



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2021 – 03:15 PM EDT

PDB ID : 1GGH  
Title : CRYSTAL STRUCTURE OF CATALASE HPII FROM ESCHERICHIA COLI, HIS128ALA VARIANT.  
Authors : Melik-Adamyan, W.R.; Bravo, J.; Carpena, X.; Switala, J.; Mate, M.J.; Fita, I.; Loewen, P.C.  
Deposited on : 2000-08-21  
Resolution : 2.15 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

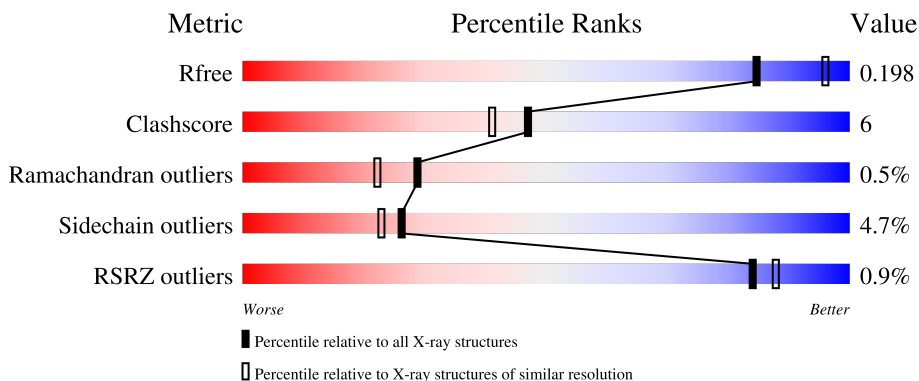
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



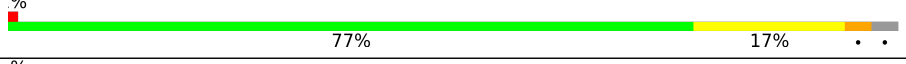

The reported resolution of this entry is 2.15 Å.

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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	 81% 14% . .
1	B	753	 79% 15% . .
1	C	753	 77% 17% . .
1	D	753	 79% 16% . . .

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25922 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 HP11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	727	5741	3644	1003	1082	12	0	0	0
1	B	727	5741	3644	1003	1082	12	0	0	0
1	C	727	5741	3644	1003	1082	12	0	0	0
1	D	727	5741	3644	1003	1082	12	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	128	ALA	HIS	engineered mutation	UNP P21179
B	128	ALA	HIS	engineered mutation	UNP P21179
C	128	ALA	HIS	engineered mutation	UNP P21179
D	128	ALA	HIS	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	
			Total	C	Fe	N			O
2	A	1	43	34	1	4	4	0	0
2	B	1	43	34	1	4	4	0	0
2	C	1	43	34	1	4	4	0	0
2	D	1	43	34	1	4	4	0	0

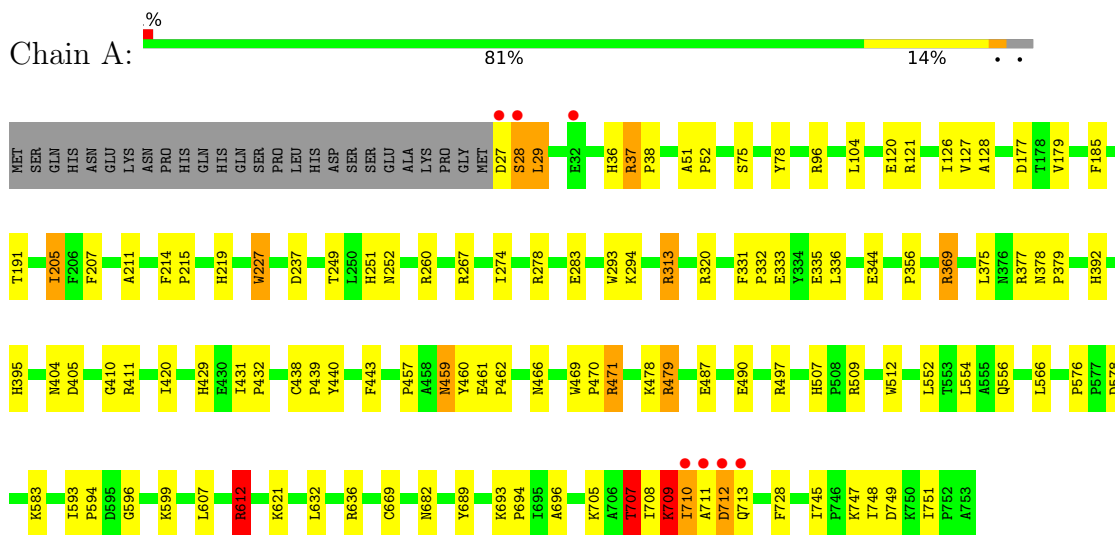
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	737	737	737	0	0
3	B	661	661	661	0	0
3	C	675	675	675	0	0
3	D	713	713	713	0	0

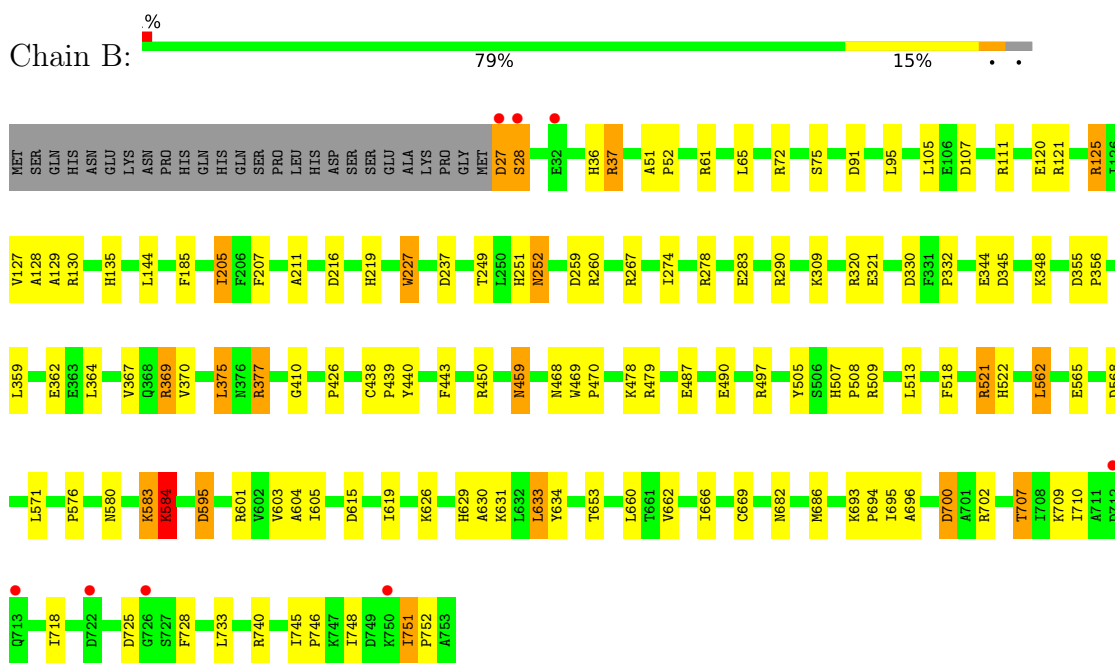
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

