



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 07:05 PM UTC

PDB ID : 1P80 / pdb_00001p80
Title : Crystal structure of the D181Q variant of catalase HP11 from E. coli
Authors : Chelikani, P.; Carpena, X.; Fita, I.; Loewen, P.C.
Deposited on : 2003-05-06
Resolution : 1.65 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

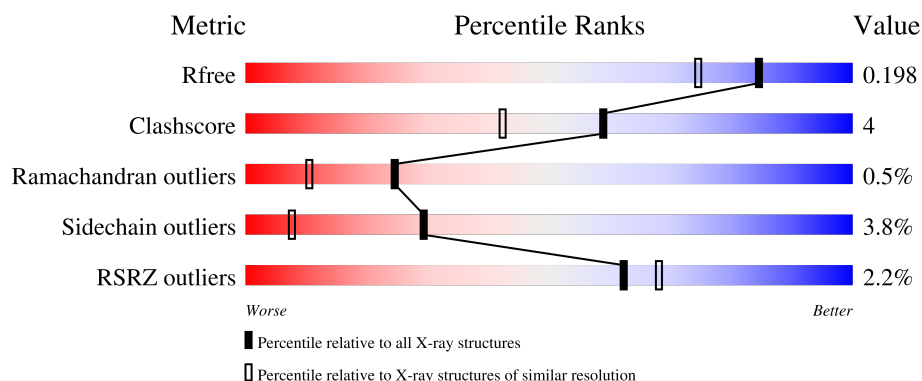
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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}	180053	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	753	2% 83% 12% ..
1	B	753	3% 80% 15% ..
1	C	753	2% 80% 15% ..
1	D	753	2% 80% 14% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26401 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.

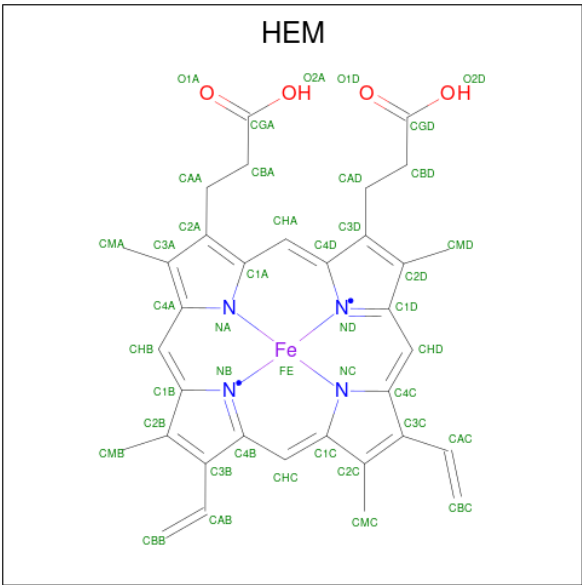
- Molecule 1 is a protein called Catalase HP11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	1	0
			5752	3651	1008	1081	12			
1	B	727	Total	C	N	O	S	0	1	0
			5752	3651	1008	1081	12			
1	C	727	Total	C	N	O	S	0	1	0
			5752	3651	1008	1081	12			
1	D	727	Total	C	N	O	S	0	1	0
			5752	3651	1008	1081	12			

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: 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

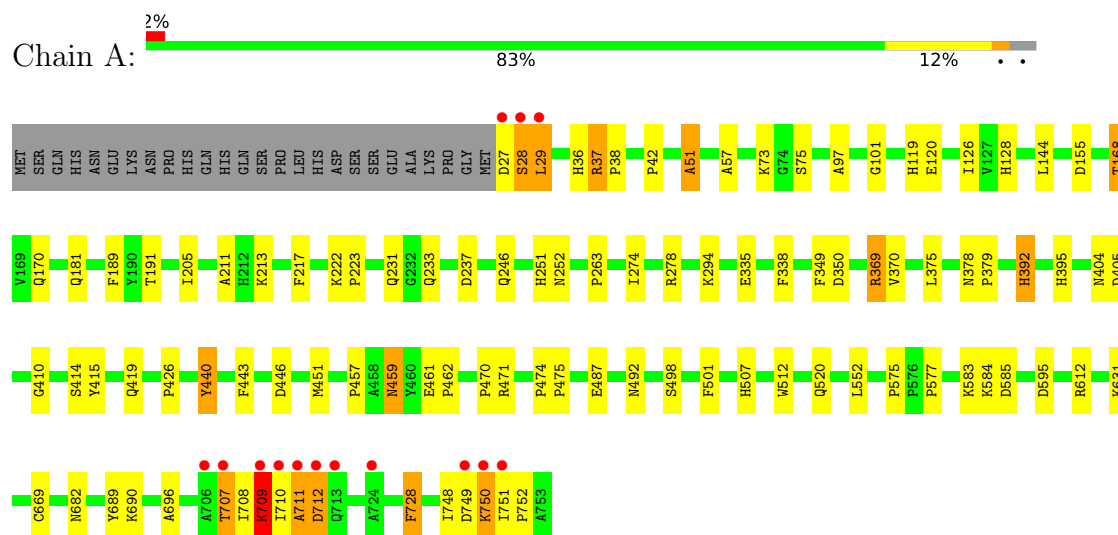
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	858	Total	O	0	0
			858	858		
3	B	740	Total	O	0	0
			740	740		
3	C	782	Total	O	0	0
			782	782		
3	D	841	Total	O	0	0
			841	841		

