



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 01:11 AM EDT

PDB ID : 1QWS  
Title : Structure of the D181N variant of catalase HP11 from E. coli  
Authors : Chelikani, P.; Carpena, X.; Fita, I.; Loewen, P.C.  
Deposited on : 2003-09-03  
Resolution : 1.90 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.

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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 : 1.8.5 (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

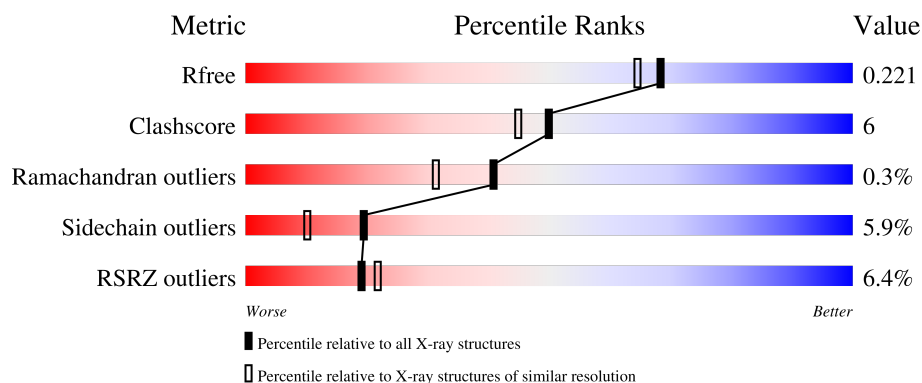
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	753	<div> <div>5%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>..</div> </div> </div>
1	B	753	<div> <div>9%</div> <div> <div></div> <div>80%</div> <div>14%</div> <div>..</div> </div> </div>
1	C	753	<div> <div>7%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>...</div> </div> </div>
1	D	753	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>15%</div> <div>..</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26230 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.

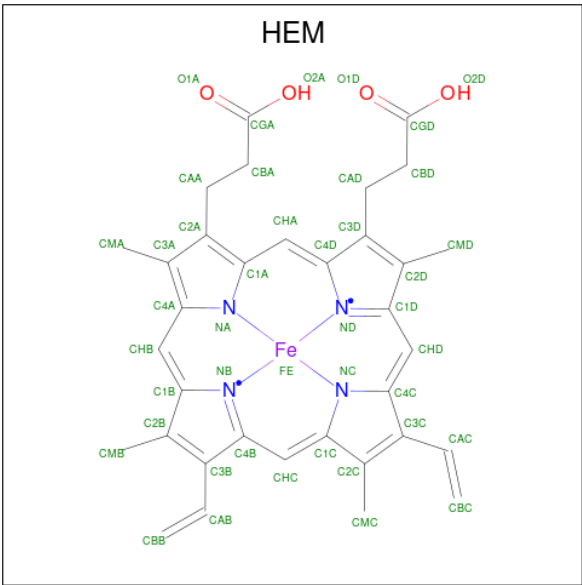
- Molecule 1 is a protein called Catalase HPIL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	3	0
			5759	3656	1009	1082	12			
1	B	727	Total	C	N	O	S	0	2	0
			5753	3652	1007	1082	12			
1	C	727	Total	C	N	O	S	0	4	0
			5760	3657	1009	1082	12			
1	D	727	Total	C	N	O	S	0	2	0
			5753	3652	1007	1082	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	ASN	ASP	engineered mutation	UNP P21179
B	181	ASN	ASP	engineered mutation	UNP P21179
C	181	ASN	ASP	engineered mutation	UNP P21179
D	181	ASN	ASP	engineered mutation	UNP P21179

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



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

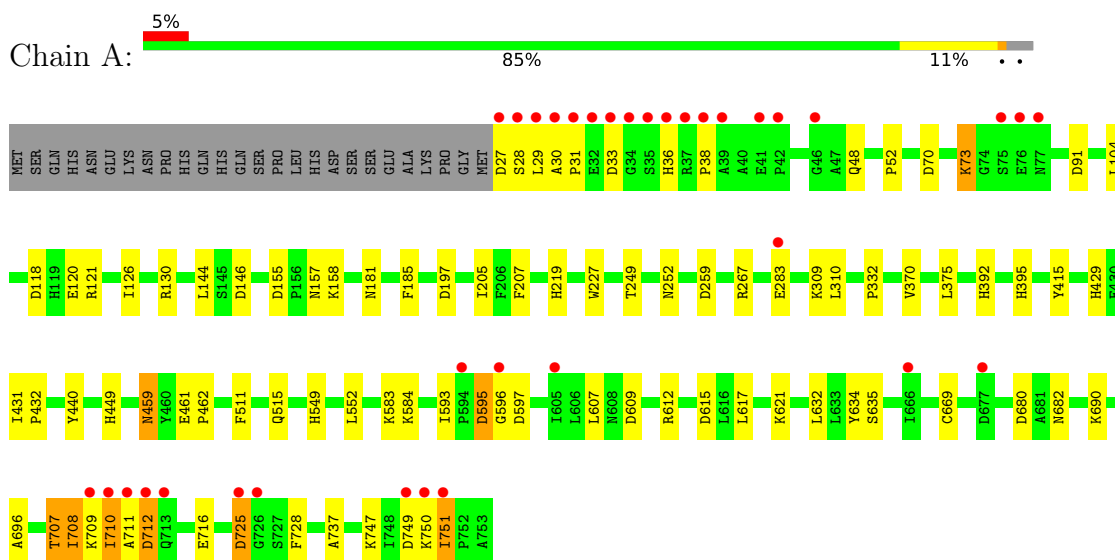
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	824	Total	O	0	0
			824	824		
3	B	670	Total	O	0	0
			670	670		
3	C	746	Total	O	0	0
			746	746		
3	D	793	Total	O	0	0
			793	793		