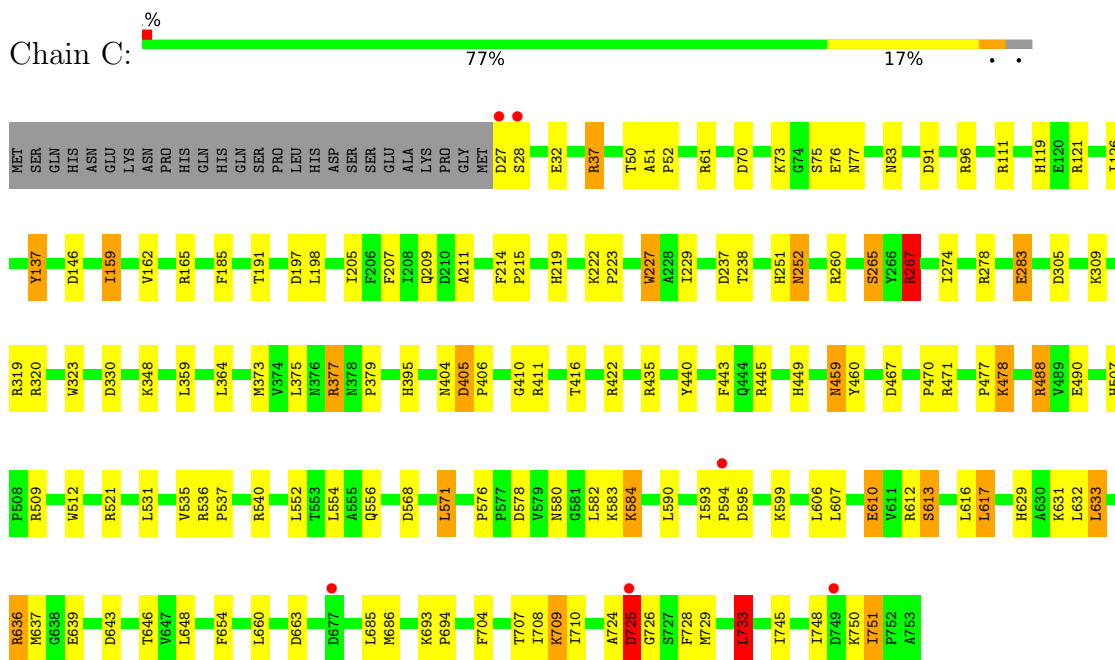
#### • Molecule 1: CATALASE HP1I



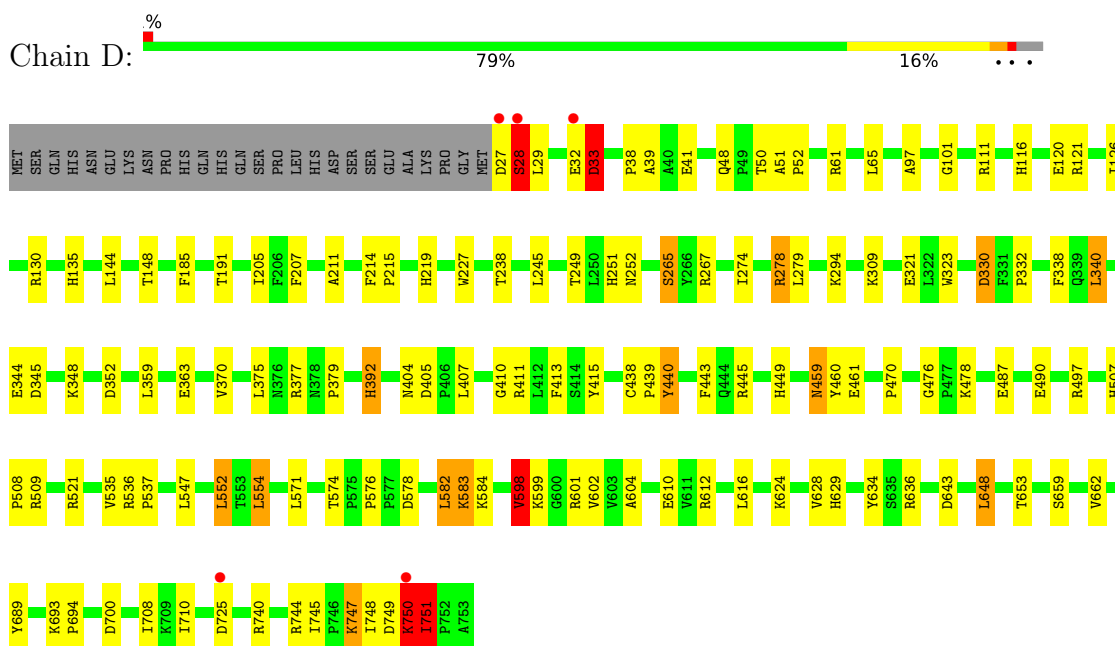
#### • Molecule 1: CATALASE HP1I



#### • Molecule 1: CATALASE HP1I



• Molecule 1: CATALASE HPII



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	93.04Å 132.34Å 121.20Å 90.00° 109.63° 90.00°	Depositor
Resolution (Å)	87.65 – 2.15 19.07 – 2.15	Depositor EDS
% Data completeness (in resolution range)	95.8 (87.65-2.15) 95.9 (19.07-2.15)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.71 (at 2.15Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.150 , 0.206 0.145 , 0.198	Depositor DCC
$R_{free}$ test set	7176 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	8.7	Xtrriage
Anisotropy	0.244	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 58.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	25922	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 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 i

### 5.1 Standard geometry i

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	0.45	0/5896	1.13	21/8016 (0.3%)
1	B	0.45	0/5896	1.16	35/8016 (0.4%)
1	C	0.46	0/5896	1.18	31/8016 (0.4%)
1	D	0.45	0/5896	1.16	29/8016 (0.4%)
All	All	0.45	0/23584	1.16	116/32064 (0.4%)

There are no bond length outliers.

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	725	ASP	C-N-CA	13.45	150.54	122.30
1	C	488	ARG	CD-NE-CZ	12.38	140.93	123.60
1	D	61	ARG	NE-CZ-NH1	-11.30	114.65	120.30
1	C	121	ARG	NE-CZ-NH1	11.30	125.95	120.30
1	D	61	ARG	NE-CZ-NH2	10.25	125.43	120.30
1	C	121	ARG	NE-CZ-NH2	-10.23	115.18	120.30
1	D	278	ARG	NE-CZ-NH1	-10.04	115.28	120.30
1	B	377	ARG	NE-CZ-NH2	-9.62	115.49	120.30
1	C	411	ARG	NE-CZ-NH1	9.52	125.06	120.30
1	C	725	ASP	CA-C-O	8.95	138.89	120.10
1	A	497	ARG	NE-CZ-NH1	8.81	124.70	120.30
1	A	278	ARG	NE-CZ-NH1	-8.80	115.90	120.30
1	D	130	ARG	NE-CZ-NH2	-8.77	115.92	120.30
1	C	37	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	B	521	ARG	NE-CZ-NH1	8.71	124.65	120.30
1	D	601	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	D	740	ARG	NE-CZ-NH2	-8.58	116.01	120.30
1	D	740	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	A	377	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	B	320	ARG	CD-NE-CZ	8.17	135.04	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	121	ARG	NE-CZ-NH2	-8.17	116.22	120.30
1	D	449	HIS	CA-CB-CG	8.12	127.41	113.60
1	C	70	ASP	CB-CG-OD2	8.11	125.60	118.30
1	D	121	ARG	NE-CZ-NH1	8.07	124.34	120.30
1	C	471	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	C	319	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	C	405	ASP	CB-CG-OD2	7.80	125.32	118.30
1	D	377	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	B	72	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	B	521	ARG	CD-NE-CZ	7.71	134.39	123.60
1	D	61	ARG	CD-NE-CZ	7.68	134.35	123.60
1	D	111	ARG	CD-NE-CZ	7.51	134.11	123.60
1	B	28	SER	N-CA-CB	7.44	121.66	110.50
1	B	125	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	A	479	ARG	CD-NE-CZ	7.03	133.44	123.60
1	D	497	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	C	146	ASP	CB-CG-OD2	6.93	124.53	118.30
1	D	497	ARG	NE-CZ-NH1	6.89	123.74	120.30
1	B	121	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	A	479	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	C	726	GLY	N-CA-C	-6.54	96.76	113.10
1	D	643	ASP	CB-CG-OD1	6.53	124.18	118.30
1	D	612	ARG	CD-NE-CZ	6.49	132.68	123.60
1	C	165	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	A	471	ARG	NE-CZ-NH1	-6.34	117.13	120.30
1	B	369	ARG	NE-CZ-NH2	6.23	123.42	120.30
1	C	445	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	D	330	ASP	CB-CG-OD2	-6.21	112.72	118.30
1	B	130	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	B	700	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	B	707	THR	N-CA-CB	6.04	121.77	110.30
1	B	740	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	A	313	ARG	NE-CZ-NH1	-6.03	117.29	120.30
1	B	320	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	D	33	ASP	CA-CB-CG	6.01	126.62	113.40
1	B	130	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	A	96	ARG	NE-CZ-NH1	-5.95	117.32	120.30
1	B	521	ARG	CA-CB-CG	5.92	126.42	113.40
1	D	445	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	C	283	GLU	CB-CG-CD	5.90	130.13	114.20
1	B	479	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	B	216	ASP	CB-CG-OD1	5.86	123.58	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	72	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	C	111	ARG	CD-NE-CZ	5.85	131.79	123.60
1	B	601	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	B	450	ARG	NE-CZ-NH1	-5.83	117.39	120.30
1	A	78	TYR	CB-CG-CD2	-5.82	117.51	121.00
1	B	669	CYS	CA-CB-SG	5.82	124.47	114.00
1	C	96	ARG	NE-CZ-NH1	-5.81	117.39	120.30
1	A	487	GLU	OE1-CD-OE2	-5.73	116.42	123.30
1	A	320	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	B	283	GLU	CA-CB-CG	5.68	125.90	113.40
1	A	612	ARG	CD-NE-CZ	5.68	131.55	123.60
1	B	290	ARG	NE-CZ-NH1	-5.67	117.47	120.30
1	C	536	ARG	CG-CD-NE	5.64	123.65	111.80
1	A	596	GLY	N-CA-C	5.64	127.20	113.10
1	B	260	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	A	278	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	C	377	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	A	121	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	C	320	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	B	497	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	D	130	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	B	740	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	B	260	ARG	NE-CZ-NH2	5.43	123.01	120.30
1	D	352	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	479	ARG	CD-NE-CZ	5.37	131.12	123.60
1	C	422	ARG	CD-NE-CZ	5.36	131.10	123.60
1	C	137	TYR	CB-CG-CD2	-5.34	117.79	121.00
1	C	267	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	C	733	LEU	CA-CB-CG	5.32	127.54	115.30
1	A	177	ASP	CB-CG-OD2	5.30	123.07	118.30
1	C	540	ARG	NE-CZ-NH2	5.29	122.94	120.30
1	C	595	ASP	CB-CG-OD2	5.28	123.05	118.30
1	C	137	TYR	CB-CG-CD1	5.26	124.16	121.00
1	D	265	SER	N-CA-CB	-5.26	102.61	110.50
1	C	278	ARG	NE-CZ-NH1	-5.23	117.68	120.30
1	B	521	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	D	536	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	595	ASP	CB-CG-OD1	5.18	122.97	118.30
1	D	636	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	636	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	B	702	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	C	725	ASP	O-C-N	-5.15	114.44	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	ARG	CD-NE-CZ	5.15	130.80	123.60
1	D	521	ARG	NE-CZ-NH2	5.15	122.87	120.30
1	D	33	ASP	N-CA-CB	5.14	119.86	110.60
1	D	648	LEU	CA-CB-CG	5.14	127.12	115.30
1	A	37	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	707	THR	N-CA-CB	5.10	120.00	110.30
1	B	111	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	C	663	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	B	61	ARG	NE-CZ-NH2	5.06	122.83	120.30
1	D	598	VAL	N-CA-CB	-5.02	100.46	111.50
1	D	440	TYR	CB-CG-CD1	5.01	124.01	121.00
1	A	260	ARG	NE-CZ-NH2	-5.01	117.80	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	5741	0	5576	74	0
1	B	5741	0	5576	77	0
1	C	5741	0	5575	81	0
1	D	5741	0	5576	78	0
2	A	43	0	30	3	0
2	B	43	0	30	1	0
2	C	43	0	30	1	0
2	D	43	0	30	3	0
3	A	737	0	0	10	0
3	B	661	0	0	9	0
3	C	675	0	0	10	0
3	D	713	0	0	7	0
All	All	25922	0	22423	280	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 6.

