.17	0.44
1:B:297:TRP:CZ3	1:B:352:ASN:HB3	2.53	0.44
1:A:649:ARG:HB3	1:A:650:PRO:HD3	1.99	0.44
1:A:656:ASP:HB3	1:A:660:TRP:CZ3	2.53	0.44
1:D:429:LYS:HE3	1:D:429:LYS:HB2	1.70	0.43
1:D:586:LYS:NZ	1:D:586:LYS:HB3	2.34	0.43
1:A:441:LYS:NZ	4:A:1718:1PE:H221	2.32	0.43
1:C:385:ARG:HG2	2:C:1720:HEM:C2C	2.53	0.43
1:D:483:ARG:HD3	1:D:524:ILE:O	2.18	0.43
1:C:109:HIS:HB2	1:C:351:ARG:HB2	2.00	0.43
1:A:398:ARG:CZ	1:B:398:ARG:CD	2.91	0.43
1:B:462:THR:HA	1:D:466:VAL:HA	2.01	0.43
1:C:297:TRP:CZ3	1:D:201:ASN:HB3	2.53	0.43
1:B:427:ILE:O	1:C:47:GLU:HA	2.18	0.43
1:C:201:ASN:HB3	1:D:297:TRP:CZ3	2.54	0.43
2:B:1717:HEM:HBB2	2:B:1717:HEM:CMB	2.49	0.43
1:B:248:ILE:HD12	2:B:1717:HEM:CBB	2.49	0.43
1:C:125:SER:OG	1:C:166:ASP:OD1	2.31	0.43
1:D:448:ASN:OD1	1:D:451:VAL:HG12	2.19	0.43
1:C:119:SER:HA	1:C:122:THR:O	2.18	0.42
1:A:602:ILE:HA	1:A:612:GLN:O	2.19	0.42
1:A:559:PHE:HB3	1:A:708:LEU:HD11	2.01	0.42
1:B:390:LEU:HG	1:C:89:GLN:OE1	2.19	0.42
1:D:551:ASN:HB3	4:D:1723:1PE:H132	2.02	0.42
1:A:82:PHE:HB2	5:D:2259:HOH:O	2.19	0.42
1:A:284:LEU:HD21	1:A:291:PHE:CD2	2.54	0.42
1:B:626:VAL:HB	1:B:665:ALA:HB3	2.00	0.42
1:C:284:LEU:HD13	1:C:620:THR:HB	2.01	0.42
1:D:248:ILE:HD12	2:D:1716:HEM:HMB1	2.00	0.42
1:D:147[A]:ARG:NH2	5:D:2084:HOH:O	2.52	0.42
1:A:429:LYS:HE2	1:A:429:LYS:HB2	1.46	0.42
1:B:398:ARG:HD2	1:C:422:GLN:OE1	2.19	0.42
1:A:638:LYS:HB3	1:A:638:LYS:HZ2	1.83	0.42
5:A:2386:HOH:O	1:C:398:ARG:NH2	2.41	0.42
1:C:589:LYS:HD2	1:C:601:VAL:HG23	2.01	0.42
1:A:398:ARG:NH2	1:B:398:ARG:CD	2.83	0.42
1:B:192:ILE:HA	1:B:195[A]:VAL:HG22	2.02	0.42
1:D:649:ARG:HB3	1:D:650:PRO:HD3	2.02	0.41
1:D:102:HIS:HA	1:D:142:THR:O	2.20	0.41
1:B:102:HIS:CE1	1:B:143:VAL:HG22	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:498:ILE:HD11	1:D:528:VAL:HG22	2.02	0.41
1:D:287:LYS:HE3	1:D:618:ASP:OD1	2.20	0.41
1:A:263:VAL:HG23	1:A:312:VAL:HB	2.02	0.41
1:C:459:PRO:O	5:C:2346:HOH:O	2.22	0.41
1:C:672:LYS:O	1:C:672:LYS:HD3	2.21	0.41
1:A:443:TYR:HA	1:A:444:PRO:C	2.40	0.41
1:B:443:TYR:HA	1:B:444:PRO:C	2.41	0.41
1:D:589:LYS:HG3	1:D:599:VAL:HB	2.02	0.41
2:D:1716:HEM:CMB	2:D:1716:HEM:HBB2	2.51	0.41
1:A:387:TYR:HB2	1:D:79:LEU:HD11	2.03	0.41
1:A:582:LEU:HD12	1:A:582:LEU:HA	1.92	0.41
1:B:631:ALA:O	1:B:634:VAL:HG22	2.21	0.41
1:D:530:LYS:O	1:D:534:VAL:HG23	2.20	0.41
1:A:202:GLU:HG2	1:A:202:GLU:O	2.21	0.41
1:B:602:ILE:HA	1:B:612:GLN:O	2.21	0.41
2:D:1716:HEM:HMB1	2:D:1716:HEM:HBB2	2.02	0.41
1:A:102:HIS:HA	1:A:142:THR:O	2.21	0.40
1:B:682:LYS:HE3	1:B:682:LYS:HB3	1.94	0.40
1:D:578:LYS:HD3	1:D:578:LYS:HA	1.76	0.40
1:D:659:ARG:HD3	5:D:2425:HOH:O	2.20	0.40
1:A:47:GLU:HA	1:D:427:ILE:O	2.21	0.40
1:A:100:VAL:O	1:A:196:LYS:HE3	2.22	0.40
1:A:680:GLU:HB3	1:A:682:LYS:CD	2.52	0.40
5:A:2085:HOH:O	1:B:398:ARG:NH2	2.53	0.40
1:B:109:HIS:HB2	1:B:351:ARG:HB2	2.04	0.40
1:C:102:HIS:HA	1:C:142:THR:O	2.21	0.40
1:C:398:ARG:HG3	1:C:398:ARG:NH1	2.37	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	684/682 (100%)	665 (97%)	19 (3%)	0	100	100
1	B	689/682 (101%)	670 (97%)	19 (3%)	0	100	100
1	C	690/682 (101%)	667 (97%)	23 (3%)	0	100	100
1	D	685/682 (100%)	662 (97%)	23 (3%)	0	100	100
All	All	2748/2728 (101%)	2664 (97%)	84 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	564/560 (101%)	549 (97%)	15 (3%)	44	29
1	B	568/560 (101%)	559 (98%)	9 (2%)	62	49
1	C	569/560 (102%)	561 (99%)	8 (1%)	67	55
1	D	564/560 (101%)	555 (98%)	9 (2%)	62	49
All	All	2265/2240 (101%)	2224 (98%)	41 (2%)	60	45