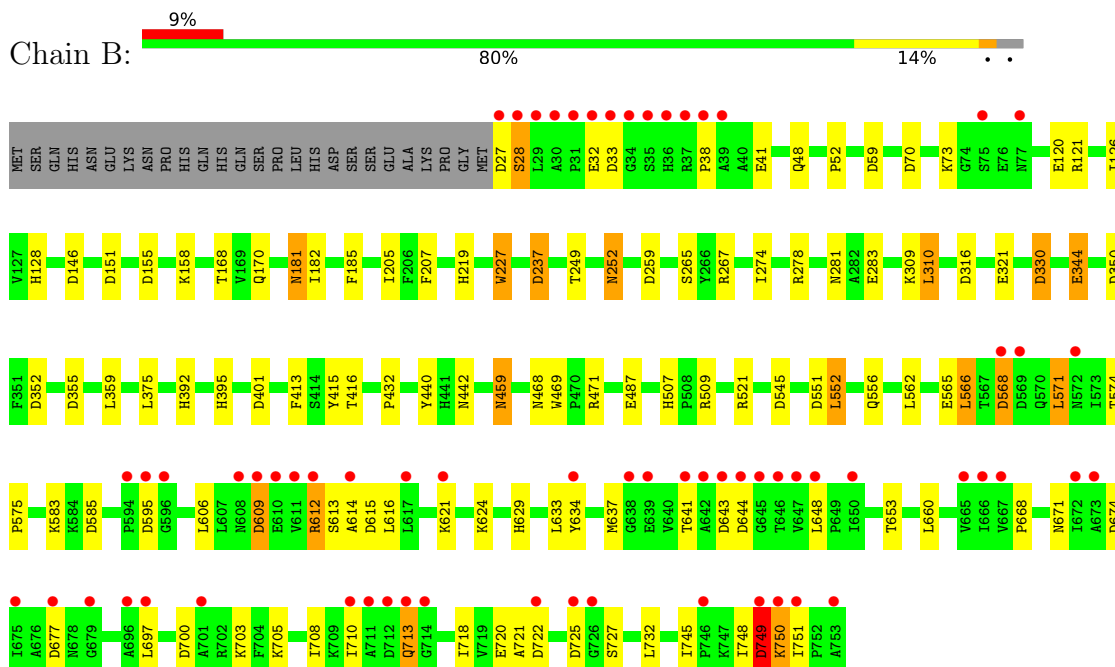
### 3 Residue-property plots

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 HPII

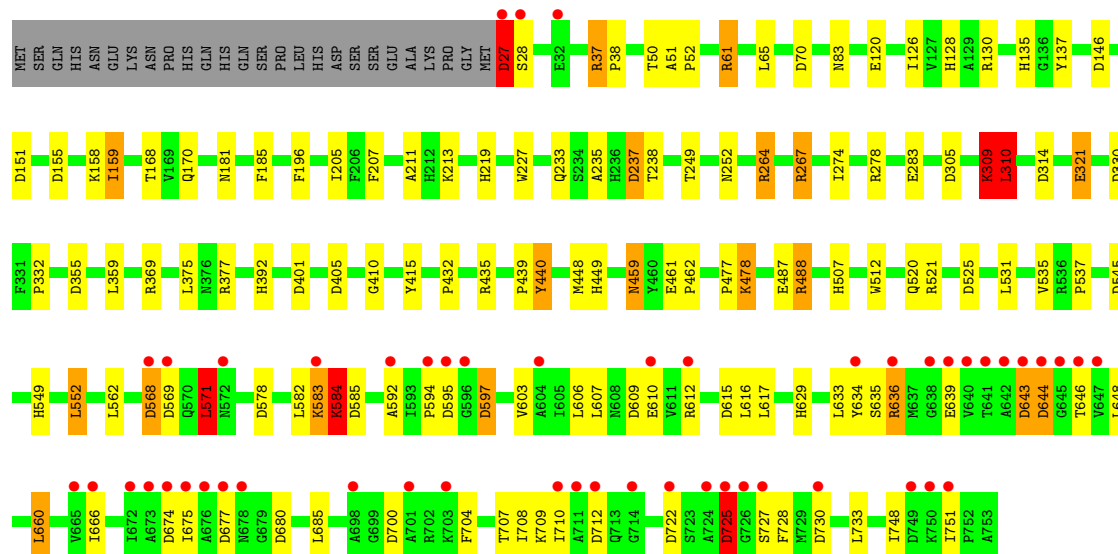


#### • Molecule 1: Catalase HPII




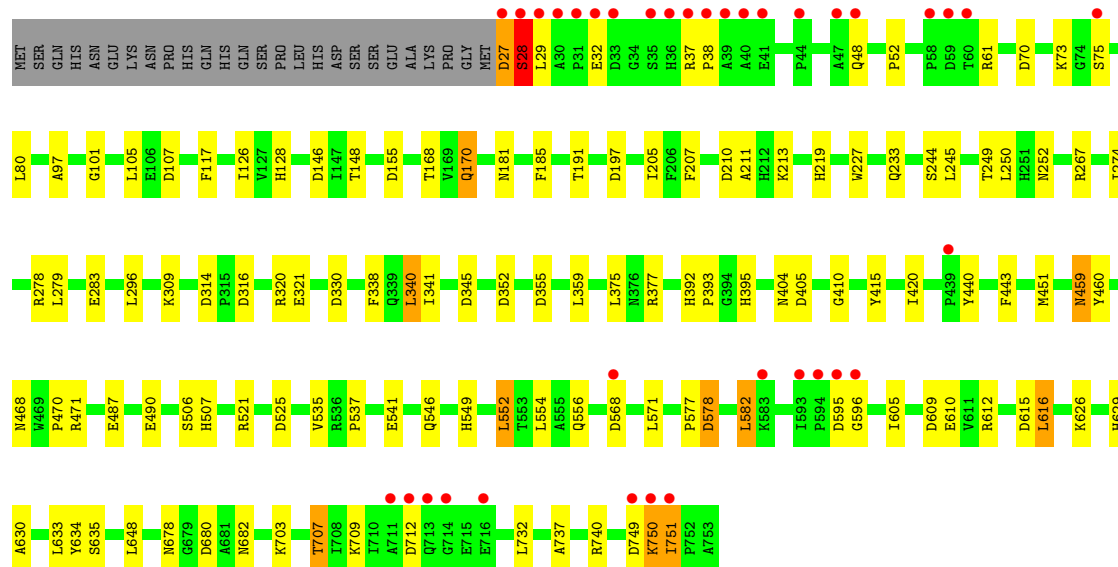
- Molecule 1: Catalase HP11

Chain C:  7% 78% 15%



- Molecule 1: Catalase HP11

Chain D:  5% 80% 15%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.43Å 132.88Å 122.10Å 90.00° 109.66° 90.00°	Depositor
Resolution (Å)	28.00 – 1.90 27.81 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (28.00-1.90) 99.5 (27.81-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.28 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.164 , 0.220 0.166 , 0.221	Depositor DCC
$R_{free}$ test set	10989 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.8	Xtriage
Anisotropy	0.018	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 54.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	26230	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.90	0/5930	0.91	12/8062 (0.1%)
1	B	0.84	0/5919	0.91	26/8047 (0.3%)
1	C	0.86	2/5938 (0.0%)	0.94	34/8072 (0.4%)
1	D	0.90	0/5919	0.94	22/8047 (0.3%)
All	All	0.88	2/23706 (0.0%)	0.93	94/32228 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	1
All	All	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	235	ALA	CA-CB	5.41	1.63	1.52
1	C	196	PHE	CE1-CZ	5.31	1.47	1.37

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	595	ASP	CB-CG-OD2	8.87	126.28	118.30
1	B	155	ASP	CB-CG-OD2	7.99	125.49	118.30
1	D	155	ASP	CB-CG-OD2	7.95	125.45	118.30
1	D	615	ASP	CB-CG-OD2	7.88	125.39	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	355	ASP	CB-CG-OD2	7.62	125.16	118.30
1	D	609	ASP	CB-CG-OD2	7.45	125.01	118.30
1	B	146	ASP	CB-CG-OD2	7.36	124.92	118.30
1	D	61	ARG	NE-CZ-NH2	7.29	123.95	120.30
1	C	155	ASP	CB-CG-OD2	7.26	124.83	118.30
1	D	355	ASP	CB-CG-OD2	7.15	124.73	118.30
1	A	259	ASP	CB-CG-OD2	7.15	124.73	118.30
1	C	725	ASP	CB-CG-OD2	7.14	124.72	118.30
1	C	569	ASP	CB-CG-OD2	7.08	124.67	118.30
1	D	146	ASP	CB-CG-OD2	7.03	124.63	118.30
1	D	61	ARG	NE-CZ-NH1	-7.00	116.80	120.30
1	A	680	ASP	CB-CG-OD2	6.93	124.54	118.30
1	C	644	ASP	CB-CG-OD2	6.87	124.48	118.30
1	C	130	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	B	352	ASP	CB-CG-OD2	6.83	124.45	118.30
1	D	197	ASP	CB-CG-OD2	6.81	124.43	118.30
1	C	27	ASP	CB-CG-OD2	6.75	124.38	118.30
1	C	615	ASP	CB-CG-OD2	6.72	124.35	118.30
1	B	615	ASP	CB-CG-OD2	6.69	124.32	118.30
1	C	680	ASP	CB-CG-OD2	6.54	124.19	118.30
1	A	197	ASP	CB-CG-OD2	6.54	124.19	118.30
1	C	545	ASP	CB-CG-OD2	6.50	124.15	118.30
1	B	350	ASP	CB-CG-OD2	6.48	124.13	118.30
1	B	259	ASP	CB-CG-OD2	6.46	124.12	118.30
1	C	674	ASP	CB-CG-OD2	6.44	124.10	118.30
1	C	310	LEU	CB-CG-CD1	6.33	121.75	111.00
1	B	316	ASP	CB-CG-OD2	6.31	123.98	118.30
1	D	578	ASP	CB-CG-OD2	6.27	123.95	118.30
1	B	609	ASP	CB-CG-OD2	6.22	123.90	118.30
1	C	730	ASP	CB-CG-OD2	6.21	123.89	118.30
1	D	316	ASP	CB-CG-OD2	6.17	123.85	118.30
1	D	314	ASP	CB-CG-OD2	6.16	123.84	118.30
1	D	70	ASP	CB-CG-OD2	6.12	123.81	118.30
1	C	405	ASP	CB-CG-OD2	6.11	123.80	118.30
1	C	585	ASP	CB-CG-OD2	6.10	123.79	118.30
1	C	525	ASP	CB-CG-OD2	6.01	123.71	118.30
1	B	677	ASP	CB-CG-OD2	5.97	123.68	118.30
1	B	350	ASP	CB-CG-OD1	-5.97	112.93	118.30
1	D	568	ASP	CB-CG-OD2	5.92	123.63	118.30
1	D	595	ASP	CB-CG-OD2	5.92	123.62	118.30
1	B	59	ASP	CB-CG-OD2	5.88	123.60	118.30
1	B	330	ASP	CB-CG-OD2	5.86	123.57	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	70	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	712	ASP	CB-CG-OD2	5.81	123.53	118.30
1	C	722	ASP	CB-CG-OD2	5.80	123.52	118.30
1	B	151	ASP	CB-CG-OD2	5.75	123.47	118.30
1	A	146	ASP	CB-CG-OD2	5.72	123.44	118.30
1	C	609	ASP	CB-CG-OD2	5.66	123.40	118.30
1	B	644	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	130	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	D	210	ASP	CB-CG-OD2	5.58	123.33	118.30
1	C	401	ASP	CB-CG-OD2	5.58	123.32	118.30
1	B	595	ASP	CB-CG-OD1	5.57	123.32	118.30
1	D	107	ASP	CB-CG-OD1	5.55	123.29	118.30
1	D	352	ASP	CB-CG-OD2	5.54	123.28	118.30
1	C	305	ASP	CB-CG-OD2	5.54	123.28	118.30
1	C	677	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	355	ASP	CB-CG-OD2	5.43	123.19	118.30
1	D	345	ASP	CB-CG-OD2	5.43	123.18	118.30
1	C	146	ASP	CB-CG-OD2	5.42	123.18	118.30
1	C	595	ASP	CB-CG-OD2	5.40	123.16	118.30
1	D	320	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	C	151	ASP	CB-CG-OD2	5.39	123.16	118.30
1	C	597	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	70	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	615	ASP	CB-CG-OD2	5.33	123.09	118.30
1	C	237	ASP	CB-CG-OD2	5.32	123.08	118.30
1	C	309	LYS	CD-CE-NZ	5.31	123.91	111.70
1	A	725	ASP	CB-CG-OD2	5.31	123.08	118.30
1	B	401	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	749	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	70	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	674	ASP	CB-CG-OD2	5.27	123.05	118.30
1	A	597	ASP	CB-CG-OD2	5.25	123.03	118.30
1	C	310	LEU	CA-CB-CG	5.25	127.37	115.30
1	B	585	ASP	CB-CG-OD2	5.24	123.01	118.30
1	B	722	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	568	ASP	CB-CG-OD2	5.19	122.97	118.30
1	D	740	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	C	643	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	643	ASP	CB-CG-OD2	5.16	122.94	118.30
1	C	314	ASP	CB-CG-OD2	5.13	122.92	118.30
1	D	712	ASP	CB-CG-OD2	5.13	122.91	118.30
1	A	609	ASP	CB-CG-OD2	5.12	122.91	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	545	ASP	CB-CG-OD2	5.10	122.89	118.30
1	B	237	ASP	CB-CG-OD2	5.08	122.87	118.30
1	C	700	ASP	CB-CG-OD2	5.06	122.86	118.30
1	C	568	ASP	CB-CG-OD2	5.06	122.85	118.30
1	D	525	ASP	CB-CG-OD2	5.03	122.83	118.30
1	C	571	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	708	ILE	Peptide
1	B	170[A]	GLN	Sidechain
1	B	170[B]	GLN	Sidechain
1	C	725	ASP	Peptide

## 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	5759	0	5593	60	0
1	B	5753	0	5591	70	0
1	C	5760	0	5591	82	0
1	D	5753	0	5591	84	0
2	A	43	0	30	0	0
2	B	43	0	30	1	0
2	C	43	0	30	1	0
2	D	43	0	30	1	0
3	A	824	0	0	16	3
3	B	670	0	0	14	2
3	C	746	0	0	20	0
3	D	793	0	0	22	1
All	All	26230	0	22486	265	3

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 6.