All (280) 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:490:GLU:HG2	1:B:490:GLU:HG2	1.57	0.87
1:D:750:LYS:HD3	1:D:751:ILE:H	1.52	0.75
1:B:468:ASN:HD22	1:D:27:ASP:N	1.86	0.73
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.72	0.72
1:B:144:LEU:HD11	1:B:370:VAL:HG13	1.72	0.70
1:D:744:ARG:HA	1:D:747:LYS:HD3	1.74	0.70
1:A:28:SER:HB2	1:D:245:LEU:HD13	1.73	0.70
1:D:267:ARG:HG3	3:D:1248:HOH:O	1.93	0.68
1:D:700:ASP:HB2	3:D:1403:HOH:O	1.93	0.68
1:C:751:ILE:HB	3:C:1414:HOH:O	1.94	0.67
1:D:552:LEU:HD11	1:D:571:LEU:HD23	1.75	0.67
1:C:477:PRO:HB2	1:C:478:LYS:HD3	1.76	0.67
1:C:724:ALA:O	1:C:725:ASP:HB2	1.94	0.67
1:B:710:ILE:HD13	1:B:718:ILE:HG13	1.74	0.67
1:B:583:LYS:O	1:B:584:LYS:HB3	1.95	0.67
1:A:612:ARG:HE	1:A:669:CYS:HB3	1.60	0.66
1:D:27:ASP:O	1:D:28:SER:HB2	1.96	0.65
1:B:345:ASP:HA	1:B:348:LYS:HD2	1.78	0.64
1:D:274:ILE:HD12	2:D:760:HEM:HMB1	1.80	0.62
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.30	0.62
1:C:330:ASP:OD2	1:C:599:LYS:HE2	2.00	0.62
1:D:32:GLU:O	1:D:33:ASP:HB3	2.00	0.62
1:C:725:ASP:HA	1:C:728:PHE:HB3	1.82	0.61
1:D:38:PRO:HA	1:D:48:GLN:HE21	1.65	0.61
1:C:490:GLU:HG3	1:D:490:GLU:HG3	1.83	0.61
1:B:583:LYS:H	1:B:583:LYS:CE	2.12	0.61
1:C:435:ARG:HD3	3:C:1110:HOH:O	2.02	0.60
1:B:748:ILE:O	1:B:751:ILE:HG22	2.01	0.60
1:B:274:ILE:HD12	2:B:760:HEM:HMB1	1.84	0.59
1:C:704:PHE:O	1:C:707:THR:HG22	2.01	0.59
1:A:335:GLU:OE1	1:A:369:ARG:HG2	2.01	0.59
1:A:748:ILE:O	1:A:751:ILE:HG13	2.03	0.59
1:B:478:LYS:HD2	3:B:1356:HOH:O	2.03	0.59
1:B:583:LYS:H	1:B:583:LYS:NZ	2.00	0.58
1:B:634:TYR:O	1:B:653:THR:HA	2.03	0.58
1:A:709:LYS:HE3	1:A:709:LYS:HA	1.86	0.58
1:C:274:ILE:HD12	2:C:760:HEM:HMB1	1.84	0.58
1:C:323:TRP:CZ3	1:C:379:PRO:HD2	2.39	0.58
1:C:613:SER:HB3	1:C:643:ASP:OD1	2.04	0.57
1:A:607:LEU:HD11	1:A:632:LEU:HB3	1.87	0.57
1:A:214:PHE:HB3	1:A:215:PRO:HD3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:686:MET:HB3	1:B:751:ILE:HD11	1.87	0.56
1:A:126:ILE:CD1	1:D:120:GLU:HB2	2.35	0.56
1:A:745:ILE:O	1:A:748:ILE:HG12	2.05	0.56
1:D:267:ARG:HG2	1:D:332:PRO:HB3	1.87	0.56
1:D:51:ALA:HB1	1:D:52:PRO:HD2	1.88	0.55
1:B:251:HIS:CE1	1:B:507:HIS:HB3	2.41	0.55
1:D:748:ILE:O	1:D:751:ILE:HG22	2.06	0.55
1:A:708:ILE:O	1:A:710:ILE:N	2.39	0.55
1:B:27:ASP:HB3	3:B:1386:HOH:O	2.07	0.55
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.22	0.55
1:B:605:ILE:HD12	1:B:630:ALA:HB1	1.88	0.55
1:A:51:ALA:HB1	1:A:52:PRO:HD2	1.88	0.55
1:D:359:LEU:H	1:D:507:HIS:HD2	1.55	0.55
1:A:705:LYS:HE3	3:A:1424:HOH:O	2.07	0.54
1:B:631:LYS:HG3	1:B:633:LEU:HD13	1.90	0.54
1:C:260:ARG:HD3	1:C:590:LEU:HD21	1.89	0.54
1:D:750:LYS:CD	1:D:751:ILE:H	2.21	0.54
1:D:27:ASP:HB2	1:D:29:LEU:HD21	1.89	0.54
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.91	0.54
1:A:438:CYS:HB2	1:A:439:PRO:CD	2.38	0.53
1:B:710:ILE:CD1	1:B:718:ILE:HG13	2.38	0.53
1:A:599:LYS:HE3	3:A:1283:HOH:O	2.08	0.53
1:D:629:HIS:HD2	3:D:1119:HOH:O	1.91	0.53
1:C:617:LEU:HD12	3:C:1326:HOH:O	2.08	0.53
1:C:636:ARG:NH2	1:C:639:GLU:O	2.40	0.53
1:D:338:PHE:HB3	1:D:340:LEU:HD13	1.89	0.53
1:A:36:HIS:CD2	1:A:36:HIS:H	2.26	0.53
1:B:521:ARG:HE	1:B:745:ILE:HG21	1.72	0.53
1:A:457:PRO:HG2	1:C:37:ARG:NH2	2.23	0.53
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.24	0.53
1:C:509:ARG:HD2	1:C:576:PRO:HD2	1.90	0.53
1:A:478:LYS:HG2	3:A:1257:HOH:O	2.09	0.53
1:B:51:ALA:HB1	1:B:52:PRO:HD2	1.90	0.53
1:D:359:LEU:H	1:D:507:HIS:CD2	2.27	0.53
1:D:32:GLU:O	1:D:33:ASP:CB	2.58	0.52
1:A:52:PRO:HG3	3:C:1004:HOH:O	2.09	0.52
2:A:760:HEM:HBC2	2:A:760:HEM:CMC	2.39	0.52
1:B:309:LYS:HG2	1:B:660:LEU:HD11	1.91	0.52
1:A:211:ALA:CB	1:A:410:GLY:HA3	2.41	0.51
1:C:552:LEU:HD22	1:C:556:GLN:HG3	1.93	0.51
1:A:127:VAL:O	1:A:128:ALA:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:631:LYS:HG3	1:C:633:LEU:HD13	1.92	0.51
1:B:267:ARG:HG3	3:B:1255:HOH:O	2.10	0.51
1:B:603:VAL:HG11	1:B:666:ILE:HD12	1.93	0.51
1:A:29:LEU:HB2	1:C:467:ASP:OD1	2.11	0.51
1:C:745:ILE:O	1:C:748:ILE:HG12	2.11	0.51
1:B:745:ILE:O	1:B:748:ILE:HG12	2.10	0.51
1:C:211:ALA:CB	1:C:410:GLY:HA3	2.41	0.51
1:A:682:ASN:HB3	1:A:707:THR:HG21	1.92	0.51
1:D:438:CYS:HB2	1:D:439:PRO:CD	2.41	0.51
1:A:751:ILE:HD12	1:A:751:ILE:O	2.11	0.50
1:C:197:ASP:OD1	1:C:395:HIS:ND1	2.41	0.50
1:D:65:LEU:HD21	1:D:135:HIS:CG	2.46	0.50
1:D:207:PHE:O	1:D:249:THR:HA	2.10	0.50
1:B:36:HIS:HD1	1:B:36:HIS:H	1.60	0.50
1:B:120:GLU:HB2	1:C:126:ILE:HD11	1.94	0.50
1:D:214:PHE:HB3	1:D:215:PRO:HD3	1.93	0.50
1:A:205:ILE:HB	1:A:356:PRO:O	2.12	0.50
1:B:359:LEU:H	1:B:507:HIS:HD2	1.58	0.50
1:C:222:LYS:HB3	1:C:223:PRO:CD	2.42	0.50
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.27	0.49
1:B:127:VAL:O	1:B:128:ALA:HB3	2.13	0.49
1:A:420:ILE:HG21	1:C:119:HIS:CE1	2.48	0.49
1:A:578:ASP:OD1	1:A:583:LYS:NZ	2.45	0.49
1:A:612:ARG:HH11	1:A:669:CYS:CB	2.25	0.49
1:A:251:HIS:CE1	1:A:507:HIS:HB3	2.47	0.49
1:D:578:ASP:OD2	1:D:583:LYS:HG3	2.12	0.49
1:D:547:LEU:HB3	1:D:554:LEU:HD13	1.95	0.49
1:D:574:THR:HG22	3:D:1165:HOH:O	2.12	0.49
1:C:416:THR:HA	3:C:1341:HOH:O	2.12	0.49
1:C:459:ASN:H	1:C:459:ASN:HD22	1.60	0.48
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.28	0.48
1:D:602:VAL:HG13	1:D:662:VAL:HA	1.94	0.48
1:B:700:ASP:HB2	3:B:1410:HOH:O	2.12	0.48
1:D:345:ASP:HA	1:D:348:LYS:HG3	1.95	0.48
1:A:443:PHE:CZ	1:A:470:PRO:HD2	2.48	0.48
1:B:207:PHE:O	1:B:249:THR:HA	2.13	0.48
1:C:251:HIS:CE1	1:C:507:HIS:HB3	2.49	0.48
1:A:179:VAL:HA	3:A:1131:HOH:O	2.14	0.47
1:B:604:ALA:HB2	1:B:662:VAL:HG11	1.96	0.47
1:A:378:ASN:HB3	1:A:379:PRO:HD2	1.97	0.47
3:A:909:HOH:O	1:C:52:PRO:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:509:ARG:HD2	1:D:576:PRO:HD2	1.97	0.47
1:C:137:TYR:HB2	1:C:159:ILE:HD12	1.96	0.47
1:C:222:LYS:HB3	1:C:223:PRO:HD2	1.97	0.47
1:A:104:LEU:HB3	3:C:781:HOH:O	2.13	0.47
1:B:344:GLU:CD	1:B:344:GLU:H	2.17	0.47
1:A:512:TRP:CZ3	1:A:554:LEU:HD13	2.48	0.47
1:A:37:ARG:HA	1:A:38:PRO:HD3	1.83	0.47
1:A:696:ALA:HB1	1:A:728:PHE:CZ	2.50	0.47
1:B:682:ASN:HB3	1:B:707:THR:HG21	1.97	0.47
1:D:745:ILE:O	1:D:748:ILE:HG12	2.14	0.47
1:C:51:ALA:HB1	1:C:52:PRO:HD2	1.97	0.46
1:C:583:LYS:O	1:C:584:LYS:HB3	2.14	0.46
1:D:211:ALA:CB	1:D:410:GLY:HA3	2.45	0.46
1:D:251:HIS:CE1	1:D:507:HIS:HB3	2.50	0.46
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.98	0.46
1:C:404:ASN:O	1:C:405:ASP:C	2.54	0.46
1:B:362:GLU:HG2	1:B:367:VAL:HG23	1.97	0.46
1:C:552:LEU:HD21	1:C:571:LEU:HD12	1.98	0.46