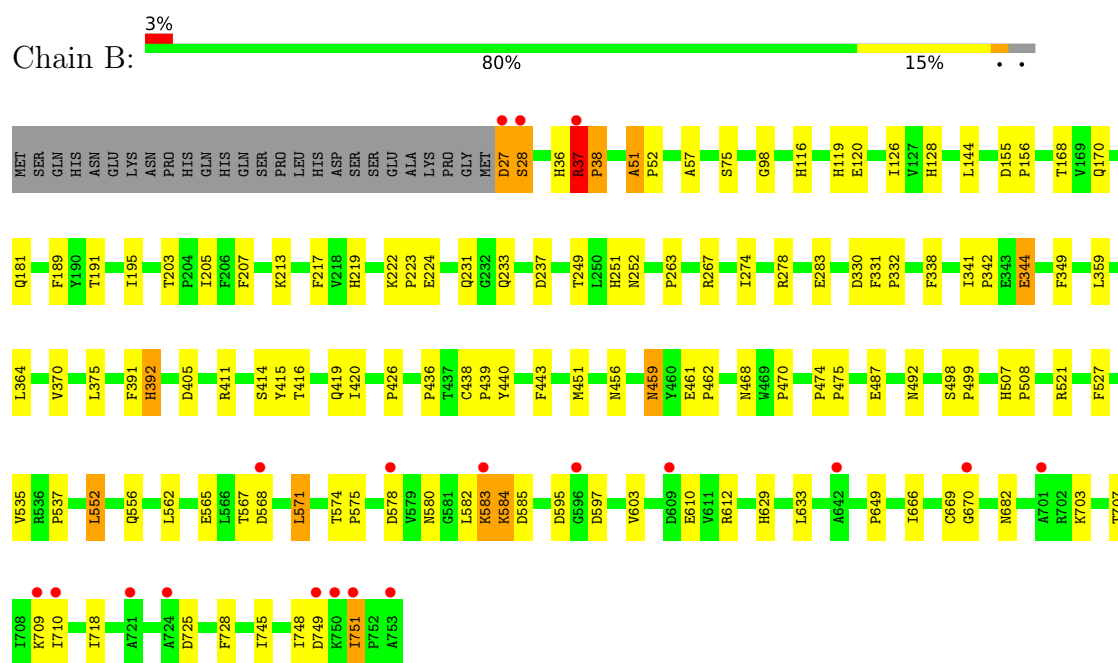
3 Residue-property plots [i](#)

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.