All (265) 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:392:HIS:ND1	1:A:415:TYR:CB	1.68	1.55
1:D:392:HIS:ND1	1:D:415:TYR:CB	1.68	1.49
1:B:392:HIS:ND1	1:B:415:TYR:CB	1.76	1.45
1:C:392:HIS:ND1	1:C:415:TYR:CB	1.76	1.45
1:A:392:HIS:CE1	1:A:415:TYR:HB2	1.65	1.31
1:D:392:HIS:CE1	1:D:415:TYR:HB2	1.65	1.29
1:D:546:GLN:HG3	3:D:3593:HOH:O	1.27	1.27
1:B:392:HIS:CE1	1:B:415:TYR:HB2	1.71	1.25
1:B:392:HIS:ND1	1:B:415:TYR:HB2	0.87	1.19
1:B:416:THR:HG21	3:D:3346:HOH:O	1.40	1.19
1:C:392:HIS:CE1	1:C:415:TYR:HB2	1.77	1.16
1:C:392:HIS:ND1	1:C:415:TYR:HB2	0.84	1.15
1:A:449[A]:HIS:CE1	3:A:4019:HOH:O	1.96	1.13
3:B:3562:HOH:O	1:D:73:LYS:HD2	1.48	1.13
1:D:392:HIS:ND1	1:D:415:TYR:HB2	0.80	1.12
1:A:392:HIS:ND1	1:A:415:TYR:HB2	0.79	1.11
1:C:449[A]:HIS:CE1	3:C:4020:HOH:O	2.03	1.10
3:B:3562:HOH:O	1:D:73:LYS:CD	1.99	1.06
1:A:28:SER:HB3	1:D:245:LEU:HD22	1.42	0.99
3:B:4016:HOH:O	1:C:126[A]:ILE:HD11	1.61	0.99
1:A:612:ARG:NH1	1:A:669:CYS:SG	2.39	0.95
3:A:4014:HOH:O	1:D:126[A]:ILE:HD11	1.66	0.95
1:B:267:ARG:HG3	3:B:2851:HOH:O	1.73	0.86
1:C:643:ASP:OD2	3:C:3873:HOH:O	1.92	0.86
1:D:267:ARG:HG3	3:D:2850:HOH:O	1.77	0.85
1:C:170[B]:GLN:OE1	3:C:4013:HOH:O	1.94	0.84
1:B:126[A]:ILE:CD1	3:C:4032:HOH:O	2.26	0.83
1:C:449[A]:HIS:NE2	3:C:4020:HOH:O	2.03	0.82
3:A:4014:HOH:O	1:D:126[A]:ILE:CD1	2.25	0.81
1:D:309:LYS:HE2	3:D:4026:HOH:O	1.80	0.81
1:C:748:ILE:O	1:C:751:ILE:HG22	1.80	0.81
1:B:309:LYS:HE3	3:B:1622:HOH:O	1.80	0.80
1:C:583:LYS:O	1:C:584:LYS:HB3	1.80	0.80
1:A:309:LYS:HE2	3:A:1213:HOH:O	1.82	0.79
1:A:449[A]:HIS:NE2	3:A:4019:HOH:O	2.08	0.79
1:B:126[A]:ILE:HD11	3:C:4032:HOH:O	1.82	0.79
1:A:120:GLU:HB2	1:D:126[B]:ILE:HD11	1.64	0.78
1:D:341:ILE:HG13	3:D:3820:HOH:O	1.83	0.78
1:B:120:GLU:HB2	1:C:126[B]:ILE:HD11	1.66	0.78
1:B:710:ILE:HD13	1:B:718:ILE:HG13	1.67	0.76
1:D:321:GLU:HG3	3:D:3063:HOH:O	1.86	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:4016:HOH:O	1:C:126[A]:ILE:CD1	2.27	0.75
1:A:392:HIS:ND1	1:A:415:TYR:CG	2.54	0.73
1:D:321:GLU:CG	3:D:3063:HOH:O	2.36	0.73
1:B:281:ASN:OD1	1:B:283:GLU:HG2	1.88	0.73
1:D:703:LYS:HE2	3:D:3594:HOH:O	1.88	0.73
1:C:264:ARG:HG3	1:C:264:ARG:HH11	1.53	0.72
1:B:309:LYS:CE	3:B:1622:HOH:O	2.35	0.72
1:D:541:GLU:HG2	3:D:3935:HOH:O	1.89	0.71
1:A:120:GLU:HB2	1:D:126[B]:ILE:CD1	2.20	0.71
1:D:27:ASP:O	1:D:28:SER:HB2	1.91	0.70
1:A:612:ARG:NH1	1:A:669:CYS:CB	2.55	0.70
1:B:392:HIS:ND1	1:B:415:TYR:HB3	2.03	0.69
1:A:395:HIS:HE1	3:A:4021:HOH:O	1.76	0.68
1:C:310:LEU:HD13	1:C:660:LEU:HB3	1.73	0.68
1:C:629:HIS:HD2	3:C:2095:HOH:O	1.76	0.67
1:D:392:HIS:ND1	1:D:415:TYR:CG	2.62	0.67
1:D:392:HIS:ND1	1:D:415:TYR:HB3	1.98	0.67
1:C:704:PHE:O	1:C:707:THR:HG22	1.94	0.66
1:D:629:HIS:HD2	3:D:2505:HOH:O	1.77	0.66
1:C:283:GLU:OE1	3:C:3190:HOH:O	2.13	0.66
1:A:690:LYS:HB2	1:A:751:ILE:HD11	1.77	0.65
1:B:629:HIS:HD2	3:B:1688:HOH:O	1.79	0.65
1:C:309:LYS:HB3	1:C:660:LEU:HD21	1.78	0.65
1:A:612:ARG:CZ	1:A:669:CYS:HB3	2.26	0.65
1:A:392:HIS:ND1	1:A:415:TYR:HB3	1.99	0.64
1:A:126[A]:ILE:HD11	3:D:4012:HOH:O	1.98	0.64
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.27	0.63
1:C:61:ARG:HG3	3:C:3513:HOH:O	1.97	0.63
1:D:274:ILE:HD12	2:D:760:HEM:HMB1	1.79	0.63
1:B:708:ILE:HD12	1:B:710:ILE:HD11	1.80	0.62
1:B:310:LEU:HD13	1:B:660:LEU:HB3	1.82	0.61
1:A:126[B]:ILE:HG12	1:D:117:PHE:CZ	2.35	0.61
1:A:449[B]:HIS:CG	1:C:449[B]:HIS:CG	2.48	0.61
1:B:27:ASP:OD2	1:D:468:ASN:HB3	2.01	0.60
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.17	0.60
1:B:521:ARG:HH21	1:B:745:ILE:HG21	1.66	0.60
1:C:439:PRO:HD3	3:C:3528:HOH:O	2.01	0.60
1:A:708:ILE:O	1:A:710:ILE:HG22	2.02	0.60
1:B:121:ARG:HG2	1:C:126[B]:ILE:HD12	1.85	0.59
1:A:144:LEU:HD11	1:A:370:VAL:HG13	1.83	0.59
3:B:3562:HOH:O	1:D:73:LYS:HD3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:552:LEU:HD21	1:B:571:LEU:HD12	1.84	0.59
1:C:274:ILE:HD12	2:C:760:HEM:HMB1	1.84	0.59
3:B:1589:HOH:O	1:D:52:PRO:HG3	2.04	0.58
1:A:392:HIS:CG	1:A:415:TYR:CB	2.77	0.57
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.87	0.57
1:C:725:ASP:HA	1:C:728:PHE:HB3	1.86	0.57
1:D:451:MET:SD	3:D:3795:HOH:O	2.57	0.57
1:C:392:HIS:ND1	1:C:415:TYR:CG	2.68	0.56
1:C:751:ILE:HD12	3:C:3261:HOH:O	2.05	0.56
1:A:716:GLU:CG	3:A:3875:HOH:O	2.52	0.56
1:D:682:ASN:HB3	1:D:707:THR:HG21	1.86	0.56
1:C:211:ALA:CB	1:C:410:GLY:HA3	2.36	0.55
1:B:552:LEU:HD22	1:B:556:GLN:HG3	1.88	0.55
1:A:30:ALA:HB1	1:A:31:PRO:HD2	1.87	0.55
1:A:725:ASP:H	1:A:728:PHE:HB3	1.72	0.55
1:D:283:GLU:OE2	3:D:3376:HOH:O	2.18	0.54
1:D:321:GLU:HG2	3:D:3063:HOH:O	2.05	0.54
1:B:265:SER:HB2	1:B:321:GLU:HG2	1.90	0.54
1:A:155:ASP:HB3	1:A:158:LYS:HB2	1.89	0.53
1:A:157:ASN:ND2	3:A:2976:HOH:O	2.19	0.53
1:C:477:PRO:HD2	1:C:478:LYS:NZ	2.23	0.53
1:C:321:GLU:OE2	3:C:2025:HOH:O	2.19	0.53
1:A:583:LYS:O	1:A:584:LYS:HB3	2.08	0.53
1:B:468:ASN:HD22	1:D:27:ASP:N	2.07	0.53
1:C:636:ARG:NH2	1:C:639:GLU:O	2.42	0.53
1:D:392:HIS:CG	1:D:415:TYR:CB	2.79	0.52
1:C:578:ASP:HB2	1:C:582:LEU:O	2.08	0.52
1:A:716:GLU:HG3	3:A:3875:HOH:O	2.10	0.52
3:A:3400:HOH:O	1:C:27:ASP:HB3	2.10	0.52
1:B:126[B]:ILE:CD1	1:C:120:GLU:HB2	2.40	0.52
1:B:697:LEU:O	1:B:720:GLU:HA	2.09	0.52
1:B:395:HIS:HE1	3:B:4022:HOH:O	1.93	0.52
1:C:137:TYR:HB2	1:C:159:ILE:HD11	1.93	0.51
1:C:488:ARG:NH1	1:D:490:GLU:OE1	2.38	0.51
1:B:52:PRO:HG3	3:D:2403:HOH:O	2.10	0.51
1:C:727:SER:HA	3:C:3570:HOH:O	2.10	0.51
1:A:595:ASP:O	3:A:2885:HOH:O	2.18	0.51
1:A:126[B]:ILE:HD13	1:D:117:PHE:O	2.10	0.51
1:B:27:ASP:HB3	1:D:471:ARG:CZ	2.41	0.51
1:A:612:ARG:CZ	1:A:669:CYS:CB	2.89	0.51
1:C:392:HIS:CG	1:C:415:TYR:CB	2.83	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126[A]:ILE:CD1	3:D:4012:HOH:O	2.57	0.50
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.94	0.50
1:C:267:ARG:HD3	1:C:332:PRO:HG3	1.93	0.50
1:A:431:ILE:HG13	1:C:449[A]:HIS:CE1	2.47	0.50
1:C:37:ARG:NH1	3:C:2803:HOH:O	2.39	0.50
1:C:392:HIS:ND1	1:C:415:TYR:HB3	2.09	0.50
1:C:359:LEU:H	1:C:507:HIS:HD2	1.60	0.49
1:D:678:ASN:OD1	1:D:680:ASP:HB2	2.13	0.49
1:D:556:GLN:NE2	3:D:3620:HOH:O	2.45	0.49