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.98	0.46
1:B:518:PHE:HB3	1:B:521:ARG:NH2	2.30	0.46
1:B:211:ALA:CB	1:B:410:GLY:HA3	2.46	0.46
1:B:369:ARG:HG3	3:B:768:HOH:O	2.15	0.46
1:A:438:CYS:HB2	1:A:439:PRO:HD2	1.97	0.46
1:C:686:MET:HB3	1:C:751:ILE:HD11	1.98	0.46
1:C:359:LEU:H	1:C:507:HIS:HD2	1.64	0.45
1:C:607:LEU:HD11	1:C:632:LEU:HB3	1.99	0.45
1:B:332:PRO:HD2	1:B:375:LEU:O	2.17	0.45
1:D:411:ARG:HG2	2:D:760:HEM:C2C	2.51	0.45
1:D:689:TYR:HA	1:D:744:ARG:NH1	2.31	0.45
1:D:634:TYR:O	1:D:653:THR:HA	2.17	0.45
1:A:126:ILE:HD11	1:D:120:GLU:HB2	1.97	0.45
1:B:438:CYS:HB2	1:B:439:PRO:HD2	1.97	0.45
1:D:404:ASN:O	1:D:405:ASP:C	2.55	0.45
1:D:535:VAL:O	1:D:537:PRO:HD3	2.15	0.45
1:C:443:PHE:CZ	1:C:470:PRO:HD2	2.52	0.45
1:D:323:TRP:CZ3	1:D:379:PRO:HD2	2.52	0.45
1:C:460:TYR:CE2	1:D:238:THR:HB	2.52	0.45
1:A:227:TRP:CZ3	1:D:50:THR:HG21	2.51	0.45
1:A:404:ASN:O	1:A:405:ASP:C	2.55	0.45
1:C:267:ARG:HD3	3:C:1245:HOH:O	2.16	0.45
1:D:148:THR:HB	1:D:279:LEU:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:745:ILE:HB	1:B:746:PRO:HD3	1.97	0.45
1:C:305:ASP:O	1:C:309:LYS:HG3	2.17	0.44
1:A:274:ILE:HD12	2:A:760:HEM:HMB1	1.98	0.44
1:A:712:ASP:HB3	3:A:1436:HOH:O	2.17	0.44
1:B:364:LEU:HD11	1:B:580:ASN:HB2	1.98	0.44
1:C:748:ILE:O	1:C:751:ILE:HG22	2.17	0.44
1:A:267:ARG:HG2	1:A:332:PRO:HB3	1.99	0.44
1:B:120:GLU:HB2	1:C:126:ILE:CD1	2.48	0.44
1:B:695:ILE:HB	1:B:718:ILE:CD1	2.48	0.44
1:D:599:LYS:HD3	3:D:1288:HOH:O	2.17	0.44
1:D:708:ILE:HG13	1:D:710:ILE:HG12	1.99	0.44
1:C:709:LYS:HD3	1:C:709:LYS:N	2.32	0.44
1:A:38:PRO:HG2	1:A:51:ALA:HB2	2.00	0.44
1:A:689:TYR:OH	1:A:710:ILE:HG21	2.17	0.44
1:B:693:LYS:HA	1:B:694:PRO:HD3	1.86	0.44
1:C:535:VAL:O	1:C:537:PRO:HD3	2.17	0.44
1:B:513:LEU:HD12	3:B:1392:HOH:O	2.18	0.44
1:C:748:ILE:HA	1:C:751:ILE:HG22	2.00	0.44
1:D:443:PHE:CZ	1:D:470:PRO:HD2	2.53	0.44
1:D:39:ALA:H	1:D:48:GLN:NE2	2.15	0.44
1:D:598:VAL:HG13	1:D:628:VAL:CG2	2.48	0.44
1:A:461:GLU:OE1	1:C:91:ASP:OD1	2.36	0.44
1:B:205:ILE:HB	1:B:356:PRO:O	2.18	0.44
1:B:105:LEU:HD11	1:D:413:PHE:HB2	2.00	0.43
1:B:521:ARG:NH2	3:B:1092:HOH:O	2.51	0.43
1:A:37:ARG:HD3	3:A:1321:HOH:O	2.18	0.43
1:A:459:ASN:HD22	1:A:460:TYR:HD2	1.66	0.43
1:A:556:GLN:HG3	1:A:566:LEU:HD12	1.99	0.43
1:A:207:PHE:O	1:A:249:THR:HA	2.18	0.43
1:B:91:ASP:OD1	1:D:461:GLU:OE1	2.36	0.43
1:B:259:ASP:OD1	1:B:522:HIS:ND1	2.42	0.43
1:B:267:ARG:HG2	1:B:332:PRO:HB3	2.00	0.43
1:D:144:LEU:HD11	1:D:370:VAL:HG13	2.00	0.43
1:C:606:LEU:HG	1:C:654:PHE:CE2	2.54	0.43
1:D:27:ASP:HB2	1:D:29:LEU:CD2	2.48	0.43
1:A:120:GLU:HB2	1:D:126:ILE:CD1	2.48	0.43
1:B:443:PHE:CZ	1:B:470:PRO:HD2	2.53	0.43
1:C:646:THR:O	1:C:648:LEU:HD13	2.19	0.43
1:D:97:ALA:O	1:D:101:GLY:HA3	2.19	0.43
1:B:631:LYS:HG3	1:B:633:LEU:CD1	2.48	0.43
1:A:593:ILE:HA	1:A:594:PRO:HD2	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:ARG:HH22	1:B:487:GLU:CD	2.22	0.43
1:B:469:TRP:HA	1:B:470:PRO:C	2.39	0.43
1:C:28:SER:HA	3:C:1435:HOH:O	2.18	0.43
1:A:429:HIS:CG	1:C:83:ASN:HB3	2.54	0.43
1:B:144:LEU:CD1	1:B:370:VAL:HG13	2.43	0.43
1:B:562:LEU:HA	1:C:637:MET:HB2	2.01	0.43
1:B:751:ILE:HD13	1:B:752:PRO:HD2	2.01	0.43
1:C:207:PHE:CD2	1:C:252:ASN:HB3	2.54	0.43
1:A:713:GLN:HG2	3:A:1319:HOH:O	2.20	0.42
1:B:583:LYS:H	1:B:583:LYS:HE2	1.83	0.42
1:D:407:LEU:HD11	2:D:760:HEM:HMC2	2.02	0.42
1:D:693:LYS:HA	1:D:694:PRO:HD3	1.93	0.42
1:A:457:PRO:HG2	1:C:37:ARG:HH21	1.84	0.42
1:B:65:LEU:HD21	1:B:135:HIS:CG	2.54	0.42
1:A:469:TRP:CE3	1:A:471:ARG:HG3	2.54	0.42
1:C:252:ASN:HD22	1:C:252:ASN:HA	1.63	0.42
1:D:583:LYS:O	1:D:584:LYS:HB3	2.19	0.42
1:A:461:GLU:HB2	1:A:462:PRO:HA	2.02	0.42
1:B:95:LEU:HB3	1:B:107:ASP:HB2	2.00	0.42
1:B:626:LYS:HG3	1:B:733:LEU:HD13	2.00	0.42
1:C:364:LEU:HD11	1:C:580:ASN:HB2	2.02	0.42
1:D:583:LYS:HB2	1:D:583:LYS:NZ	2.35	0.42
1:B:227:TRP:CZ3	1:C:50:THR:HG21	2.54	0.42
1:C:265:SER:OG	1:C:267:ARG:HB2	2.19	0.42
1:A:27:ASP:O	1:A:29:LEU:HG	2.20	0.42
1:A:509:ARG:HD2	1:A:576:PRO:HD2	2.01	0.42
1:A:612:ARG:HG3	3:A:1487:HOH:O	2.19	0.42
1:C:729:MET:O	1:C:733:LEU:HB2	2.19	0.42
1:D:321:GLU:HG3	3:D:1316:HOH:O	2.20	0.42
1:A:294:LYS:NZ	3:A:1135:HOH:O	2.53	0.41
1:C:76:GLU:O	1:C:77:ASN:HB2	2.18	0.41
1:B:505:TYR:HA	1:B:508:PRO:HG2	2.02	0.41
1:A:293:TRP:CZ3	1:A:336:LEU:HB2	2.56	0.41
1:B:509:ARG:HD2	1:B:576:PRO:HD2	2.02	0.41
1:A:431:ILE:HG13	1:C:449:HIS:CE1	2.55	0.41
1:B:125:ARG:HB2	1:B:129:ALA:HA	2.02	0.41
1:C:209:GLN:O	1:C:406:PRO:HG2	2.20	0.41
1:B:426:PRO:HB2	1:D:116:HIS:CD2	2.55	0.41
1:C:162:VAL:HG21	1:C:373:MET:SD	2.60	0.41
1:C:227:TRP:CE2	1:C:229:ILE:HB	2.56	0.41
1:D:547:LEU:HD22	1:D:554:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:ARG:HD3	3:C:1163:HOH:O	2.21	0.41
1:B:615:ASP:O	1:B:619:ILE:HG13	2.20	0.41
1:C:578:ASP:HB2	1:C:582:LEU:O	2.21	0.41
1:D:438:CYS:HB2	1:D:439:PRO:HD2	2.01	0.41
1:D:507:HIS:N	1:D:508:PRO:HD2	2.35	0.41
1:A:429:HIS:CD2	1:C:83:ASN:HB3	2.55	0.41
1:B:37:ARG:HD2	3:B:1358:HOH:O	2.21	0.41
1:B:696:ALA:HB1	1:B:728:PHE:CZ	2.55	0.41
1:B:252:ASN:HD22	1:B:252:ASN:HA	1.63	0.41
1:B:459:ASN:HD22	1:B:459:ASN:H	1.68	0.41
1:D:278:ARG:HH12	1:D:487:GLU:CD	2.24	0.41
1:D:476:GLY:HA3	3:D:872:HOH:O	2.20	0.41
1:A:313:ARG:NH1	1:D:309:LYS:HD2	2.36	0.41
1:A:331:PHE:O	1:A:333:GLU:HG3	2.20	0.41
1:B:355:ASP:HA	1:B:356:PRO:HD2	1.97	0.41
1:C:686:MET:HG2	1:C:751:ILE:HD11	2.02	0.41
1:D:211:ALA:HB3	1:D:410:GLY:HA3	2.02	0.41
1:D:507:HIS:N	1:D:508:PRO:CD	2.83	0.41
1:D:604:ALA:HB2	1:D:662:VAL:HG11	2.03	0.41
1:C:507:HIS:HE1	3:C:923:HOH:O	2.03	0.41
1:C:512:TRP:CZ3	1:C:554:LEU:HD13	2.56	0.40
1:C:593:ILE:HA	1:C:594:PRO:HD2	1.90	0.40
1:A:411:ARG:HG2	2:A:760:HEM:C2C	2.56	0.40
1:C:238:THR:HB	1:D:460:TYR:CE2	2.57	0.40
1:C:610:GLU:O	1:C:610:GLU:HG3	2.20	0.40
1:A:392:HIS:HB3	1:A:395:HIS:CG	2.57	0.40
1:B:629:HIS:HD2	3:B:1034:HOH:O	2.03	0.40
1:C:214:PHE:HB3	1:C:215:PRO:HD3	2.02	0.40
1:C:693:LYS:HA	1:C:694:PRO:HD3	1.97	0.40
1:D:392:HIS:CE1	1:D:415:TYR:HB2	2.57	0.40
1:A:466:ASN:HA	1:C:37:ARG:HH22	1.86	0.40
1:A:748:ILE:HG13	1:A:749:ASP:N	2.35	0.40
1:A:693:LYS:HA	1:A:694:PRO:HD3	1.86	0.40
1:D:363:GLU:HB2	1:D:582:LEU:HD21	2.04	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	725/753 (96%)	701 (97%)	20 (3%)	4 (1%)	25	18
1	B	725/753 (96%)	700 (97%)	21 (3%)	4 (1%)	25	18
1	C	725/753 (96%)	701 (97%)	22 (3%)	2 (0%)	41	37
1	D	725/753 (96%)	693 (96%)	28 (4%)	4 (1%)	25	18
All	All	2900/3012 (96%)	2795 (96%)	91 (3%)	14 (0%)	29	22