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	GLU
1	A	147[A]	ARG
1	A	147[B]	ARG
1	A	159	PHE
1	A	211	ASP
1	A	301	GLU
1	A	433	HIS
1	A	471	LEU
1	A	554[A]	ARG
1	A	554[B]	ARG
1	A	582	LEU
1	A	592	LEU
1	A	595	ASP

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Mol	Chain	Res	Type
1	A	682	LYS
1	A	696	LYS
1	B	44	LYS
1	B	65	GLU
1	B	159	PHE
1	B	398	ARG
1	B	433	HIS
1	B	582	LEU
1	B	626	VAL
1	B	659	ARG
1	B	682	LYS
1	C	65	GLU
1	C	159	PHE
1	C	211	ASP
1	C	295	ASP
1	C	398	ARG
1	C	433	HIS
1	C	638	LYS
1	C	692	ASP
1	D	65	GLU
1	D	159	PHE
1	D	211	ASP
1	D	315	ILE
1	D	347	MET
1	D	433	HIS
1	D	582	LEU
1	D	659	ARG
1	D	672	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	157	HIS
1	D	422	GLN

### 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](#)

36 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	ACT	C	1722	-	3,3,3	0.73	0	3,3,3	1.66	1 (33%)
2	HEM	A	1715	1	41,50,50	1.87	7 (17%)	45,82,82	1.73	7 (15%)
2	HEM	D	1716	1	41,50,50	1.93	6 (14%)	45,82,82	1.80	9 (20%)
4	1PE	C	1724	-	2,2,15	0.36	0	1,1,14	0.33	0
4	1PE	B	1720	-	2,2,15	0.35	0	1,1,14	0.34	0
4	1PE	B	1724	-	5,5,15	0.53	0	4,4,14	1.53	1 (25%)
4	1PE	C	1725	-	5,5,15	0.55	0	4,4,14	1.46	1 (25%)
4	1PE	B	1723	-	5,5,15	0.55	0	4,4,14	1.47	1 (25%)
4	1PE	B	1726	-	11,11,15	0.91	0	10,10,14	1.57	1 (10%)
3	ACT	C	1721	-	3,3,3	0.81	0	3,3,3	1.46	0
4	1PE	B	1725	-	11,11,15	0.90	0	10,10,14	1.59	2 (20%)
4	1PE	A	1720	-	2,2,15	0.35	0	1,1,14	0.30	0
4	1PE	A	1724	-	8,8,15	0.57	0	7,7,14	1.41	0
4	1PE	A	1722	-	5,5,15	0.55	0	4,4,14	1.24	0
4	1PE	A	1721	-	2,2,15	0.36	0	1,1,14	0.26	0
4	1PE	D	1722	-	5,5,15	0.48	0	4,4,14	1.54	1 (25%)
2	HEM	C	1720	1	41,50,50	1.92	7 (17%)	45,82,82	1.60	6 (13%)
3	ACT	D	1718	-	3,3,3	0.78	0	3,3,3	1.57	1 (33%)
3	ACT	A	1717	-	3,3,3	0.78	0	3,3,3	1.51	0
3	ACT	D	1717	-	3,3,3	0.69	0	3,3,3	1.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	1PE	D	1723	-	8,8,15	0.58	0	7,7,14	1.55	0
3	ACT	B	1719	-	3,3,3	0.75	0	3,3,3	1.62	1 (33%)
4	1PE	A	1723	-	5,5,15	0.52	0	4,4,14	1.37	0
4	1PE	D	1721	-	2,2,15	0.35	0	1,1,14	0.29	0
4	1PE	C	1723	-	2,2,15	0.36	0	1,1,14	0.27	0
4	1PE	A	1719	-	2,2,15	0.34	0	1,1,14	0.34	0
3	ACT	B	1718	-	3,3,3	0.67	0	3,3,3	1.25	0
4	1PE	B	1722	-	5,5,15	0.56	0	4,4,14	1.48	1 (25%)
2	HEM	B	1717	1	41,50,50	1.87	6 (14%)	45,82,82	1.55	8 (17%)
4	1PE	B	1721	-	2,2,15	0.35	0	1,1,14	0.37	0
4	1PE	A	1718	-	2,2,15	0.35	0	1,1,14	0.33	0
4	1PE	C	1727	-	8,8,15	0.61	0	7,7,14	1.46	0
3	ACT	A	1716	-	3,3,3	0.74	0	3,3,3	1.41	0
4	1PE	D	1720	-	2,2,15	0.37	0	1,1,14	0.25	0
4	1PE	D	1719	-	2,2,15	0.34	0	1,1,14	0.41	0
4	1PE	C	1726	-	5,5,15	0.52	0	4,4,14	1.42	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	C	1720	1	-	4/12/54/54	-
4	1PE	C	1725	-	-	0/3/3/13	-
4	1PE	B	1723	-	-	2/3/3/13	-
2	HEM	A	1715	1	-	3/12/54/54	-
4	1PE	B	1726	-	-	2/9/9/13	-
2	HEM	B	1717	1	-	4/12/54/54	-
2	HEM	D	1716	1	-	2/12/54/54	-
4	1PE	B	1725	-	-	4/9/9/13	-
4	1PE	C	1727	-	-	4/6/6/13	-
4	1PE	A	1724	-	-	4/6/6/13	-
4	1PE	A	1722	-	-	1/3/3/13	-
4	1PE	D	1723	-	-	4/6/6/13	-
4	1PE	A	1723	-	-	1/3/3/13	-
4	1PE	D	1722	-	-	2/3/3/13	-
4	1PE	C	1726	-	-	1/3/3/13	-
4	1PE	B	1724	-	-	1/3/3/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	1PE	B	1722	-	-	2/3/3/13	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1717	HEM	C3D-C2D	7.54	1.52	1.36
2	D	1716	HEM	C3D-C2D	7.51	1.52	1.36
2	C	1720	HEM	C3D-C2D	7.49	1.52	1.36
2	A	1715	HEM	C3D-C2D	7.45	1.52	1.36
2	C	1720	HEM	C3C-C2C	-4.57	1.34	1.40
2	D	1716	HEM	C3C-C2C	-4.57	1.34	1.40
2	A	1715	HEM	C3C-C2C	-4.24	1.34	1.40
2	B	1717	HEM	C3C-C2C	-4.06	1.34	1.40
2	B	1717	HEM	C3C-CAC	3.35	1.54	1.47
2	A	1715	HEM	C3C-CAC	3.29	1.54	1.47
2	D	1716	HEM	C3C-CAC	3.24	1.54	1.47
2	D	1716	HEM	FE-ND	3.24	2.12	1.96
2	B	1717	HEM	CAB-C3B	3.00	1.55	1.47
2	D	1716	HEM	CAB-C3B	3.00	1.55	1.47
2	C	1720	HEM	C3C-CAC	2.95	1.53	1.47
2	C	1720	HEM	CAB-C3B	2.86	1.55	1.47
2	C	1720	HEM	FE-ND	2.81	2.10	1.96
2	A	1715	HEM	CAB-C3B	2.67	1.54	1.47
2	A	1715	HEM	FE-ND	2.62	2.09	1.96
2	C	1720	HEM	CAA-C2A	2.48	1.55	1.52
2	A	1715	HEM	CMB-C2B	2.44	1.56	1.50
2	B	1717	HEM	CMB-C2B	2.14	1.55	1.50
2	A	1715	HEM	FE-NB	2.06	2.07	1.96
2	D	1716	HEM	CMD-C2D	2.03	1.55	1.50
2	B	1717	HEM	FE-NB	2.02	2.06	1.96
2	C	1720	HEM	CMB-C2B	2.02	1.55	1.50