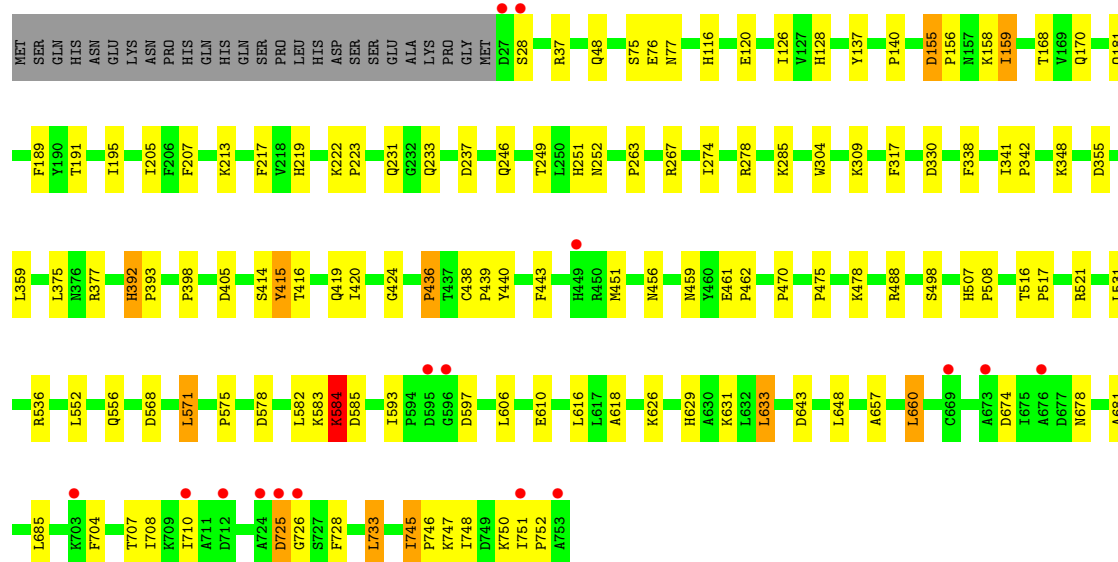
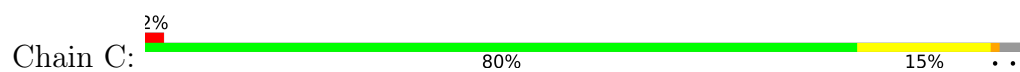
• Molecule 1: Catalase HPII



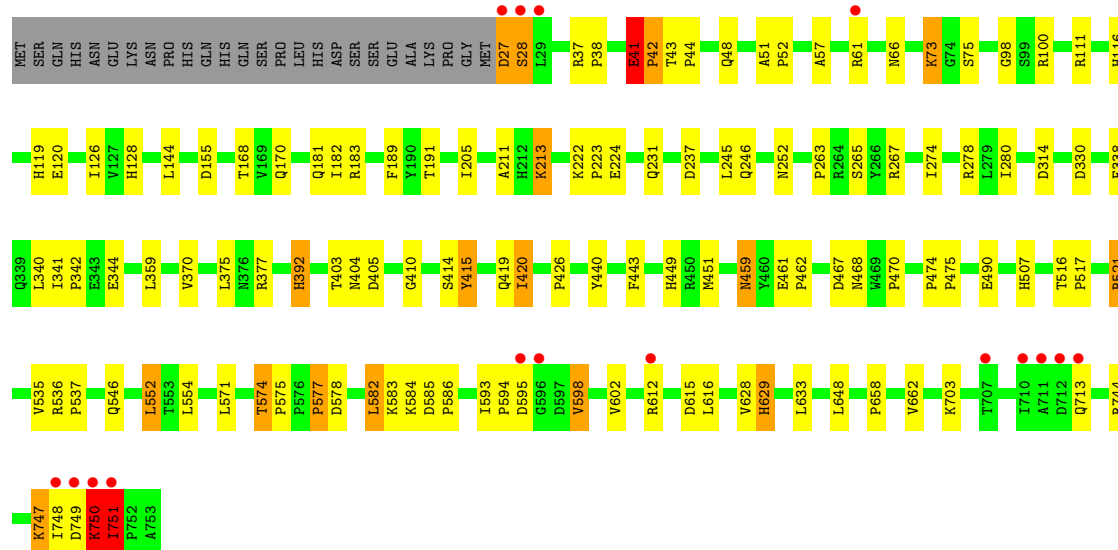
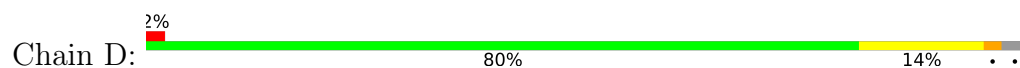
• Molecule 1: Catalase HPII



• Molecule 1: Catalase HPII



• Molecule 1: Catalase HP11



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.76Å 133.13Å 122.50Å 90.00° 109.50° 90.00°	Depositor
Resolution (Å)	29.80 – 1.65 29.80 – 1.65	Depositor EDS
% Data completeness (in resolution range)	96.0 (29.80-1.65) 95.4 (29.80-1.65)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 1.65Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.168 , 0.202 0.168 , 0.198	Depositor DCC
R_{free} test set	16400 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	16.2	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	26401	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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	0.55	0/5914	1.40	49/8041 (0.6%)
1	B	0.53	0/5914	1.40	48/8041 (0.6%)
1	C	0.52	0/5914	1.38	54/8041 (0.7%)
1	D	0.55	0/5914	1.41	57/8041 (0.7%)
All	All	0.54	0/23656	1.40	208/32164 (0.6%)

There are no bond length outliers.