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	A	709	LYS
1	B	28	SER
1	C	725	ASP
1	D	28	SER
1	D	750	LYS
1	D	751	ILE
1	B	725	ASP
1	C	75	SER
1	D	33	ASP
1	A	75	SER
1	A	711	ALA
1	B	584	LYS
1	B	75	SER

### 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	611/635 (96%)	589 (96%)	22 (4%)	35	33
1	B	611/635 (96%)	589 (96%)	22 (4%)	35	33
1	C	611/635 (96%)	570 (93%)	41 (7%)	16	11
1	D	611/635 (96%)	580 (95%)	31 (5%)	24	20
All	All	2444/2540 (96%)	2328 (95%)	116 (5%)	26	23

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	185	PHE
1	A	191	THR
1	A	205	ILE
1	A	227	TRP
1	A	237	ASP
1	A	252	ASN
1	A	283	GLU
1	A	344	GLU
1	A	369	ARG
1	A	375	LEU
1	A	432	PRO
1	A	440	TYR
1	A	459	ASN
1	A	552	LEU
1	A	612	ARG
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	B	27	ASP
1	B	37	ARG
1	B	185	PHE
1	B	205	ILE
1	B	227	TRP
1	B	237	ASP
1	B	252	ASN
1	B	321	GLU
1	B	375	LEU
1	B	377	ARG
1	B	440	TYR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	459	ASN
1	B	562	LEU
1	B	565	GLU
1	B	568	ASP
1	B	571	LEU
1	B	583	LYS
1	B	584	LYS
1	B	595	ASP
1	B	633	LEU
1	B	709	LYS
1	B	751	ILE
1	C	27	ASP
1	C	32	GLU
1	C	61	ARG
1	C	73	LYS
1	C	159	ILE
1	C	185	PHE
1	C	191	THR
1	C	198	LEU
1	C	205	ILE
1	C	227	TRP
1	C	237	ASP
1	C	252	ASN
1	C	265	SER
1	C	267	ARG
1	C	283	GLU
1	C	348	LYS
1	C	375	LEU
1	C	377	ARG
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	568	ASP
1	C	571	LEU
1	C	584	LYS
1	C	610	GLU
1	C	612	ARG
1	C	613	SER
1	C	616	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	617	LEU
1	C	633	LEU
1	C	636	ARG
1	C	660	LEU
1	C	685	LEU
1	C	709	LYS
1	C	725	ASP
1	C	733	LEU
1	C	750	LYS
1	C	751	ILE
1	D	28	SER
1	D	41	GLU
1	D	185	PHE
1	D	191	THR
1	D	205	ILE
1	D	227	TRP
1	D	252	ASN
1	D	265	SER
1	D	294	LYS
1	D	340	LEU
1	D	344	GLU
1	D	375	LEU
1	D	392	HIS
1	D	440	TYR
1	D	459	ASN
1	D	478	LYS
1	D	552	LEU
1	D	554	LEU
1	D	582	LEU
1	D	583	LYS
1	D	598	VAL
1	D	610	GLU
1	D	616	LEU
1	D	624	LYS
1	D	648	LEU
1	D	659	SER
1	D	725	ASP
1	D	747	LYS
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 (23)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	252	ASN
1	A	368	GLN
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	C	252	ASN
1	C	449	HIS
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
1	D	546	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	C	760	1	27,50,50	1.95	5 (18%)	17,82,82	1.91	6 (35%)
2	HEM	A	760	1	27,50,50	1.96	4 (14%)	17,82,82	1.39	2 (11%)
2	HEM	B	760	1	27,50,50	2.00	5 (18%)	17,82,82	1.81	5 (29%)
2	HEM	D	760	1	27,50,50	1.92	5 (18%)	17,82,82	1.88	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	C	760	1	-	0/6/54/54	-
2	HEM	A	760	1	-	0/6/54/54	-
2	HEM	B	760	1	-	0/6/54/54	-
2	HEM	D	760	1	-	0/6/54/54	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	760	HEM	C3B-C2B	-4.95	1.33	1.40
2	B	760	HEM	C3C-C2C	-4.92	1.33	1.40
2	B	760	HEM	C3B-C2B	-4.84	1.33	1.40
2	D	760	HEM	C3B-C2B	-4.73	1.33	1.40
2	A	760	HEM	C3B-C2B	-4.72	1.33	1.40
2	A	760	HEM	C3C-C2C	-4.57	1.34	1.40
2	C	760	HEM	C3C-C2C	-4.33	1.34	1.40
2	D	760	HEM	C3C-C2C	-4.16	1.34	1.40
2	A	760	HEM	C3C-CAC	3.72	1.55	1.47
2	D	760	HEM	C3B-CAB	3.56	1.55	1.47
2	D	760	HEM	C3C-CAC	3.39	1.54	1.47
2	C	760	HEM	C3B-CAB	3.38	1.54	1.47
2	B	760	HEM	C3B-CAB	3.30	1.54	1.47
2	C	760	HEM	C3C-CAC	3.30	1.54	1.47
2	A	760	HEM	C3B-CAB	3.22	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	760	HEM	C3C-CAC	3.01	1.54	1.47
2	D	760	HEM	CAD-C3D	2.29	1.56	1.52
2	C	760	HEM	CAD-C3D	2.05	1.55	1.52
2	B	760	HEM	CAD-C3D	2.02	1.55	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	760	HEM	CAD-CBD-CGD	4.81	120.74	112.67
2	B	760	HEM	CMD-C2D-C1D	-4.33	121.82	128.46
2	C	760	HEM	CAD-CBD-CGD	3.81	119.06	112.67
2	C	760	HEM	CMD-C2D-C1D	-3.50	123.08	128.46
2	B	760	HEM	CMD-C2D-C3D	3.13	130.84	124.94
2	C	760	HEM	CMA-C3A-C4A	-3.13	123.66	128.46
2	D	760	HEM	CMD-C2D-C1D	-3.09	123.72	128.46
2	A	760	HEM	CMA-C3A-C4A	-2.81	124.15	128.46
2	C	760	HEM	CMB-C2B-C3B	2.67	129.67	124.68
2	A	760	HEM	CMD-C2D-C1D	-2.67	124.37	128.46
2	B	760	HEM	CAD-CBD-CGD	2.51	116.88	112.67
2	B	760	HEM	CMC-C2C-C3C	2.44	129.25	124.68
2	C	760	HEM	CMA-C3A-C2A	2.43	129.52	124.94
2	D	760	HEM	CMD-C2D-C3D	2.34	129.35	124.94
2	C	760	HEM	CMD-C2D-C3D	2.21	129.12	124.94
2	B	760	HEM	CMA-C3A-C4A	-2.17	125.13	128.46
2	D	760	HEM	CMA-C3A-C4A	-2.14	125.18	128.46