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1716	HEM	C4D-ND-C1D	6.85	112.14	105.07
2	A	1715	HEM	C4D-ND-C1D	5.97	111.24	105.07
2	C	1720	HEM	C4D-ND-C1D	5.60	110.86	105.07
2	B	1717	HEM	C4D-ND-C1D	5.43	110.68	105.07
2	A	1715	HEM	C1B-NB-C4B	3.91	109.11	105.07
2	D	1716	HEM	C4C-CHD-C1D	3.81	127.58	122.56
2	A	1715	HEM	CAA-CBA-CGA	-3.19	104.83	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1720	HEM	C1B-NB-C4B	3.05	108.22	105.07
2	A	1715	HEM	C4C-CHD-C1D	2.88	126.36	122.56
2	A	1715	HEM	CHD-C1D-ND	2.85	127.53	124.43
2	B	1717	HEM	CAA-CBA-CGA	-2.79	105.94	113.76
2	D	1716	HEM	C1B-NB-C4B	2.78	107.94	105.07
2	B	1717	HEM	C4C-CHD-C1D	2.78	126.22	122.56
2	D	1716	HEM	CBD-CAD-C3D	-2.72	105.06	112.63
2	B	1717	HEM	C1B-NB-C4B	2.62	107.78	105.07
2	C	1720	HEM	CMA-C3A-C4A	-2.53	124.58	128.46
2	A	1715	HEM	CBD-CAD-C3D	-2.52	105.63	112.63
2	D	1716	HEM	CAA-CBA-CGA	-2.37	107.10	113.76
4	B	1725	1PE	C25-OH5-C14	2.36	121.34	112.90
2	D	1716	HEM	CHD-C1D-ND	2.35	126.99	124.43
2	C	1720	HEM	C1D-C2D-C3D	-2.31	104.53	106.96
4	B	1722	1PE	C23-OH3-C22	2.23	120.90	112.90
2	B	1717	HEM	CBD-CAD-C3D	-2.20	106.52	112.63
4	B	1724	1PE	C23-OH3-C22	2.17	120.66	112.90
4	B	1723	1PE	OH3-C22-C12	2.14	119.47	110.07
4	B	1726	1PE	C25-OH5-C14	2.13	120.55	112.90
3	C	1722	ACT	OXT-C-CH3	2.13	123.97	115.18
4	D	1722	1PE	C23-OH3-C22	2.12	120.50	112.90
2	C	1720	HEM	C4C-CHD-C1D	2.12	125.36	122.56
2	D	1716	HEM	CAD-CBD-CGD	-2.11	109.06	113.60
2	B	1717	HEM	C1D-C2D-C3D	-2.11	104.74	106.96
2	B	1717	HEM	CHC-C4B-NB	2.11	126.72	124.43
2	A	1715	HEM	CMA-C3A-C4A	-2.10	125.24	128.46
4	C	1725	1PE	C23-OH3-C22	2.09	120.39	112.90
2	C	1720	HEM	CBD-CAD-C3D	-2.08	106.86	112.63
2	D	1716	HEM	C3D-C4D-ND	-2.06	107.87	110.17
3	D	1718	ACT	OXT-C-O	-2.05	114.48	122.05
3	B	1719	ACT	OXT-C-CH3	2.05	123.65	115.18
2	D	1716	HEM	CMA-C3A-C4A	-2.05	125.31	128.46
4	B	1725	1PE	OH5-C14-C24	2.01	119.46	110.39
2	B	1717	HEM	C3B-C2B-C1B	2.00	107.97	106.49

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1723	1PE	OH2-C12-C22-OH3
4	B	1724	1PE	C12-C22-OH3-C23
4	D	1723	1PE	OH4-C13-C23-OH3