1:B:274:ILE:HD12	2:B:760:HEM:HMB1	1.93	0.49
1:B:634:TYR:O	1:B:653:THR:HA	2.12	0.49
1:A:118:ASP:O	1:D:126[A]:ILE:HD11	2.12	0.49
3:A:1180:HOH:O	1:C:52:PRO:HG3	2.12	0.49
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.28	0.49
1:A:549:HIS:HE1	3:A:3618:HOH:O	1.95	0.49
1:B:120:GLU:HB2	1:C:126[B]:ILE:CD1	2.40	0.48
1:D:506:SER:HB2	1:D:577:PRO:O	2.13	0.48
1:B:38:PRO:HA	1:B:48:GLN:OE1	2.13	0.48
1:A:38:PRO:HA	1:A:48:GLN:OE1	2.13	0.48
1:D:596:GLY:HA3	1:D:737:ALA:O	2.13	0.48
1:A:104:LEU:HB3	3:C:1170:HOH:O	2.13	0.48
1:B:359:LEU:H	1:B:507:HIS:HD2	1.61	0.48
1:B:749:ASP:HB3	1:B:750:LYS:HE2	1.94	0.48
1:D:170[B]:GLN:HE22	1:D:233:GLN:C	2.17	0.48
1:D:244:SER:HA	3:D:3593:HOH:O	2.13	0.48
1:B:27:ASP:HB3	1:D:471:ARG:NH2	2.29	0.47
1:C:448:MET:HG3	1:C:449[B]:HIS:CD2	2.50	0.47
1:D:27:ASP:HB2	1:D:29:LEU:HG	1.95	0.47
1:B:637:MET:HB2	1:C:562:LEU:HA	1.96	0.47
1:C:603:VAL:HG11	1:C:666:ILE:HG13	1.95	0.47
1:B:442:ASN:HA	1:D:80:LEU:HD12	1.96	0.47
1:A:73:LYS:NZ	1:C:440:TYR:O	2.46	0.47
1:C:552:LEU:HD21	1:C:571:LEU:HD12	1.96	0.47
1:D:709:LYS:HG3	1:D:750:LYS:HE3	1.97	0.47
1:A:309:LYS:HD2	3:A:4025:HOH:O	2.14	0.47
1:C:137:TYR:HB2	1:C:159:ILE:HD12	1.96	0.47
1:B:469:TRP:CE3	1:B:471:ARG:HG3	2.50	0.47
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.30	0.47
1:D:359:LEU:H	1:D:507:HIS:HD2	1.63	0.47
1:B:713:GLN:H	1:B:713:GLN:HG3	1.54	0.46
1:D:552:LEU:HD21	1:D:571:LEU:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:750:LYS:HZ2	1:D:751:ILE:HA	1.81	0.46
1:B:413:PHE:HB2	1:D:105:LEU:HD11	1.96	0.46
1:D:27:ASP:O	1:D:28:SER:CB	2.63	0.46
1:C:264:ARG:HH11	1:C:264:ARG:CG	2.22	0.46
1:A:696:ALA:HB1	1:A:728:PHE:CZ	2.50	0.46
1:C:238:THR:HB	1:D:460:TYR:CE2	2.50	0.46
1:A:267:ARG:HG2	1:A:332:PRO:HG3	1.98	0.46
1:C:170[B]:GLN:HE22	1:C:233:GLN:C	2.20	0.46
1:C:583:LYS:O	1:C:584:LYS:CB	2.57	0.46
1:A:52:PRO:HG3	3:C:1993:HOH:O	2.15	0.45
1:D:750:LYS:HZ2	1:D:750:LYS:C	2.20	0.45
1:C:634:TYR:CG	1:C:635:SER:N	2.84	0.45
1:D:37:ARG:HA	1:D:38:PRO:HD2	1.85	0.45
1:D:392:HIS:CE1	1:D:415:TYR:CB	2.59	0.45
1:A:716:GLU:HG2	3:A:3875:HOH:O	2.13	0.45
1:C:435:ARG:HD3	3:C:2147:HOH:O	2.17	0.45
1:D:750:LYS:HD3	1:D:751:ILE:HG22	1.99	0.45
1:A:121:ARG:HG2	1:D:126[B]:ILE:HD12	1.98	0.45
1:A:596:GLY:HA3	1:A:737:ALA:O	2.17	0.45
1:A:461:GLU:HA	1:A:462:PRO:C	2.36	0.45
1:B:392:HIS:ND1	1:B:415:TYR:CG	2.72	0.44
1:C:330:ASP:OD1	1:C:629:HIS:HE1	2.00	0.44
1:D:97:ALA:O	1:D:101:GLY:HA3	2.17	0.44
1:B:616:LEU:CD1	1:B:648:LEU:HD22	2.47	0.44
1:C:461:GLU:HA	1:C:462:PRO:C	2.38	0.44
1:B:750:LYS:NZ	1:B:750:LYS:HB3	2.33	0.44
1:B:721:ALA:HB2	3:B:2194:HOH:O	2.16	0.44
1:C:207:PHE:O	1:C:249:THR:HA	2.18	0.44
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.33	0.44
1:A:429:HIS:CD2	1:C:83:ASN:HB3	2.52	0.44
1:B:181:ASN:HB3	1:B:182:ILE:O	2.17	0.44
1:B:705:LYS:NZ	1:B:720:GLU:OE2	2.42	0.44
1:D:341:ILE:CG1	3:D:3820:HOH:O	2.53	0.44
1:A:459:ASN:HD22	1:A:459:ASN:C	2.20	0.44
1:D:278:ARG:HH12	1:D:487:GLU:CD	2.22	0.44
1:C:359:LEU:H	1:C:507:HIS:CD2	2.36	0.43
1:D:126[A]:ILE:HG12	3:D:2343:HOH:O	2.17	0.43
1:D:605:ILE:HD12	1:D:630:ALA:HB1	1.99	0.43
1:B:126[B]:ILE:HD11	1:C:120:GLU:HB2	1.99	0.43
1:C:128:HIS:HA	1:C:168:THR:O	2.17	0.43
1:A:511:PHE:O	1:A:515:GLN:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:GLU:CD	1:B:344:GLU:H	2.22	0.43
1:B:612:ARG:O	1:B:614:ALA:N	2.52	0.43
1:D:732:LEU:C	1:D:732:LEU:HD13	2.39	0.43
1:A:309:LYS:CE	3:A:1213:HOH:O	2.56	0.43
1:B:207:PHE:O	1:B:249:THR:HA	2.18	0.43
1:C:708:ILE:HG13	1:C:710:ILE:HG12	2.00	0.43
1:D:211:ALA:CB	1:D:410:GLY:HA3	2.48	0.43
1:B:359:LEU:H	1:B:507:HIS:CD2	2.37	0.42
1:B:392:HIS:CE1	1:B:415:TYR:CB	2.65	0.42
1:B:745:ILE:O	1:B:748:ILE:HG12	2.19	0.42
1:C:278:ARG:HH12	1:C:487:GLU:CD	2.22	0.42
1:D:535:VAL:O	1:D:537:PRO:HD3	2.18	0.42
1:B:128:HIS:HA	1:B:168:THR:O	2.20	0.42
1:D:148:THR:HB	1:D:279:LEU:HB3	2.01	0.42
1:B:227:TRP:CZ3	1:C:50:THR:HG21	2.54	0.42
1:C:477:PRO:HD2	1:C:478:LYS:HZ1	1.84	0.42
1:C:592:ALA:O	1:C:594:PRO:HD3	2.20	0.42
1:A:392:HIS:CE1	1:A:415:TYR:CB	2.60	0.42
1:B:556:GLN:HG2	1:B:566:LEU:HD23	2.01	0.42
1:C:535:VAL:O	1:C:537:PRO:HD3	2.18	0.42
1:D:128:HIS:HA	1:D:168:THR:O	2.19	0.42
1:D:395:HIS:HE1	3:D:4024:HOH:O	2.02	0.42
1:D:549:HIS:HD2	3:D:3114:HOH:O	2.03	0.42
1:C:38:PRO:HG2	1:C:51:ALA:HB2	2.01	0.42
1:D:634:TYR:CG	1:D:635:SER:N	2.87	0.42
1:B:708:ILE:CD1	1:B:710:ILE:HD11	2.49	0.42
1:C:264:ARG:CG	1:C:264:ARG:NH1	2.81	0.42
1:D:338:PHE:HB3	1:D:340:LEU:HD13	2.02	0.42
1:B:609:ASP:OD2	1:B:671:ASN:ND2	2.52	0.42
1:D:578:ASP:HB3	1:D:582:LEU:O	2.19	0.42
1:D:616:LEU:HD23	1:D:616:LEU:HA	1.82	0.42
1:C:607:LEU:O	1:C:634:TYR:HD1	2.03	0.41
1:B:278:ARG:HH22	1:B:487:GLU:CD	2.24	0.41
1:B:509:ARG:NH2	1:B:551:ASP:OD2	2.50	0.41
1:B:606:LEU:O	1:B:668:PRO:HD2	2.20	0.41
1:C:65:LEU:HD21	1:C:135:HIS:CG	2.55	0.41
1:B:267:ARG:HD2	3:B:1630:HOH:O	2.19	0.41
1:D:278:ARG:HH21	1:D:278:ARG:HD2	1.73	0.41
1:D:207:PHE:O	1:D:249:THR:HA	2.20	0.41
1:A:607:LEU:HD11	1:A:632:LEU:HB3	2.02	0.41
1:B:252:ASN:HD22	1:B:252:ASN:HA	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:521:ARG:NH2	1:B:745:ILE:HG21	2.34	0.41
1:C:512:TRP:CH2	1:C:520:GLN:HB3	2.56	0.41
1:C:584:LYS:NZ	3:C:2710:HOH:O	2.50	0.41
1:D:250:LEU:HD11	1:D:546:GLN:HE21	1.85	0.41
1:D:443:PHE:CZ	1:D:470:PRO:HD2	2.56	0.41
1:A:207:PHE:O	1:A:249:THR:HA	2.21	0.41
1:D:393:PRO:HD2	1:D:415:TYR:CG	2.55	0.41
1:A:634:TYR:CG	1:A:635:SER:N	2.89	0.41
1:B:267:ARG:NH1	3:B:1630:HOH:O	2.48	0.41
1:C:549:HIS:HE1	3:C:3758:HOH:O	2.04	0.41
1:D:296:LEU:HD23	1:D:296:LEU:HA	1.91	0.41
1:D:404:ASN:O	1:D:405:ASP:C	2.59	0.41
1:A:682:ASN:HB3	1:A:707:THR:HG21	2.03	0.41
1:B:725:ASP:OD2	1:B:727:SER:N	2.54	0.40
1:B:574:THR:HA	1:B:575:PRO:HD2	1.96	0.40
1:C:644:ASP:OD2	1:C:646:THR:OG1	2.32	0.40
1:C:751:ILE:HB	3:C:3261:HOH:O	2.20	0.40
1:A:91:ASP:OD1	1:C:461:GLU:OE1	2.39	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3290:HOH:O	3:D:3196:HOH:O[1_455]	1.54	0.66
3:A:1050:HOH:O	3:B:3771:HOH:O[2_545]	1.93	0.27
3:A:3831:HOH:O	3:B:3771:HOH:O[2_545]	2.14	0.06