All (208) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	231	GLN	N-CA-C	11.98	124.33	111.03
1	A	728	PHE	CA-CB-CG	11.43	125.23	113.80
1	C	419	GLN	OE1-CD-NE2	-10.79	111.81	122.60
1	B	231	GLN	N-CA-C	10.69	122.90	111.03
1	D	449	HIS	CA-CB-CG	10.32	124.12	113.80
1	A	233	GLN	OE1-CD-NE2	-10.15	112.45	122.60
1	A	575	PRO	N-CA-CB	10.09	108.84	103.19
1	A	231	GLN	N-CA-C	9.84	121.95	111.03
1	C	341	ILE	CA-C-O	9.50	124.88	119.94
1	B	749	ASP	CA-CB-CG	9.23	121.83	112.60
1	A	181	GLN	OE1-CD-NE2	9.21	131.81	122.60
1	D	181	GLN	OE1-CD-NE2	9.18	131.78	122.60
1	C	575	PRO	N-CA-CB	9.07	108.27	103.19
1	B	575	PRO	N-CA-CB	8.92	108.19	103.19
1	D	575	PRO	N-CA-CB	8.78	108.11	103.19
1	B	181	GLN	OE1-CD-NE2	8.74	131.34	122.60
1	D	612	ARG	CD-NE-CZ	8.58	136.41	124.40
1	B	728	PHE	CA-CB-CG	8.57	122.37	113.80
1	B	233	GLN	OE1-CD-NE2	-8.49	114.11	122.60
1	D	419	GLN	OE1-CD-NE2	-8.36	114.24	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	338	PHE	CA-CB-CG	8.33	122.13	113.80
1	A	170	GLN	CG-CD-NE2	8.29	128.83	116.40
1	C	233	GLN	OE1-CD-NE2	-8.17	114.43	122.60
1	C	338	PHE	CA-CB-CG	8.11	121.91	113.80
1	B	283	GLU	CB-CG-CD	8.05	126.28	112.60
1	C	231	GLN	N-CA-C	8.01	119.92	111.03
1	C	728	PHE	CA-CB-CG	7.88	121.68	113.80
1	C	28	SER	N-CA-C	-7.84	101.64	112.30
1	B	595	ASP	CA-CB-CG	7.82	120.42	112.60
1	D	43	THR	CA-C-N	7.71	125.21	119.66
1	D	43	THR	C-N-CA	7.71	125.21	119.66
1	B	155	ASP	CA-CB-CG	7.67	120.27	112.60
1	B	341	ILE	CA-C-O	7.63	123.91	119.94
1	B	338	PHE	CA-CB-CG	7.58	121.38	113.80
1	D	155	ASP	CA-CB-CG	7.43	120.03	112.60
1	D	170	GLN	CG-CD-NE2	7.33	127.40	116.40
1	C	726	GLY	N-CA-C	-7.30	95.89	113.18
1	C	674	ASP	CA-CB-CG	7.15	119.75	112.60
1	A	338	PHE	CA-CB-CG	7.13	120.93	113.80
1	B	414	SER	N-CA-C	7.07	118.64	111.07
1	D	341	ILE	CA-C-O	7.01	123.59	119.94
1	A	189	PHE	CA-CB-CG	6.88	120.68	113.80
1	C	414	SER	N-CA-C	6.85	118.40	111.07
1	D	231	GLN	CA-C-O	-6.79	113.91	120.90
1	A	414	SER	N-CA-C	6.78	118.67	111.28
1	C	189	PHE	CA-CB-CG	6.67	120.47	113.80
1	D	44	PRO	N-CA-CB	6.66	106.68	103.22
1	C	170	GLN	N-CA-C	6.65	119.51	111.40
1	C	231	GLN	CA-C-O	-6.53	114.17	120.90
1	D	100	ARG	CD-NE-CZ	6.53	133.54	124.40
1	C	263	PRO	N-CA-CB	6.48	108.99	103.35
1	C	355	ASP	CA-C-O	6.45	123.48	119.29
1	A	708	ILE	CA-C-N	6.43	133.83	121.54
1	A	708	ILE	C-N-CA	6.43	133.83	121.54
1	A	712	ASP	CA-CB-CG	6.42	119.02	112.60
1	A	233	GLN	CG-CD-OE1	6.41	133.61	120.80
1	C	158	LYS	CA-C-N	-6.37	115.29	123.19
1	C	158	LYS	C-N-CA	-6.37	115.29	123.19