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Mol	Chain	Res	Type	Atoms
4	C	1727	1PE	OH4-C13-C23-OH3
4	A	1723	1PE	OH2-C12-C22-OH3
4	D	1723	1PE	C14-C24-OH4-C13
4	B	1725	1PE	OH5-C14-C24-OH4
4	B	1722	1PE	OH2-C12-C22-OH3
4	B	1723	1PE	OH2-C12-C22-OH3
4	C	1727	1PE	C14-C24-OH4-C13
4	B	1725	1PE	C15-C25-OH5-C14
4	A	1724	1PE	C14-C24-OH4-C13
4	D	1722	1PE	C13-C23-OH3-C22
4	B	1725	1PE	OH2-C12-C22-OH3
4	C	1726	1PE	C12-C22-OH3-C23
4	A	1724	1PE	C23-C13-OH4-C24
4	A	1724	1PE	OH2-C12-C22-OH3
4	C	1727	1PE	C12-C22-OH3-C23
4	D	1723	1PE	C13-C23-OH3-C22
4	D	1722	1PE	C12-C22-OH3-C23
4	A	1722	1PE	C12-C22-OH3-C23
4	B	1725	1PE	C24-C14-OH5-C25
4	B	1726	1PE	OH5-C14-C24-OH4
2	B	1717	HEM	CAA-CBA-CGA-O2A
2	C	1720	HEM	CAA-CBA-CGA-O2A
4	B	1723	1PE	C13-C23-OH3-C22
4	B	1726	1PE	C14-C24-OH4-C13
2	A	1715	HEM	CAA-CBA-CGA-O2A
2	B	1717	HEM	CAA-CBA-CGA-O1A
2	D	1716	HEM	CAA-CBA-CGA-O1A
2	D	1716	HEM	CAA-CBA-CGA-O2A
2	C	1720	HEM	CAA-CBA-CGA-O1A
2	A	1715	HEM	CAA-CBA-CGA-O1A
4	B	1722	1PE	C13-C23-OH3-C22
4	C	1727	1PE	C13-C23-OH3-C22
4	A	1724	1PE	OH4-C13-C23-OH3
2	B	1717	HEM	CAD-CBD-CGD-O2D
2	B	1717	HEM	CAD-CBD-CGD-O1D
2	A	1715	HEM	CAD-CBD-CGD-O2D
2	C	1720	HEM	CAD-CBD-CGD-O2D
2	C	1720	HEM	CAD-CBD-CGD-O1D

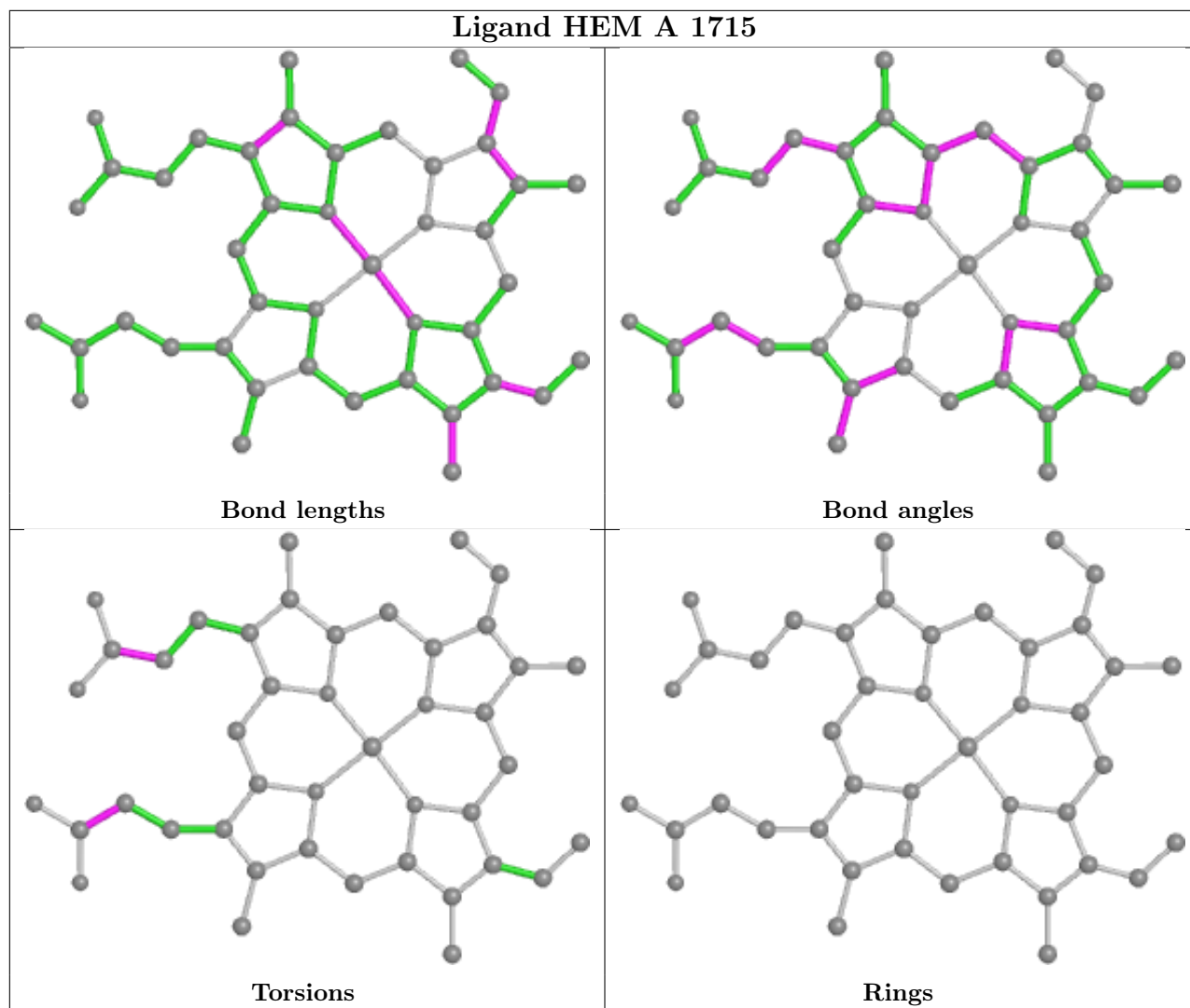
There are no ring outliers.