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	728/753 (97%)	701 (96%)	26 (4%)	1 (0%)	51 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	727/753 (96%)	706 (97%)	19 (3%)	2 (0%)	41	31
1	C	729/753 (97%)	705 (97%)	21 (3%)	3 (0%)	34	24
1	D	727/753 (96%)	705 (97%)	20 (3%)	2 (0%)	41	31
All	All	2911/3012 (97%)	2817 (97%)	86 (3%)	8 (0%)	41	31

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	711	ALA
1	B	613	SER
1	D	28	SER
1	B	28	SER
1	C	584	LYS
1	C	612	ARG
1	C	725	ASP
1	D	75	SER

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	615/636 (97%)	587 (95%)	28 (5%)	27	17
1	B	614/636 (96%)	577 (94%)	37 (6%)	19	9
1	C	616/636 (97%)	568 (92%)	48 (8%)	12	5
1	D	614/636 (96%)	581 (95%)	33 (5%)	22	13
All	All	2459/2544 (97%)	2313 (94%)	146 (6%)	19	10

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASP
1	A	29	LEU
1	A	33	ASP

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Mol	Chain	Res	Type
1	A	36	HIS
1	A	73	LYS
1	A	181	ASN
1	A	185	PHE
1	A	205	ILE
1	A	227	TRP
1	A	252	ASN
1	A	283	GLU
1	A	310	LEU
1	A	375	LEU
1	A	432	PRO
1	A	440	TYR
1	A	459	ASN
1	A	552	LEU
1	A	593	ILE
1	A	617	LEU
1	A	621	LYS
1	A	707	THR
1	A	709	LYS
1	A	710	ILE
1	A	712	ASP
1	A	747	LYS
1	A	749	ASP
1	A	750	LYS
1	A	751	ILE
1	B	28	SER
1	B	32	GLU
1	B	33	ASP
1	B	41	GLU
1	B	73	LYS
1	B	158	LYS
1	B	181	ASN
1	B	185	PHE
1	B	205	ILE
1	B	227	TRP
1	B	237	ASP
1	B	252	ASN
1	B	310	LEU
1	B	344	GLU
1	B	375	LEU
1	B	432	PRO
1	B	440	TYR

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Mol	Chain	Res	Type
1	B	459	ASN
1	B	552	LEU
1	B	562	LEU
1	B	565	GLU
1	B	566	LEU
1	B	568	ASP
1	B	571	LEU
1	B	583	LYS
1	B	612	ARG
1	B	621	LYS
1	B	624	LYS
1	B	633	LEU
1	B	641	THR
1	B	700	ASP
1	B	703	LYS
1	B	713	GLN
1	B	732	LEU
1	B	749	ASP
1	B	750	LYS
1	B	751	ILE
1	C	27	ASP
1	C	28	SER
1	C	37	ARG
1	C	61	ARG
1	C	158	LYS
1	C	159	ILE
1	C	181	ASN
1	C	185	PHE
1	C	205	ILE
1	C	213	LYS
1	C	227	TRP
1	C	237	ASP
1	C	252	ASN
1	C	264	ARG
1	C	267	ARG
1	C	309	LYS
1	C	310	LEU
1	C	321	GLU
1	C	369	ARG
1	C	375	LEU
1	C	377	ARG
1	C	432	PRO

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Mol	Chain	Res	Type
1	C	440	TYR
1	C	459	ASN
1	C	478	LYS
1	C	488	ARG
1	C	521	ARG
1	C	531	LEU
1	C	552	LEU
1	C	568	ASP
1	C	571	LEU
1	C	583	LYS
1	C	584	LYS
1	C	597	ASP
1	C	606	LEU
1	C	610	GLU
1	C	616	LEU
1	C	617	LEU
1	C	633	LEU
1	C	636	ARG
1	C	648	LEU
1	C	660	LEU
1	C	675	ILE
1	C	685	LEU
1	C	709	LYS
1	C	712	ASP
1	C	725	ASP
1	C	733	LEU
1	D	27	ASP
1	D	28	SER
1	D	32	GLU
1	D	48	GLN
1	D	170[A]	GLN
1	D	170[B]	GLN
1	D	181	ASN
1	D	185	PHE
1	D	191	THR
1	D	205	ILE
1	D	213	LYS
1	D	227	TRP
1	D	252	ASN
1	D	340	LEU
1	D	375	LEU
1	D	377	ARG

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Mol	Chain	Res	Type
1	D	420	ILE
1	D	440	TYR
1	D	459	ASN
1	D	521	ARG
1	D	552	LEU
1	D	554	LEU
1	D	582	LEU
1	D	610	GLU
1	D	612	ARG
1	D	616	LEU
1	D	626	LYS
1	D	633	LEU
1	D	648	LEU
1	D	707	THR
1	D	749	ASP
1	D	750	LYS
1	D	751	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	252	ASN
1	A	459	ASN
1	A	515	GLN
1	B	252	ASN
1	B	459	ASN
1	B	507	HIS
1	B	629	HIS
1	B	713	GLN
1	C	252	ASN
1	C	368	GLN
1	C	459	ASN
1	C	507	HIS
1	C	572	ASN
1	C	629	HIS
1	C	671	ASN
1	D	48	GLN
1	D	252	ASN
1	D	449	HIS
1	D	459	ASN
1	D	507	HIS

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Mol	Chain	Res	Type
1	D	546	GLN
1	D	549	HIS
1	D	556	GLN
1	D	629	HIS

### 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](#)

4 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	HEM	B	760	1	27,50,50	2.01	9 (33%)	17,82,82	2.35	6 (35%)
2	HEM	D	760	1	27,50,50	2.26	8 (29%)	17,82,82	2.62	6 (35%)
2	HEM	A	760	1	27,50,50	2.16	9 (33%)	17,82,82	3.20	9 (52%)
2	HEM	C	760	1	27,50,50	1.96	6 (22%)	17,82,82	2.48	4 (23%)

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	B	760	1	-	0/6/54/54	-
2	HEM	D	760	1	-	0/6/54/54	-
2	HEM	A	760	1	-	0/6/54/54	-
2	HEM	C	760	1	-	0/6/54/54	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	760	HEM	C3D-C2D	4.98	1.52	1.37
2	A	760	HEM	C3C-C2C	-4.77	1.33	1.40
2	D	760	HEM	C3B-CAB	4.33	1.56	1.47
2	C	760	HEM	C3D-C2D	4.31	1.50	1.37
2	D	760	HEM	C3B-C2B	-4.19	1.34	1.40
2	A	760	HEM	CAA-C2A	4.14	1.58	1.52
2	C	760	HEM	C3B-C2B	-4.11	1.34	1.40
2	B	760	HEM	C3B-C2B	-4.09	1.34	1.40
2	A	760	HEM	C3D-C2D	4.03	1.49	1.37
2	B	760	HEM	C3C-C2C	-4.00	1.34	1.40
2	D	760	HEM	C3C-C2C	-3.96	1.34	1.40
2	C	760	HEM	C3B-CAB	3.94	1.56	1.47
2	B	760	HEM	C3D-C2D	3.92	1.49	1.37
2	A	760	HEM	C3B-C2B	-3.87	1.35	1.40
2	C	760	HEM	C3C-CAC	3.70	1.55	1.47
2	B	760	HEM	C3C-CAC	3.64	1.55	1.47
2	D	760	HEM	C3C-CAC	3.51	1.55	1.47
2	A	760	HEM	C3B-CAB	3.36	1.54	1.47
2	D	760	HEM	CAA-C2A	2.83	1.56	1.52
2	A	760	HEM	C3C-CAC	2.82	1.53	1.47
2	B	760	HEM	C3B-CAB	2.82	1.53	1.47
2	A	760	HEM	C4B-NB	2.68	1.41	1.36
2	C	760	HEM	CAA-C2A	2.56	1.55	1.52
2	C	760	HEM	CMA-C3A	2.33	1.56	1.51
2	B	760	HEM	CMA-C3A	2.22	1.56	1.51
2	A	760	HEM	CMC-C2C	2.19	1.56	1.51
2	A	760	HEM	C1D-ND	2.18	1.40	1.36
2	B	760	HEM	C1D-ND	2.17	1.40	1.36
2	B	760	HEM	CMC-C2C	2.14	1.56	1.51
2	D	760	HEM	CAD-C3D	2.09	1.55	1.52
2	B	760	HEM	CAA-C2A	2.04	1.55	1.52
2	D	760	HEM	C1C-C2C	2.02	1.47	1.42

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	760	HEM	CBD-CAD-C3D	-7.09	99.42	112.48
2	A	760	HEM	CBD-CAD-C3D	-7.08	99.44	112.48
2	D	760	HEM	CBD-CAD-C3D	-7.00	99.58	112.48
2	A	760	HEM	CAA-CBA-CGA	-6.14	102.37	112.67
2	B	760	HEM	CBD-CAD-C3D	-5.68	102.02	112.48
2	C	760	HEM	CAA-CBA-CGA	-4.71	104.77	112.67
2	D	760	HEM	CAA-CBA-CGA	-4.64	104.88	112.67
2	A	760	HEM	CMA-C3A-C4A	-4.57	121.44	128.46
2	B	760	HEM	CAA-CBA-CGA	-4.07	105.84	112.67
2	A	760	HEM	C4A-C3A-C2A	3.85	109.68	107.00
2	A	760	HEM	C4C-C3C-C2C	3.62	109.43	106.90
2	A	760	HEM	CAD-CBD-CGD	-3.43	106.92	112.67
2	D	760	HEM	C1D-C2D-C3D	-3.42	104.62	107.00
2	D	760	HEM	CMA-C3A-C4A	-3.38	123.26	128.46
2	D	760	HEM	CAD-CBD-CGD	-3.29	107.14	112.67
2	B	760	HEM	CMA-C3A-C4A	-3.15	123.62	128.46
2	A	760	HEM	C3C-C4C-NC	-2.50	106.23	110.94
2	C	760	HEM	CAD-CBD-CGD	-2.44	108.57	112.67
2	B	760	HEM	CAD-CBD-CGD	-2.43	108.60	112.67
2	B	760	HEM	CBA-CAA-C2A	-2.39	108.07	112.49
2	B	760	HEM	CMC-C2C-C3C	2.32	129.02	124.68
2	A	760	HEM	CMB-C2B-C3B	2.09	128.59	124.68
2	C	760	HEM	C4C-C3C-C2C	2.06	108.34	106.90
2	A	760	HEM	CMA-C3A-C2A	2.05	128.81	124.94
2	D	760	HEM	C4A-C3A-C2A	2.01	108.40	107.00

There are no chirality outliers.