There are no chirality outliers.

There are no torsion outliers.

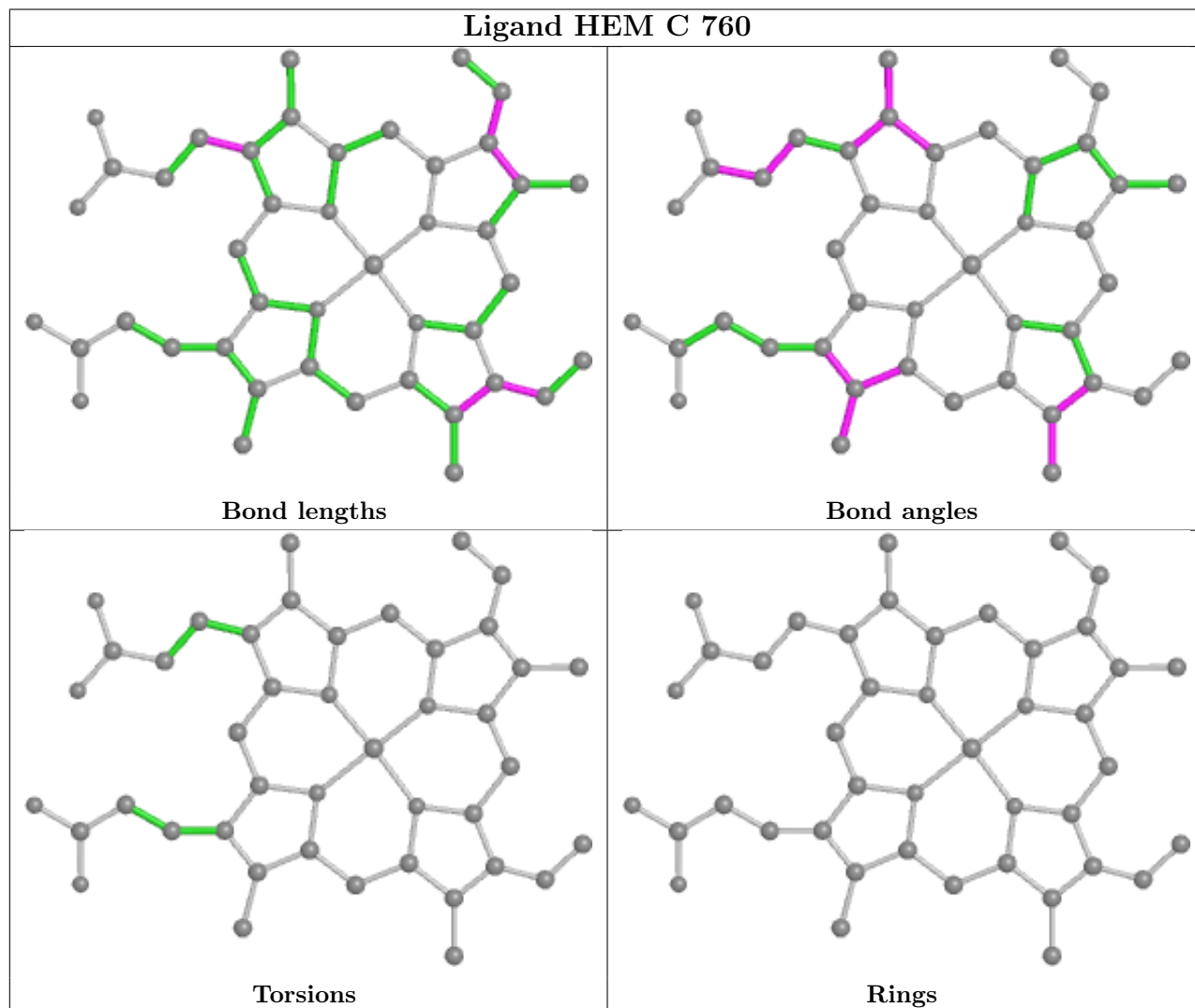
There are no ring outliers.

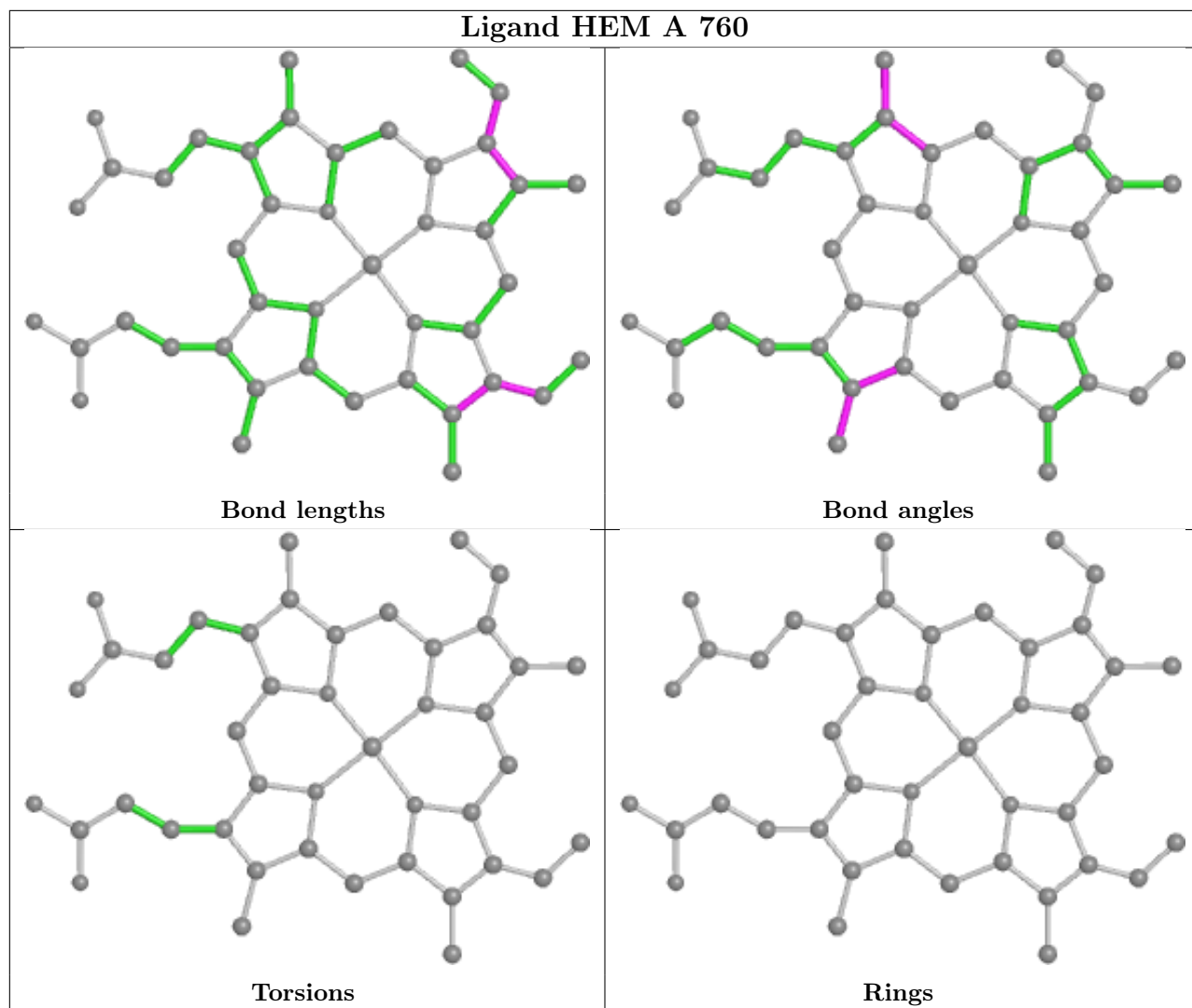
4 monomers are involved in 8 short contacts:

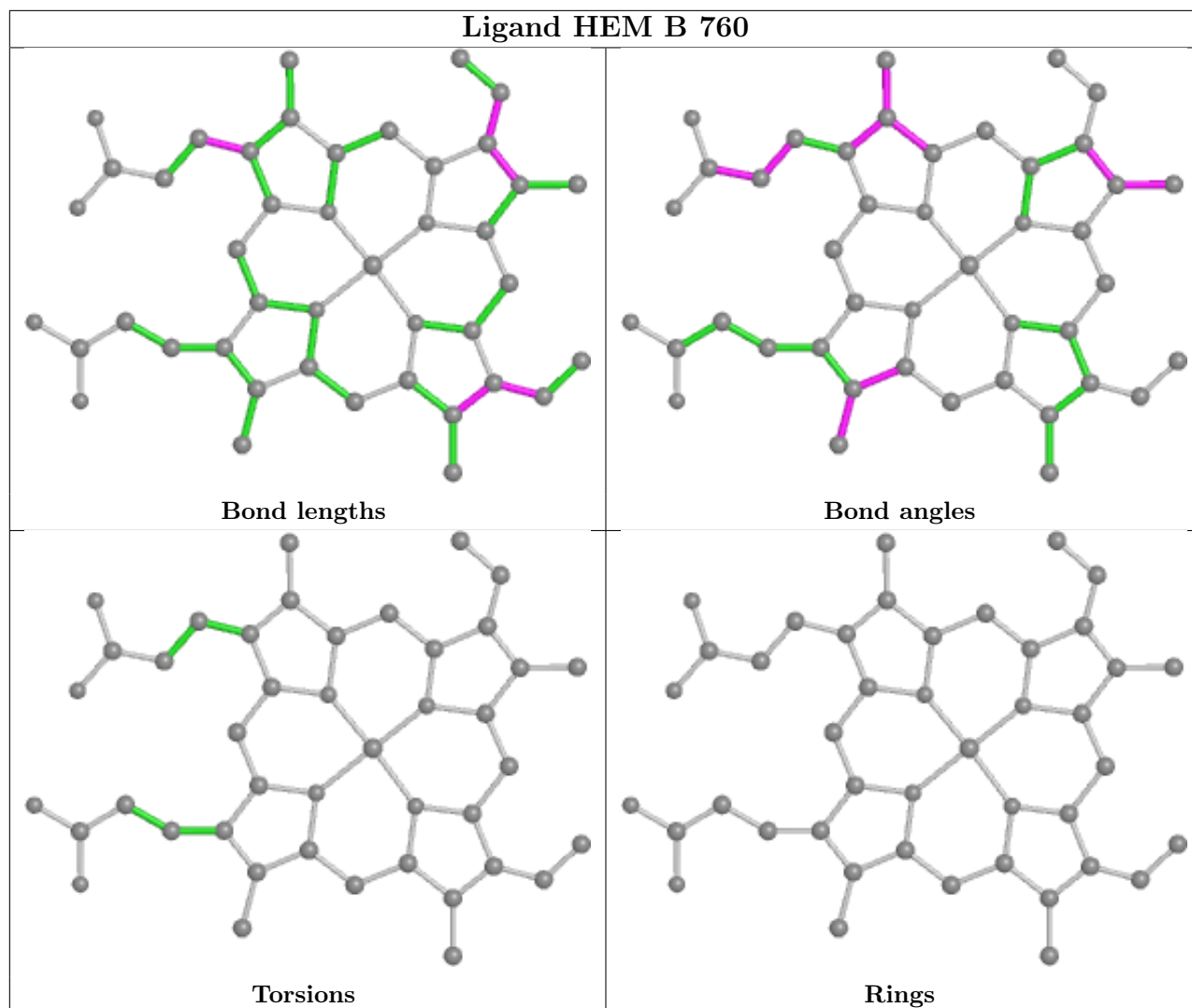
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	760	HEM	1	0
2	A	760	HEM	3	0
2	B	760	HEM	1	0
2	D	760	HEM	3	0

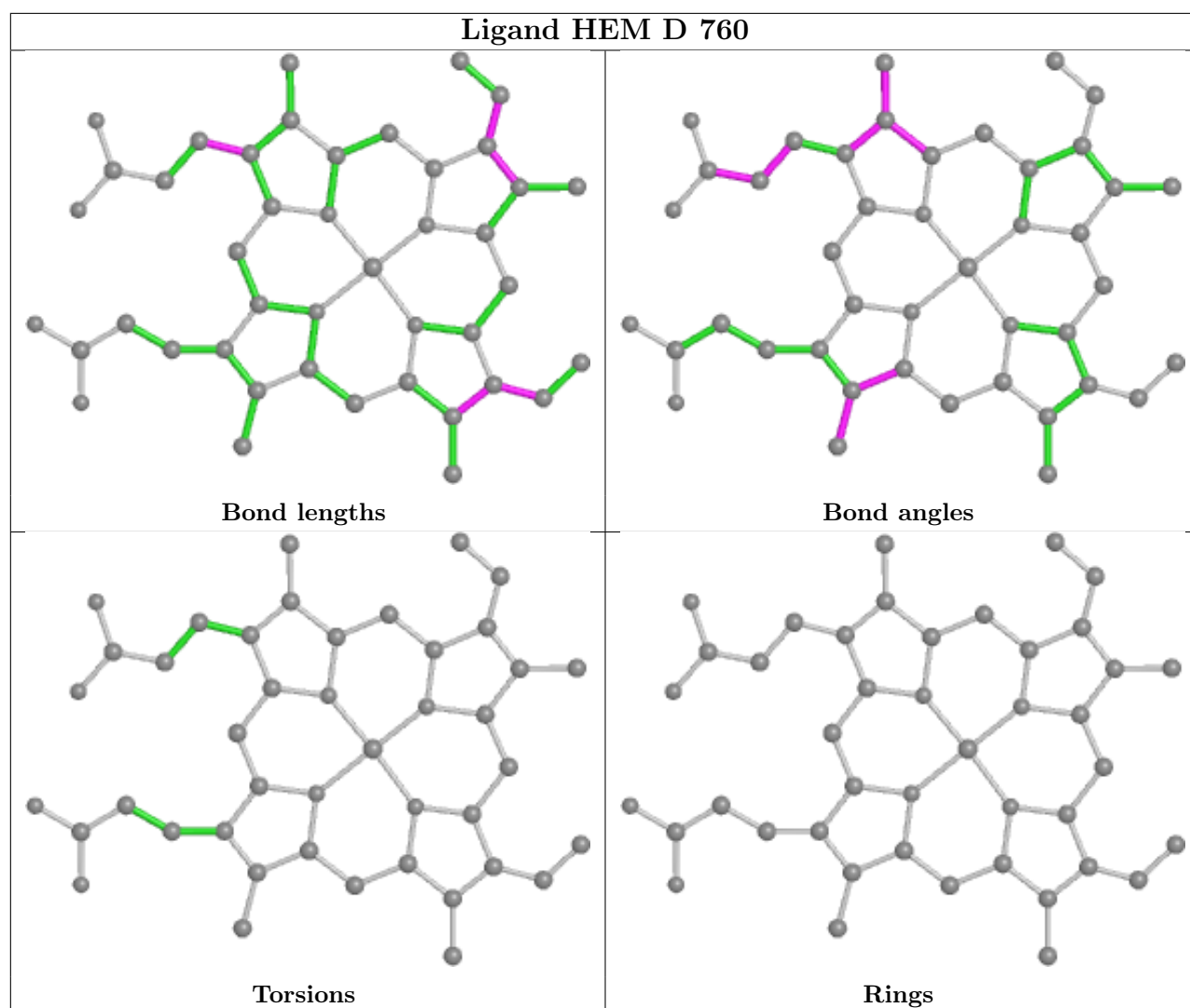
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	727/753 (96%)	-0.63	7 (0%) 82 86	3, 8, 26, 50	1 (0%)
1	B	727/753 (96%)	-0.58	8 (1%) 80 85	3, 9, 28, 47	1 (0%)
1	C	727/753 (96%)	-0.59	6 (0%) 86 89	3, 9, 28, 46	1 (0%)
1	D	727/753 (96%)	-0.64	5 (0%) 87 91	3, 8, 27, 47	1 (0%)
All	All	2908/3012 (96%)	-0.61	26 (0%) 84 88	3, 8, 27, 50	4 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	ASP	10.6
1	A	711	ALA	5.9
1	A	28	SER	5.7
1	A	710	ILE	5.3
1	C	28	SER	4.5
1	A	712	ASP	4.5
1	B	726	GLY	4.4
1	C	27	ASP	4.2
1	D	27	ASP	4.1
1	B	27	ASP	4.0
1	A	713	GLN	3.4
1	D	32	GLU	3.3
1	D	28	SER	3.2
1	A	32	GLU	3.1
1	B	28	SER	3.0
1	B	750	LYS	2.9
1	D	750	LYS	2.7
1	B	32	GLU	2.7
1	C	594	PRO	2.7
1	C	725	ASP	2.6
1	D	725	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	713	GLN	2.2
1	C	677	ASP	2.2
1	B	712	ASP	2.1
1	B	722	ASP	2.0
1	C	749	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](#)