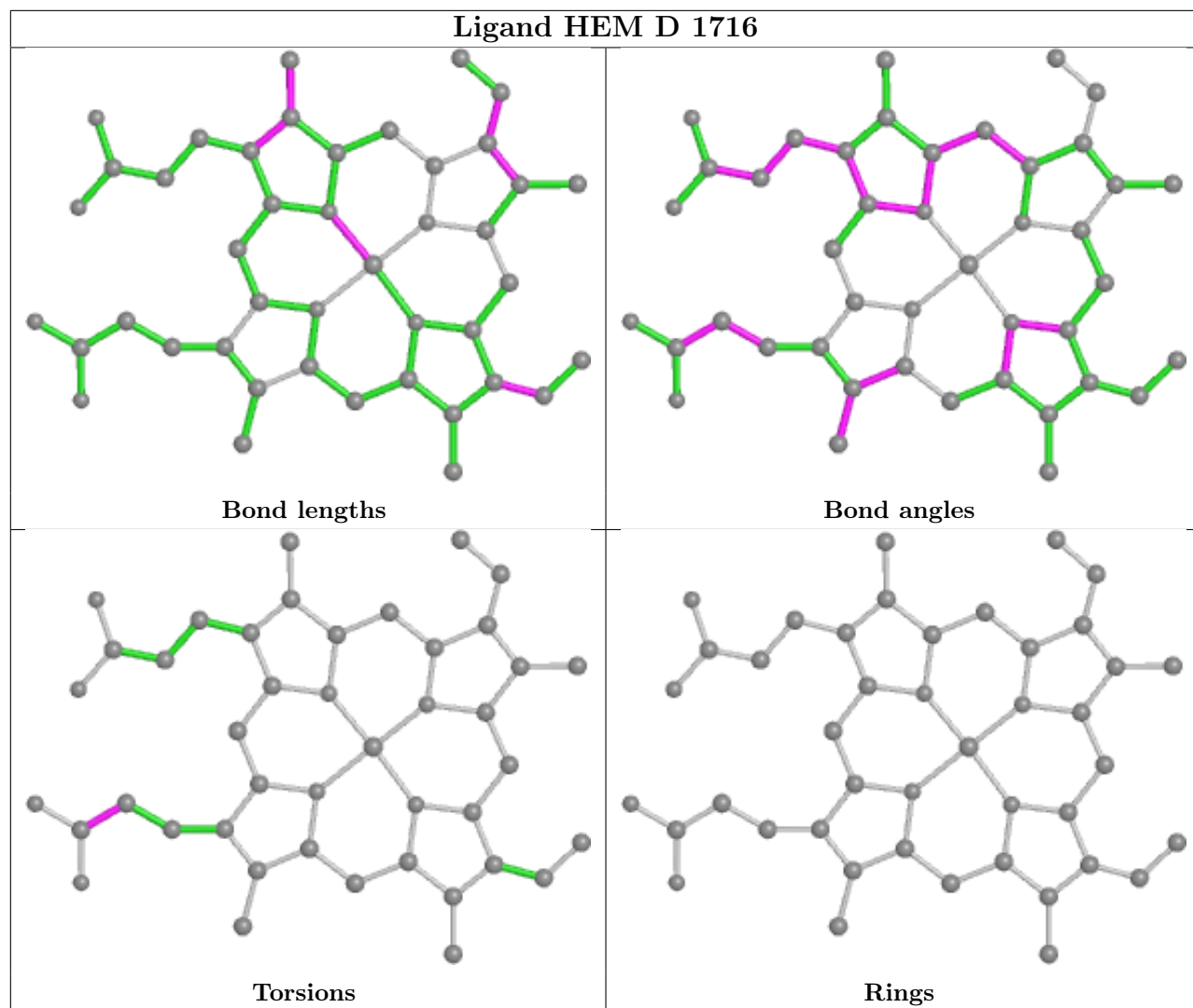
15 monomers are involved in 21 short contacts:

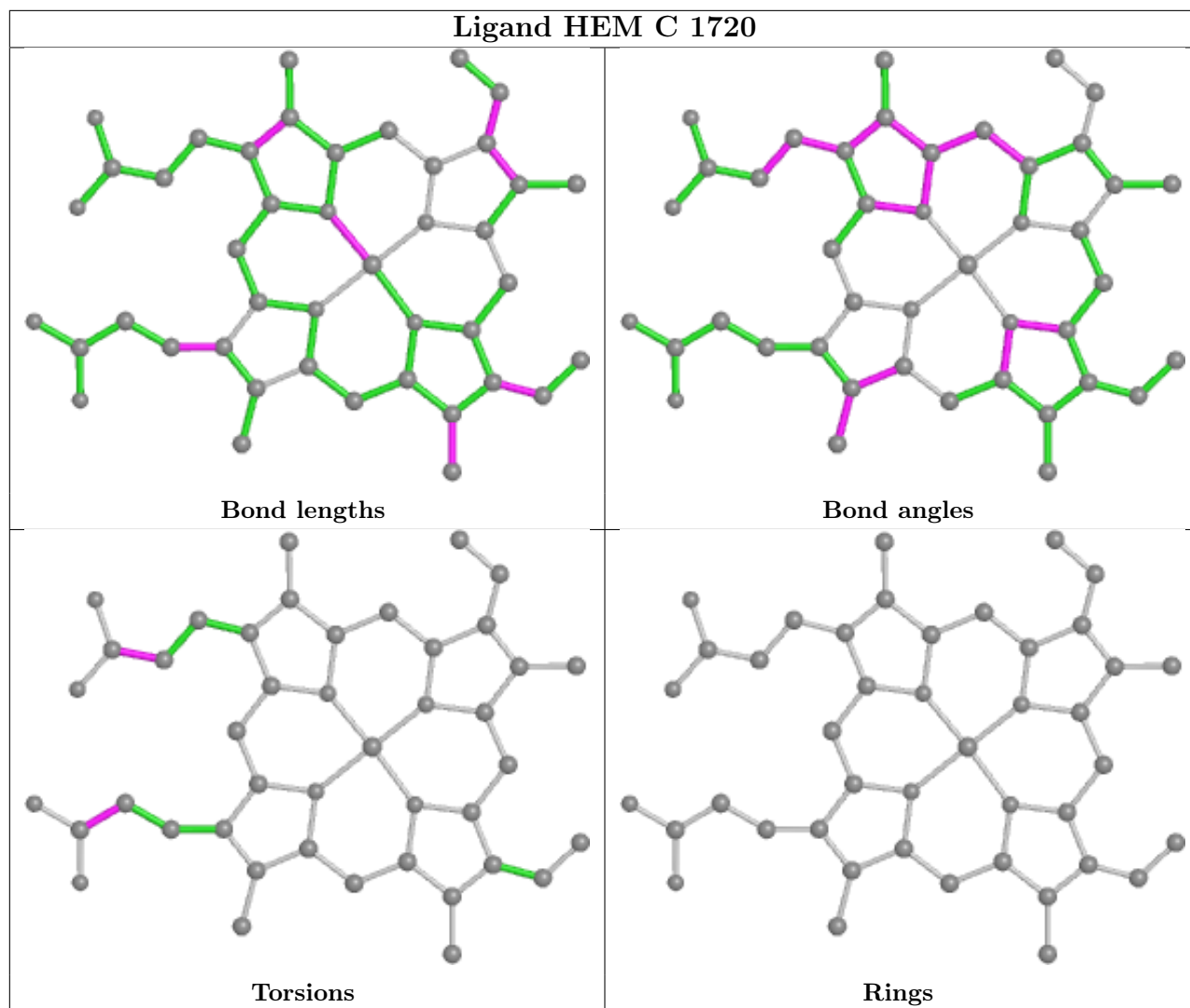
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1722	ACT	1	0
2	A	1715	HEM	2	0
2	D	1716	HEM	3	0
4	B	1720	1PE	1	0
4	B	1726	1PE	1	0
4	A	1724	1PE	1	0
4	A	1722	1PE	2	0
2	C	1720	HEM	1	0
3	D	1717	ACT	1	0
4	D	1723	1PE	1	0
3	B	1719	ACT	1	0
2	B	1717	HEM	3	0
4	A	1718	1PE	1	0
3	A	1716	ACT	1	0
4	C	1726	1PE	1	0