There are no torsion outliers.

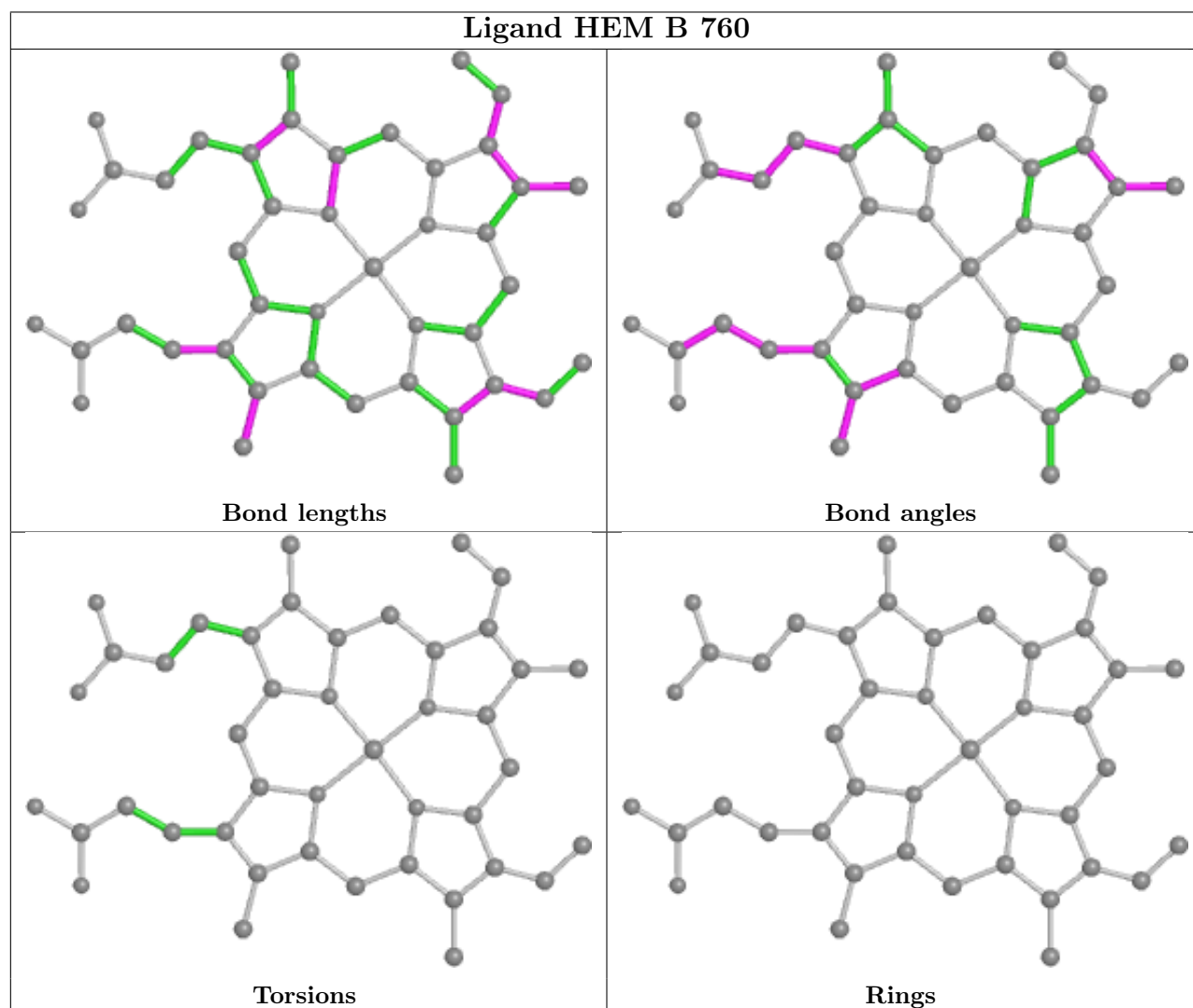
There are no ring outliers.

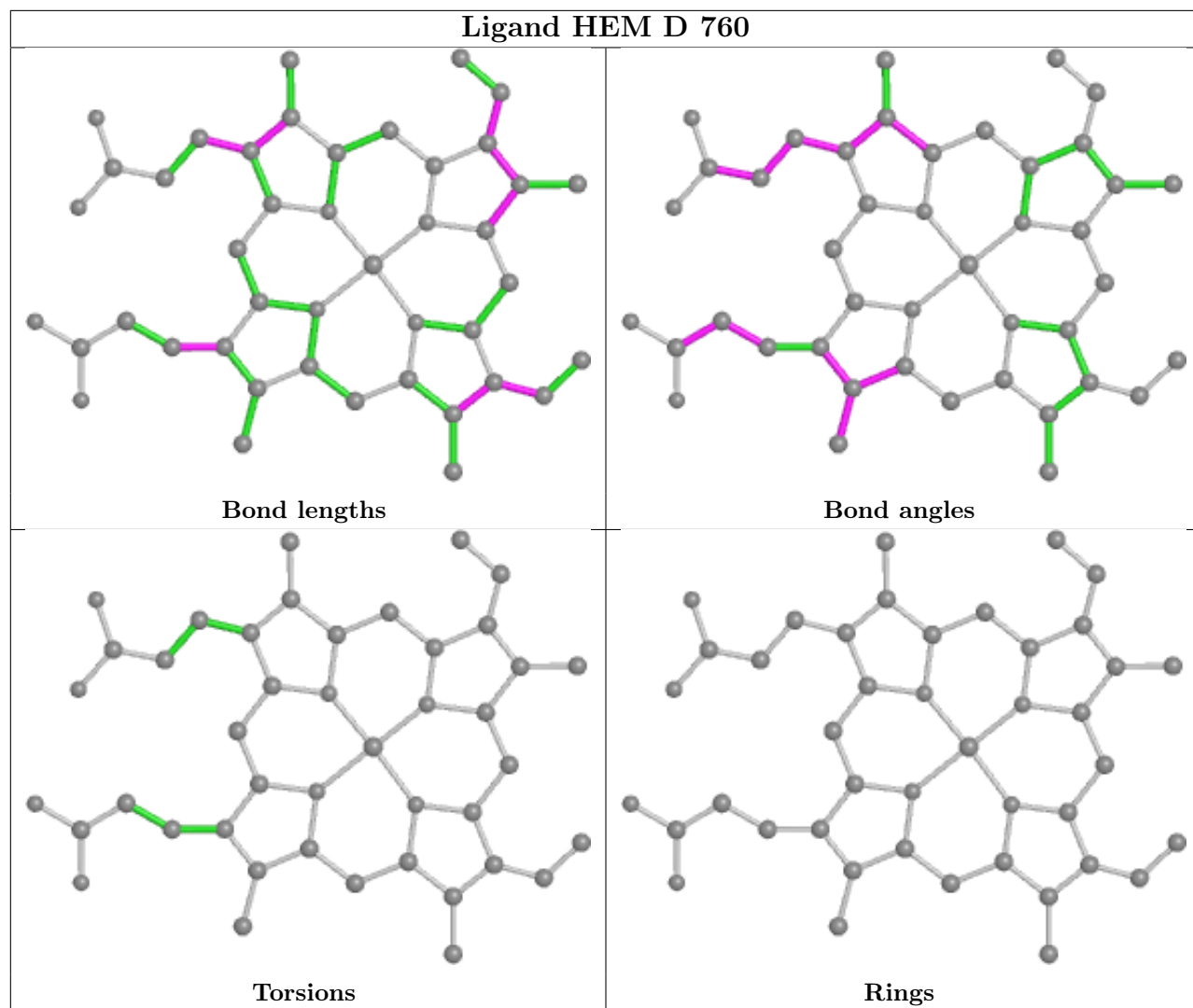
3 monomers are involved in 3 short contacts:

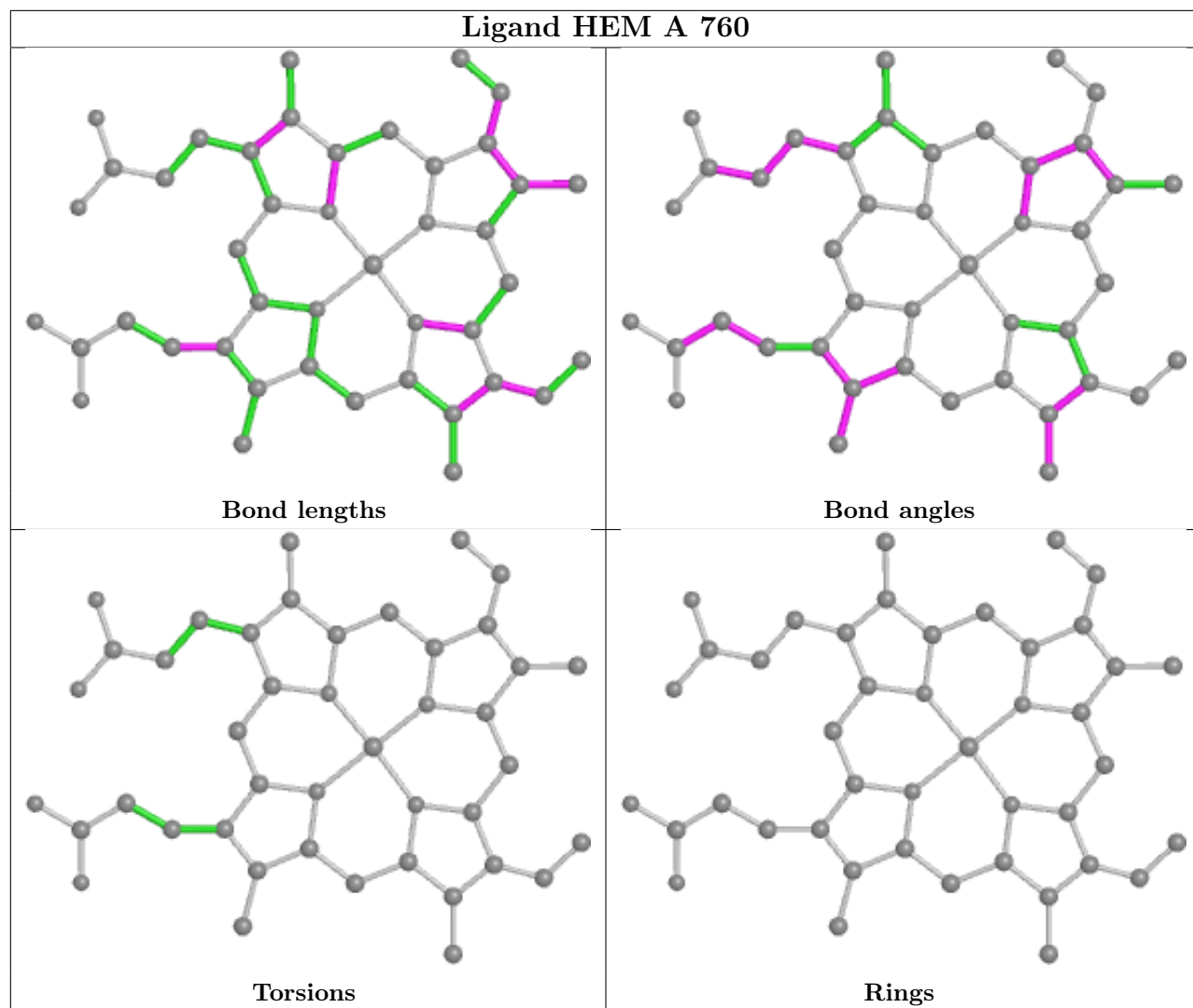
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	760	HEM	1	0
2	D	760	HEM	1	0
2	C	760	HEM	1	0