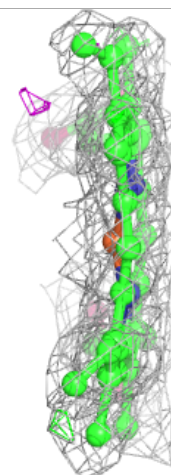
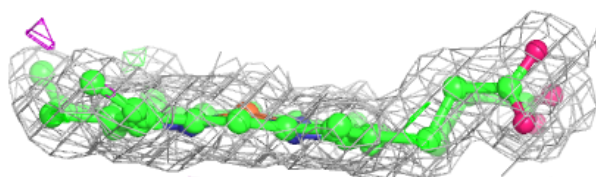
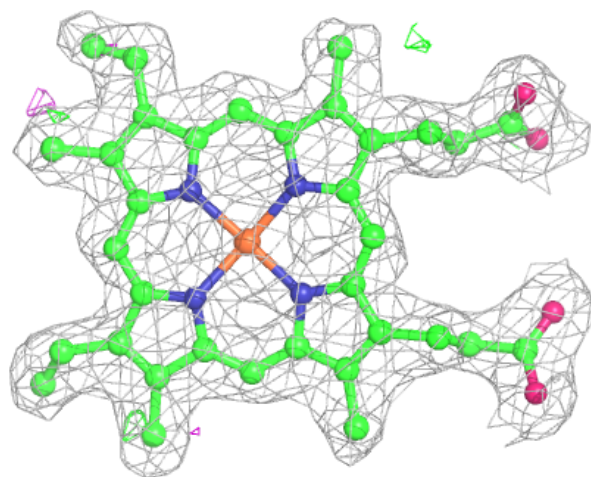
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	HEM	A	760	43/43	0.99	0.06	2,5,6,7	0
2	HEM	B	760	43/43	0.99	0.08	3,5,6,6	0
2	HEM	C	760	43/43	0.99	0.07	2,5,7,8	0
2	HEM	D	760	43/43	0.99	0.07	2,5,6,6	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:**

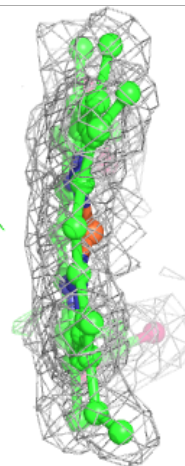
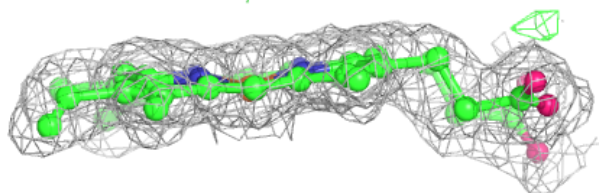
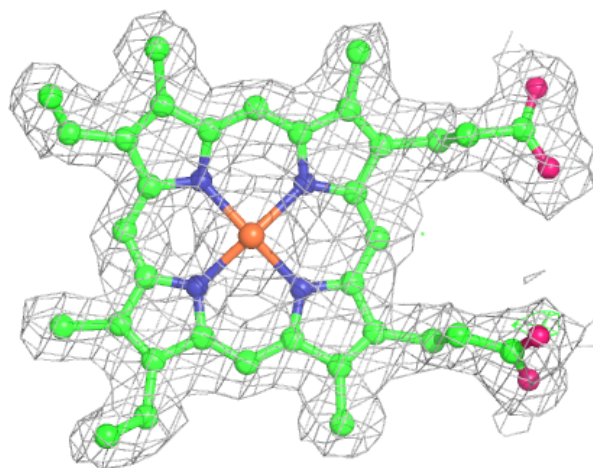
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





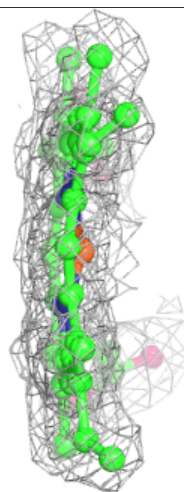
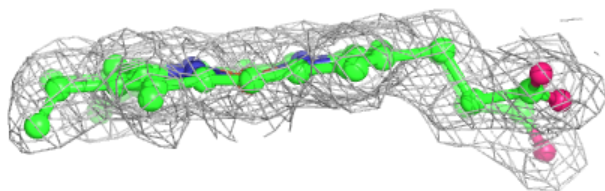
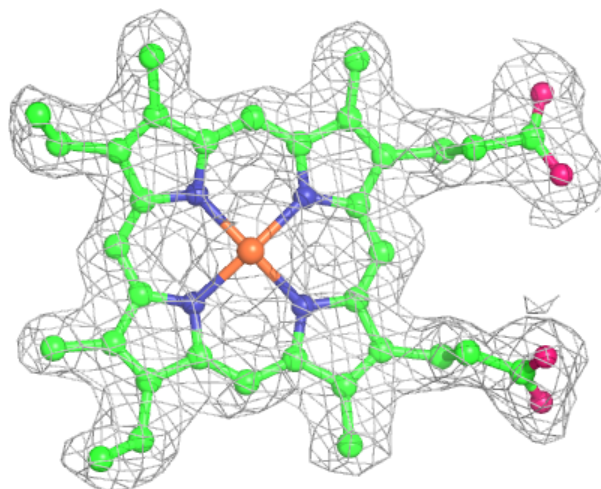
**Electron density around HEM B 760:**

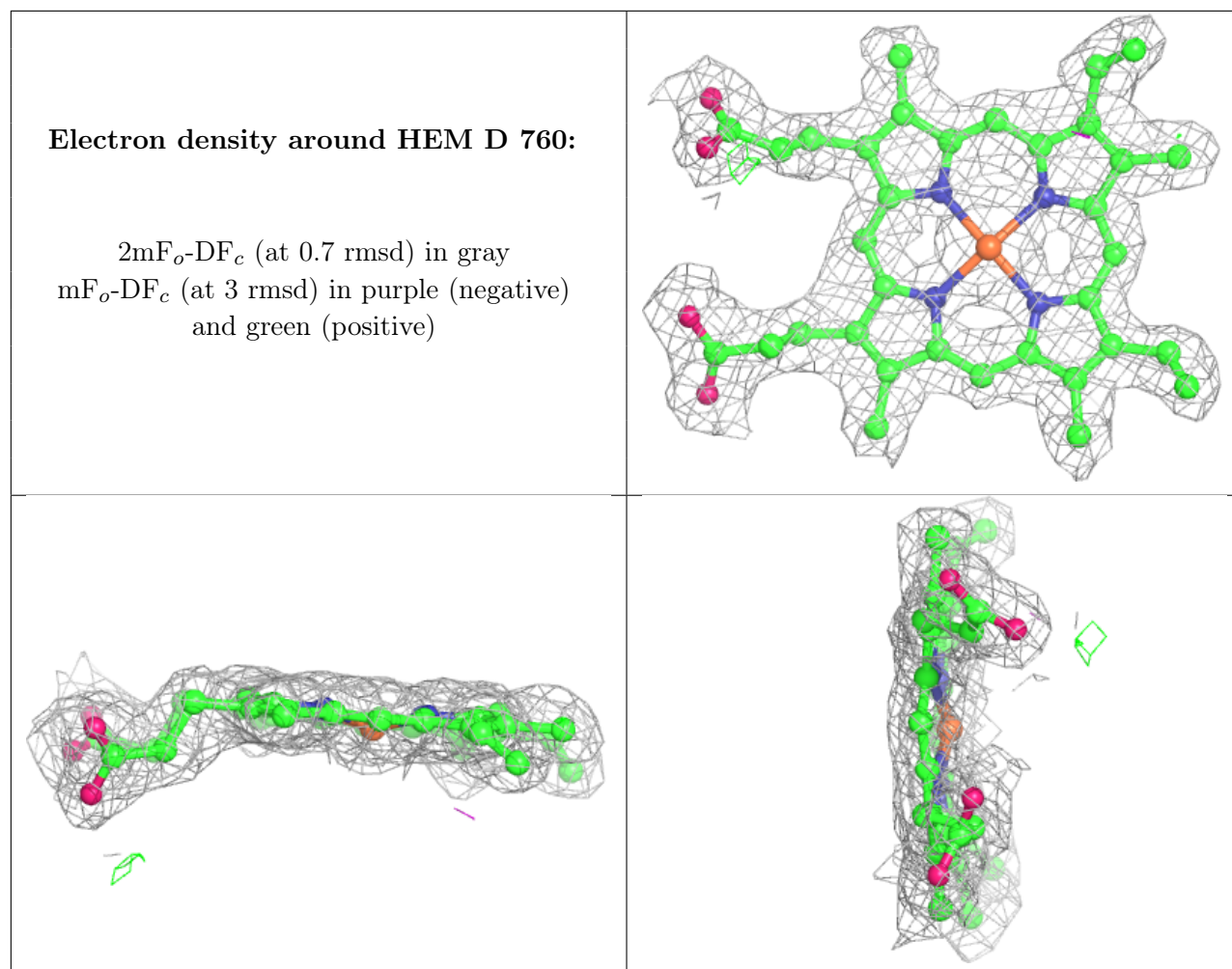
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**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.