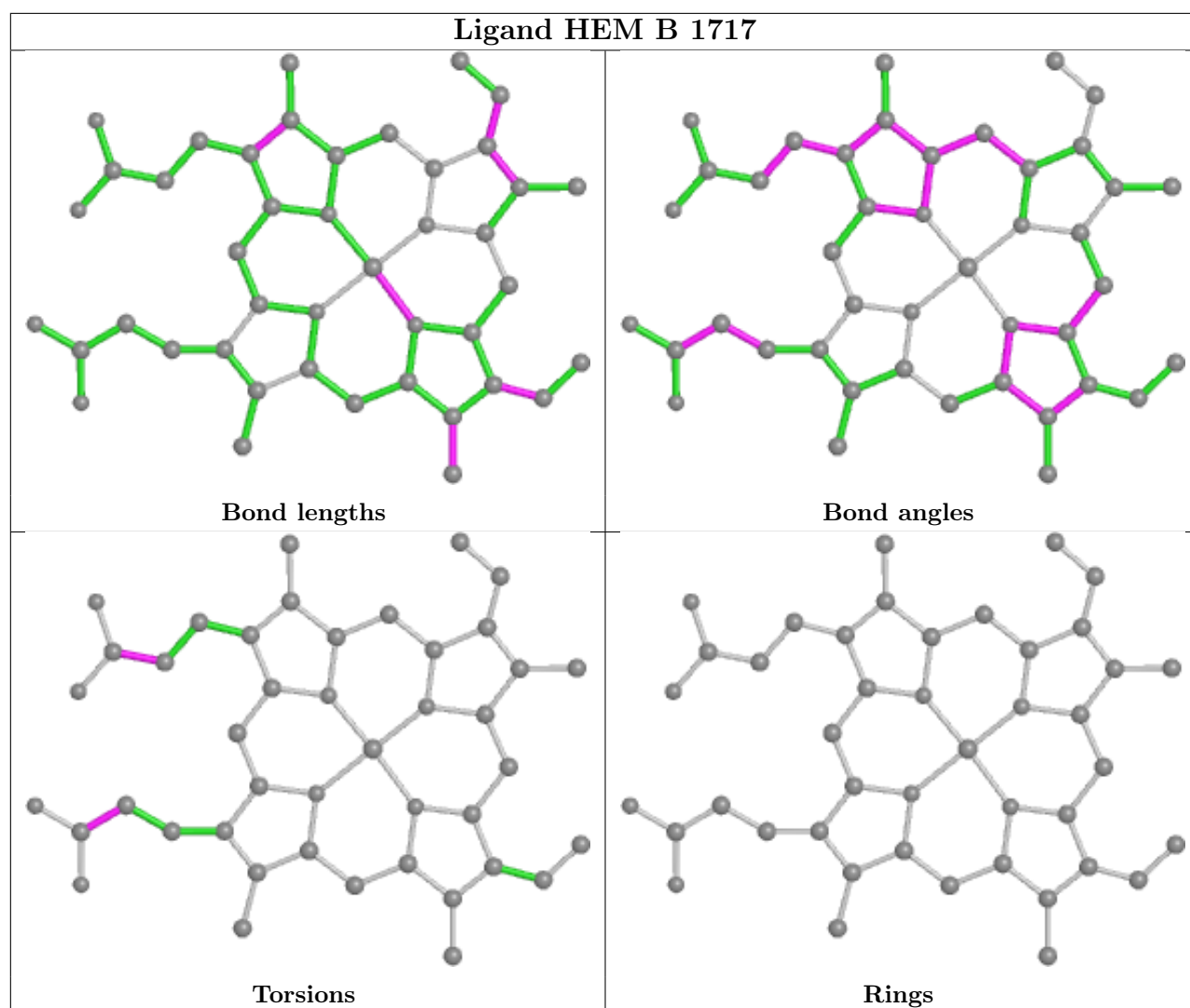
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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, 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	677/682 (99%)	-0.26	9 (1%) 77 78	2, 8, 24, 51	0
1	B	679/682 (99%)	-0.24	12 (1%) 68 68	2, 8, 25, 55	0
1	C	682/682 (100%)	-0.18	14 (2%) 63 63	2, 9, 29, 50	0
1	D	678/682 (99%)	-0.21	9 (1%) 77 78	3, 9, 26, 55	0
All	All	2716/2728 (99%)	-0.22	44 (1%) 72 72	2, 8, 26, 55	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	540	ALA	4.2
1	D	641	MET	3.9
1	B	716	ASP	3.8
1	D	680	GLU	3.8
1	C	540	ALA	3.6
1	A	637	GLY	3.5
1	D	715	GLY	3.4
1	A	680	GLU	3.4
1	C	39	ALA	3.3
1	C	38	ASP	3.2
1	C	638	LYS	3.2
1	A	638	LYS	3.1
1	C	718	GLU	3.0
1	B	637	GLY	3.0
1	C	641	MET	3.0
1	A	41	GLN	2.9
1	C	637	GLY	2.9
1	C	579	GLY	2.9
1	C	41	GLN	2.8
1	D	682	LYS	2.7
1	A	682	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	641	MET	2.6
1	C	541[A]	PRO	2.5
1	A	681	GLU	2.5
1	B	451	VAL	2.5
1	D	637	GLY	2.5
1	B	680	GLU	2.4
1	B	450	THR	2.4
1	B	682	LYS	2.3
1	C	719	GLU	2.3
1	C	681	GLU	2.3
1	D	638	LYS	2.3
1	B	638	LYS	2.3
1	B	38	ASP	2.3
1	B	681	GLU	2.2
1	A	540	ALA	2.2
1	D	464	SER	2.2
1	B	579	GLY	2.2
1	C	626[A]	VAL	2.2
1	A	539	GLU	2.2
1	C	692	ASP	2.1
1	D	41	GLN	2.0
1	A	38	ASP	2.0
1	D	38	ASP	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, 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.