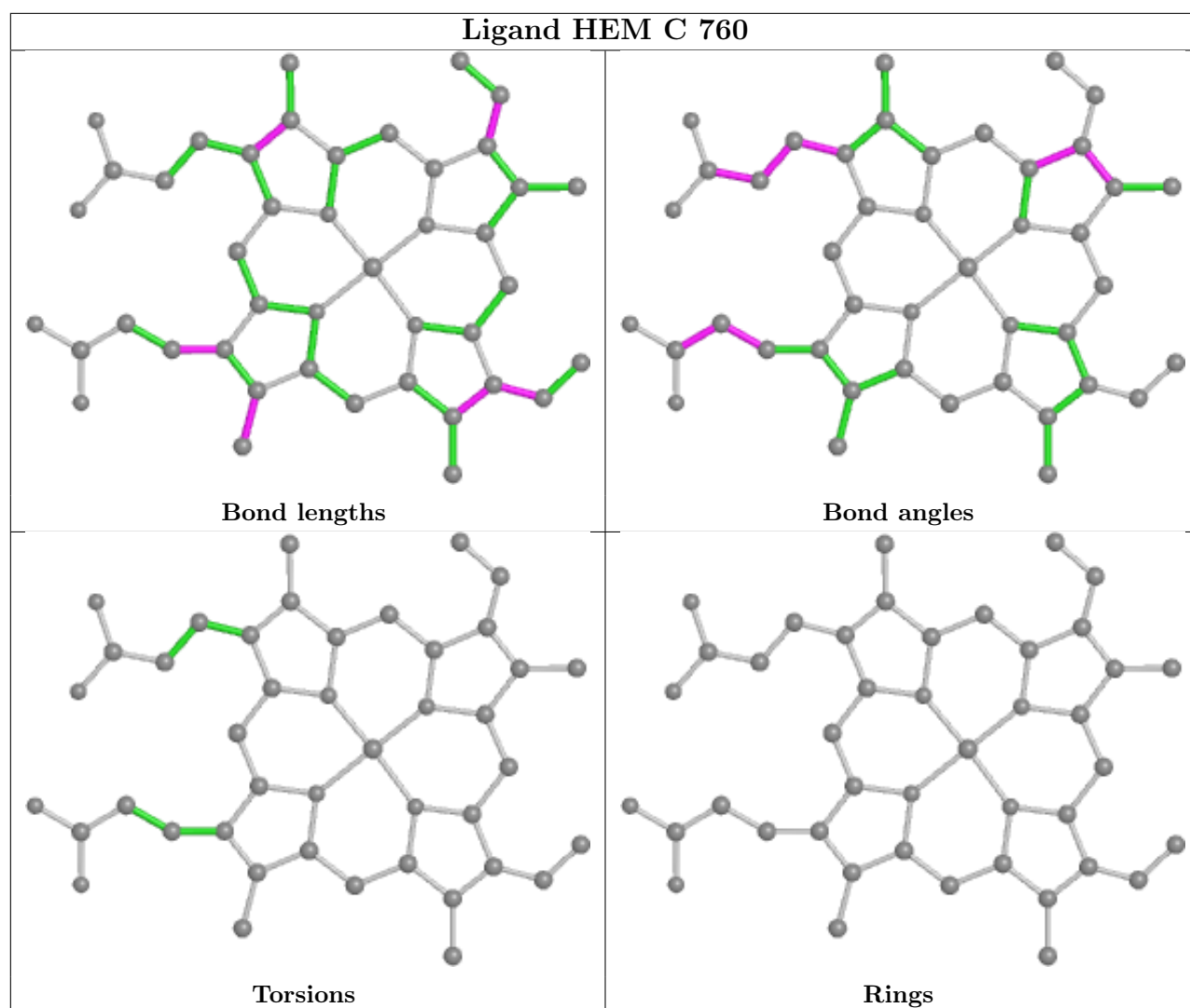
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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

### 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	727/753 (96%)	-0.19	35 (4%)	30	33	8, 14, 37, 74	1 (0%)
1	B	727/753 (96%)	0.08	65 (8%)	9	11	9, 17, 53, 70	1 (0%)
1	C	727/753 (96%)	-0.04	51 (7%)	16	18	9, 17, 47, 57	1 (0%)
1	D	727/753 (96%)	-0.16	36 (4%)	28	32	7, 15, 37, 68	1 (0%)
All	All	2908/3012 (96%)	-0.08	187 (6%)	19	22	7, 16, 47, 74	4 (0%)

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	ASP	8.5
1	A	711	ALA	8.2
1	B	32	GLU	8.1
1	A	28	SER	7.7
1	D	27	ASP	7.0
1	D	28	SER	6.8
1	D	29	LEU	6.7
1	B	27	ASP	6.6
1	B	29	LEU	6.5
1	C	28	SER	6.3
1	A	32	GLU	6.1
1	C	27	ASP	5.8
1	A	37	ARG	5.7
1	B	711	ALA	5.5
1	B	726	GLY	5.3
1	B	28	SER	5.2
1	B	30	ALA	5.2
1	D	35	SER	5.1
1	A	29	LEU	5.1
1	A	39	ALA	4.9
1	B	642	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	36	HIS	4.8
1	A	710	ILE	4.7
1	A	35	SER	4.7
1	A	33	ASP	4.6
1	A	34	GLY	4.6
1	D	32	GLU	4.5
1	B	713	GLN	4.5
1	C	675	ILE	4.5
1	B	610	GLU	4.4
1	C	595	ASP	4.4
1	C	751	ILE	4.4
1	D	33	ASP	4.4
1	B	641	THR	4.3
1	B	677	ASP	4.3
1	B	645	GLY	4.3
1	B	750	LYS	4.3
1	B	33	ASP	4.2
1	D	751	ILE	4.2
1	C	641	THR	4.2
1	B	646	THR	4.1
1	B	749	ASP	4.1
1	C	701	ALA	4.1
1	A	726	GLY	4.1
1	A	713	GLN	4.0
1	B	608	ASN	4.0
1	A	38	PRO	4.0
1	D	749	ASP	3.9
1	B	34	GLY	3.8
1	A	596	GLY	3.8
1	B	612	ARG	3.8
1	B	572	ASN	3.8
1	D	37	ARG	3.7
1	B	673	ALA	3.6
1	C	726	GLY	3.6
1	B	647	VAL	3.6
1	D	750	LYS	3.6
1	D	595	ASP	3.5
1	C	666	ILE	3.5
1	B	35	SER	3.5
1	B	37	ARG	3.5
1	B	712	ASP	3.5
1	C	594	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	44	PRO	3.4
1	D	39	ALA	3.4
1	C	596	GLY	3.4
1	C	749	ASP	3.4
1	C	677	ASP	3.3
1	C	676	ALA	3.3
1	C	569	ASP	3.3
1	C	673	ALA	3.2
1	D	41	GLU	3.2
1	B	665	VAL	3.2
1	C	711	ALA	3.2
1	C	636	ARG	3.1
1	B	38	PRO	3.1
1	A	750	LYS	3.1
1	D	713	GLN	3.1
1	B	568	ASP	3.1
1	B	614	ALA	3.1
1	D	30	ALA	3.1
1	C	645	GLY	3.1
1	A	41	GLU	3.0
1	B	595	ASP	3.0
1	B	611	VAL	3.0
1	C	640	VAL	3.0
1	C	678	ASN	3.0
1	B	594	PRO	3.0
1	B	675	ILE	2.9
1	D	711	ALA	2.9
1	A	31	PRO	2.9
1	C	638	GLY	2.9
1	C	714	GLY	2.9
1	B	617	LEU	2.9
1	D	38	PRO	2.9
1	D	712	ASP	2.9
1	B	596	GLY	2.9
1	B	31	PRO	2.8
1	B	722	ASP	2.8
1	C	722	ASP	2.8
1	B	644	ASP	2.8
1	B	725	ASP	2.8
1	D	59	ASP	2.8
1	B	751	ILE	2.7
1	D	36	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	568	ASP	2.7
1	B	714	GLY	2.7
1	D	596	GLY	2.7
1	B	36	HIS	2.7
1	C	703	LYS	2.6
1	B	697	LEU	2.6
1	D	60	THR	2.6
1	D	40	ALA	2.6
1	B	710	ILE	2.6
1	B	701	ALA	2.6
1	A	712	ASP	2.6
1	B	648	LEU	2.6
1	C	32	GLU	2.5
1	B	666	ILE	2.5
1	A	749	ASP	2.5
1	B	569	ASP	2.5
1	C	750	LYS	2.5
1	C	646	THR	2.5
1	C	610	GLU	2.5
1	A	709	LYS	2.5
1	A	30	ALA	2.5
1	A	283	GLU	2.5
1	B	39	ALA	2.5
1	C	643	ASP	2.4
1	C	727	SER	2.4
1	B	746	PRO	2.4
1	D	714	GLY	2.4
1	B	609	ASP	2.4
1	B	643	ASP	2.4
1	A	46	GLY	2.4
1	A	594	PRO	2.4
1	A	677	ASP	2.4
1	C	674	ASP	2.4
1	D	47	ALA	2.4
1	B	679	GLY	2.4
1	A	666	ILE	2.4
1	A	751	ILE	2.4
1	C	665	VAL	2.4
1	C	698	ALA	2.3
1	B	638	GLY	2.3
1	C	710	ILE	2.3
1	C	712	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	696	ALA	2.3
1	B	621	LYS	2.3
1	C	730	ASP	2.3
1	A	77	ASN	2.2
1	D	31	PRO	2.2
1	C	642	ALA	2.2
1	C	612	ARG	2.2
1	B	75	SER	2.2
1	C	583	LYS	2.2
1	B	672	ILE	2.2
1	A	42	PRO	2.2
1	C	724	ALA	2.2
1	C	725	ASP	2.2
1	D	48	GLN	2.2
1	D	439	PRO	2.2
1	C	604	ALA	2.2
1	A	725	ASP	2.2
1	C	647	VAL	2.2
1	B	77	ASN	2.1
1	A	76	GLU	2.1
1	D	75	SER	2.1
1	D	583	LYS	2.1
1	C	672	ILE	2.1
1	D	568	ASP	2.1
1	D	594	PRO	2.1
1	B	667	VAL	2.1
1	C	639	GLU	2.1
1	D	58	PRO	2.1
1	B	634	TYR	2.1
1	C	572	ASN	2.1
1	C	634	TYR	2.0
1	C	644	ASP	2.0
1	C	592	ALA	2.0
1	B	639	GLU	2.0
1	D	716	GLU	2.0
1	A	75	SER	2.0
1	B	753	ALA	2.0
1	A	605	ILE	2.0
1	B	650	ILE	2.0
1	D	593	ILE	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](#)

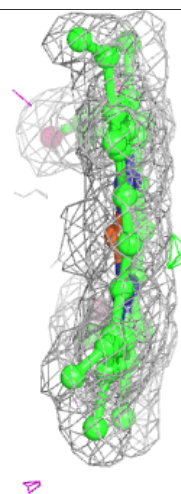
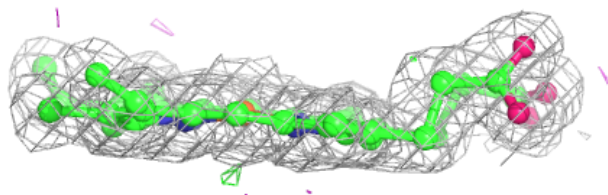
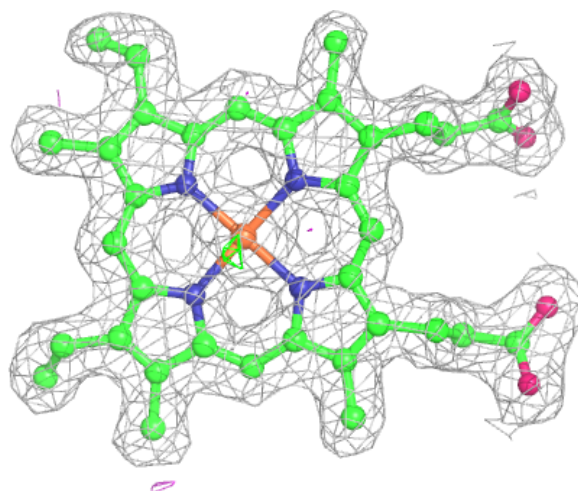
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	HEM	A	760	43/43	0.98	0.06	7,9,14,14	0
2	HEM	B	760	43/43	0.98	0.07	7,11,13,15	0
2	HEM	C	760	43/43	0.98	0.07	7,12,14,16	0
2	HEM	D	760	43/43	0.98	0.07	6,10,13,14	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.

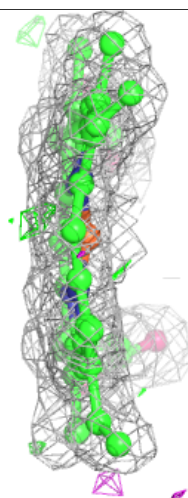
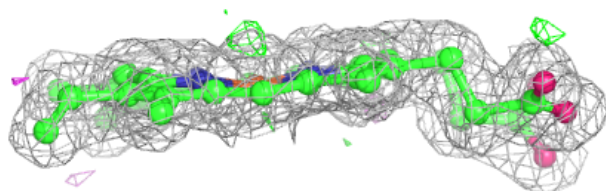
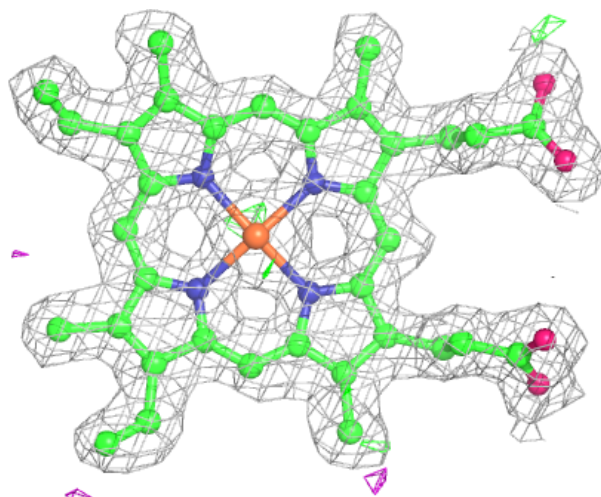
**Electron density around HEM A 760:**

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



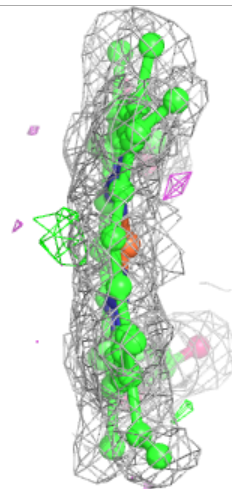
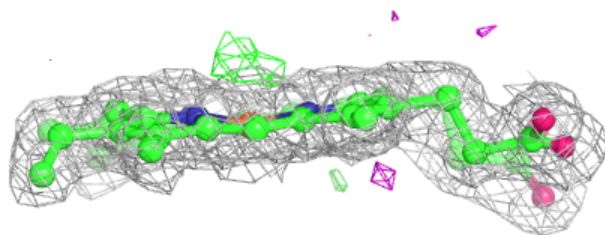
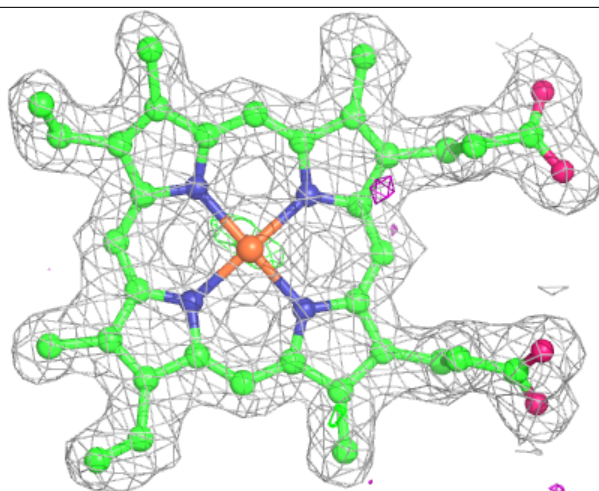
**Electron density around HEM B 760:**

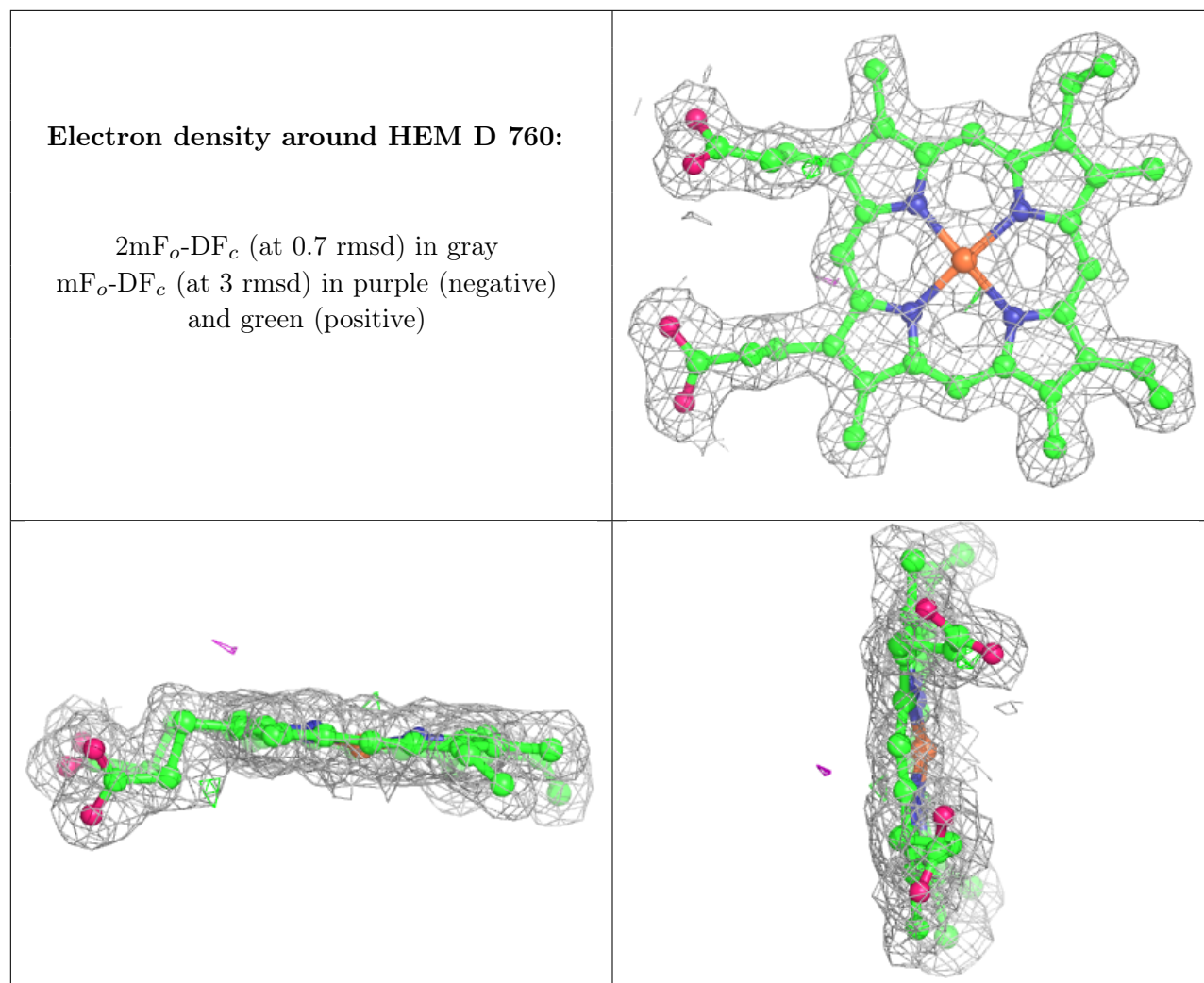
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM C 760:**

$2mF_o-DF_c$  (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.