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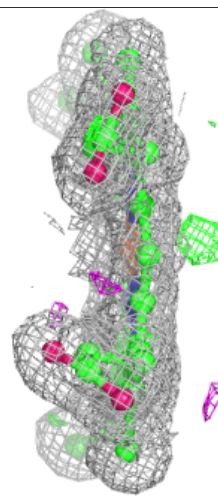
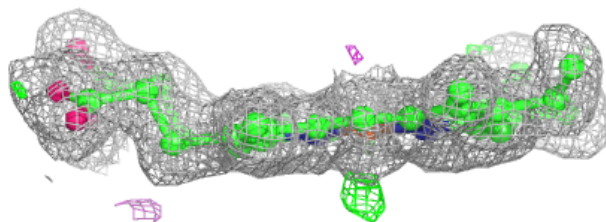
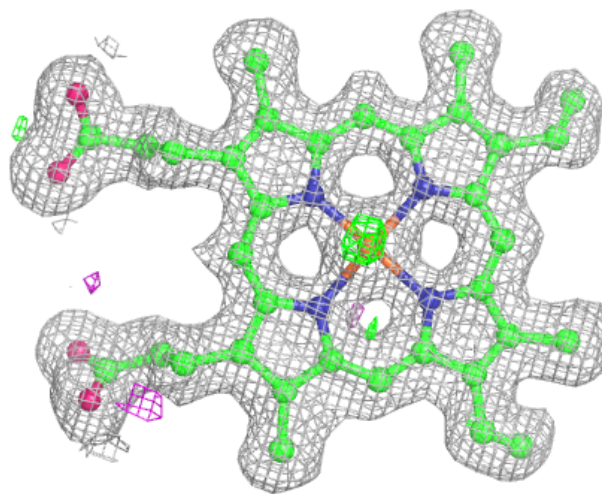
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	1PE	D	1722	6/16	0.73	0.20	23,28,34,34	0
4	1PE	D	1719	3/16	0.79	0.13	26,26,30,31	0
4	1PE	D	1723	9/16	0.80	0.20	22,33,37,40	0
4	1PE	C	1724	3/16	0.81	0.16	22,22,23,36	0
4	1PE	A	1724	9/16	0.81	0.17	19,26,33,34	0
4	1PE	A	1720	3/16	0.82	0.18	23,23,30,31	0
4	1PE	D	1720	3/16	0.82	0.17	26,26,27,39	0
4	1PE	B	1720	3/16	0.82	0.13	14,14,27,33	0
4	1PE	A	1723	6/16	0.82	0.22	28,31,31,32	0
4	1PE	C	1723	3/16	0.83	0.14	18,18,22,31	0
4	1PE	B	1722	6/16	0.84	0.15	26,37,40,42	0
3	ACT	D	1718	4/4	0.85	0.17	6,12,17,20	0
4	1PE	A	1721	3/16	0.85	0.10	24,24,25,35	0
4	1PE	A	1719	3/16	0.86	0.13	24,24,25,27	0
4	1PE	B	1723	6/16	0.86	0.15	16,25,32,37	0
4	1PE	B	1725	12/16	0.86	0.15	16,23,36,41	0
4	1PE	A	1718	3/16	0.88	0.10	25,25,28,33	0
4	1PE	B	1721	3/16	0.89	0.12	16,16,25,32	0
4	1PE	C	1725	6/16	0.89	0.10	24,29,33,38	0
4	1PE	B	1726	12/16	0.90	0.14	12,20,28,37	0
3	ACT	B	1719	4/4	0.90	0.16	5,7,19,23	0
4	1PE	C	1726	6/16	0.90	0.13	17,24,35,37	0
4	1PE	C	1727	9/16	0.90	0.13	21,25,35,40	0
3	ACT	A	1717	4/4	0.91	0.16	5,8,13,18	0
4	1PE	B	1724	6/16	0.93	0.10	16,22,24,44	0
4	1PE	D	1721	3/16	0.93	0.08	16,16,21,30	0
3	ACT	C	1721	4/4	0.93	0.10	7,7,10,15	0
4	1PE	A	1722	6/16	0.93	0.15	15,24,26,31	0
3	ACT	C	1722	4/4	0.94	0.12	8,8,21,25	0
2	HEM	C	1720	43/43	0.97	0.09	0,4,8,11	0
3	ACT	D	1717	4/4	0.97	0.08	5,6,8,11	0
3	ACT	B	1718	4/4	0.97	0.07	8,10,12,13	0
3	ACT	A	1716	4/4	0.98	0.07	6,6,7,8	0
2	HEM	B	1717	43/43	0.98	0.10	0,2,6,7	0
2	HEM	A	1715	43/43	0.98	0.09	0,3,6,8	0
2	HEM	D	1716	43/43	0.98	0.08	1,4,5,7	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 C 1720:**

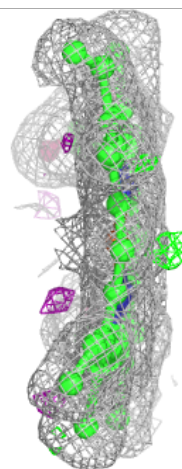
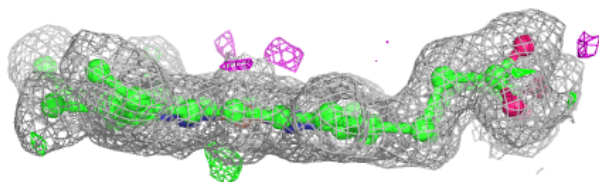
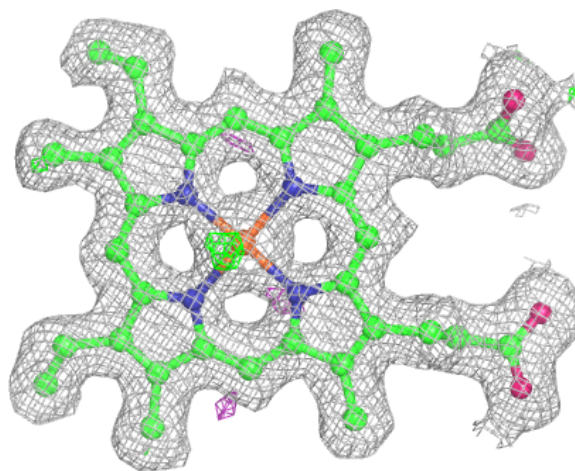
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





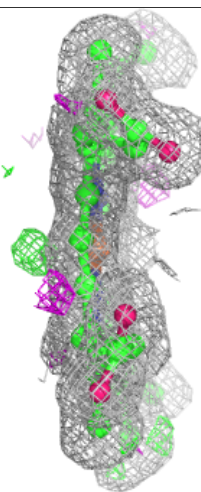
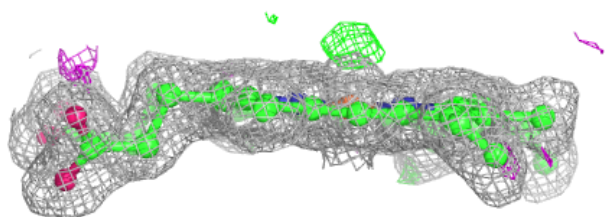
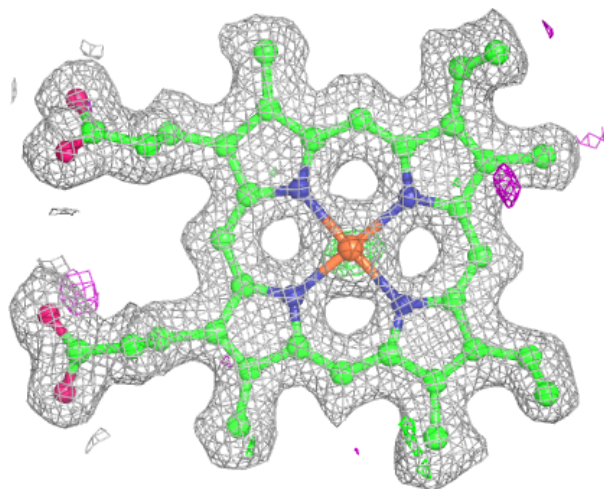
**Electron density around HEM B 1717:**

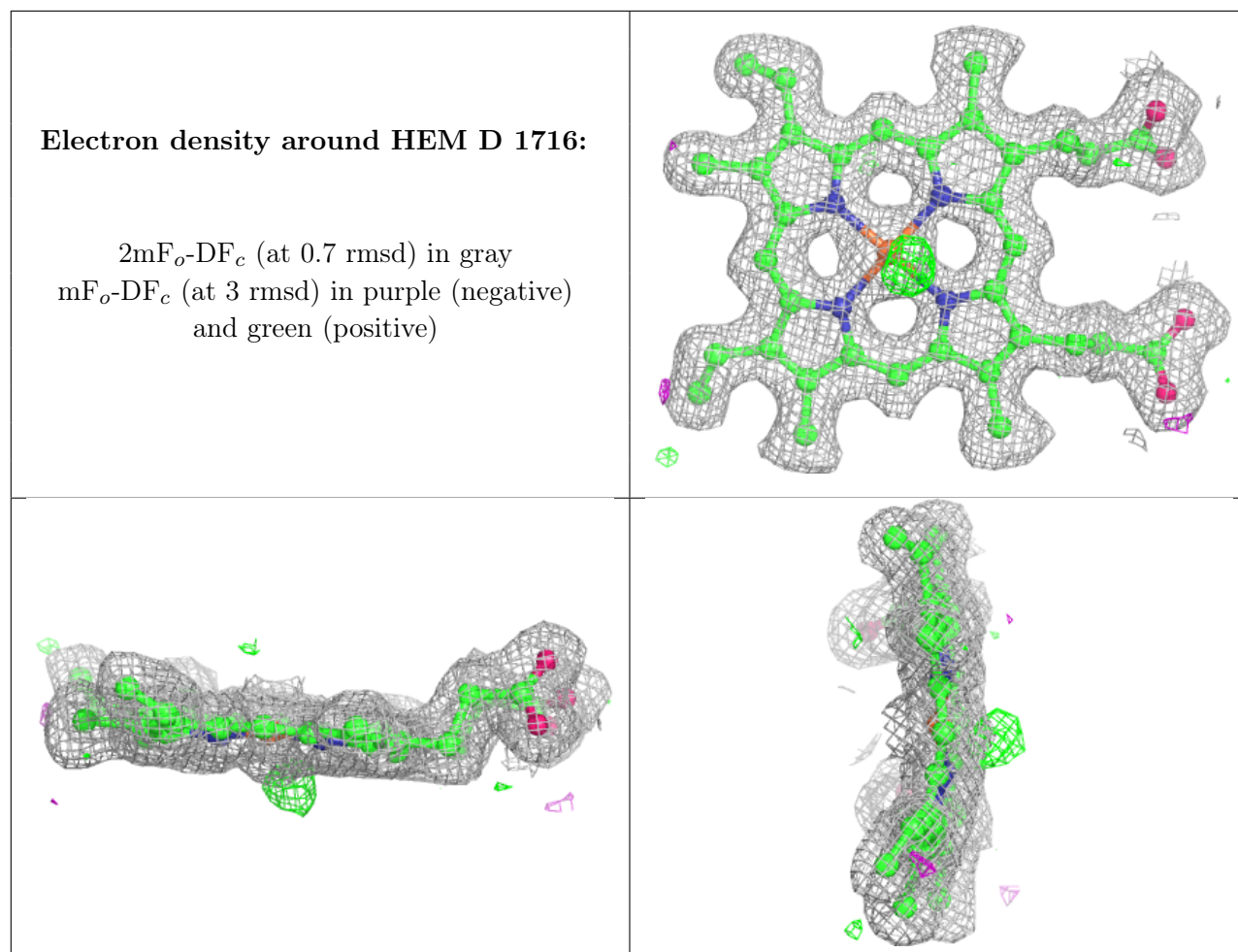
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM A 1715:**

$2mF_o-DF_c$  (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.