1	A	501	PHE	CA-CB-CG	6.36	120.16	113.80
1	B	263	PRO	N-CA-CB	6.33	108.85	103.35
1	D	615	ASP	CA-CB-CG	6.29	118.89	112.60
1	D	280	ILE	CA-C-O	-6.27	113.87	120.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	567	THR	CA-C-N	6.26	128.99	120.54
1	B	567	THR	C-N-CA	6.26	128.99	120.54
1	C	419	GLN	CG-CD-NE2	6.23	125.75	116.40
1	B	98	GLY	N-CA-C	-6.16	105.03	112.48
1	C	725	ASP	CA-CB-CG	-6.06	106.54	112.60
1	B	405	ASP	CA-CB-CG	6.05	118.65	112.60
1	C	536	ARG	CA-C-O	6.05	123.22	119.29
1	B	492	ASN	CA-CB-CG	-6.05	106.55	112.60
1	B	57	ALA	CA-C-N	6.04	125.72	119.56
1	B	57	ALA	C-N-CA	6.04	125.72	119.56
1	D	474	PRO	N-CA-CB	5.99	106.55	103.19
1	A	37	ARG	CD-NE-CZ	5.99	132.78	124.40
1	A	595	ASP	CA-CB-CG	5.97	118.57	112.60
1	D	536	ARG	CA-C-O	5.95	123.16	119.29
1	B	475	PRO	N-CA-CB	5.94	108.52	103.35
1	D	278	ARG	NE-CZ-NH1	-5.90	115.60	121.50
1	A	474	PRO	N-CA-CB	5.89	106.49	103.19
1	A	350	ASP	CA-CB-CG	5.87	118.47	112.60
1	A	237	ASP	N-CA-C	5.85	118.13	111.11
1	D	414	SER	N-CA-C	5.83	117.64	111.28
1	A	42	PRO	N-CA-CB	5.83	108.52	103.27
1	B	391	PHE	CA-CB-CG	5.80	119.61	113.80
1	B	585	ASP	CA-C-N	5.77	125.44	119.56
1	B	585	ASP	C-N-CA	5.77	125.44	119.56
1	C	456	ASN	CA-C-N	5.76	125.62	119.28
1	C	456	ASN	C-N-CA	5.76	125.62	119.28
1	B	474	PRO	N-CA-CB	5.76	106.41	103.19
1	A	471	ARG	N-CA-C	5.74	119.42	110.17
1	C	246	GLN	CA-C-N	5.74	125.41	119.56
1	C	246	GLN	C-N-CA	5.74	125.41	119.56
1	C	237	ASP	N-CA-C	5.74	118.00	111.11
1	B	527	PHE	CA-CB-CG	5.74	119.54	113.80
1	C	155	ASP	CA-CB-CG	5.73	118.33	112.60
1	A	631	LYS	N-CA-CB	5.72	119.75	110.77
1	A	585	ASP	CA-C-N	5.72	125.39	119.56
1	A	585	ASP	C-N-CA	5.72	125.39	119.56
1	D	475	PRO	N-CA-CB	5.72	108.65	103.33
1	A	752	PRO	N-CA-CB	5.68	106.51	102.65
1	D	595	ASP	CA-CB-CG	5.68	118.28	112.60
1	B	349	PHE	CA-CB-CG	-5.64	108.16	113.80
1	D	237	ASP	N-CA-C	5.63	117.87	111.11
1	D	170	GLN	N-CA-C	5.62	118.25	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	419	GLN	OE1-CD-NE2	-5.61	116.99	122.60
1	D	403	THR	N-CA-CB	5.58	120.04	111.22
1	D	27	ASP	CA-CB-CG	5.57	118.17	112.60
1	D	658	PRO	N-CA-CB	5.57	108.63	103.39
1	A	440	TYR	N-CA-CB	5.57	119.84	110.77
1	A	492	ASN	CA-CB-CG	-5.57	107.03	112.60
1	B	203	THR	O-C-N	-5.56	117.02	121.80
1	C	342	PRO	N-CA-CB	5.55	108.18	103.35
1	A	498	SER	CA-C-O	5.55	125.94	120.17
1	A	231	GLN	CA-C-O	-5.54	115.19	120.90
1	B	419	GLN	OE1-CD-NE2	-5.54	117.06	122.60
1	C	475	PRO	N-CA-CB	5.54	108.48	103.33
1	A	349	PHE	CA-CB-CG	-5.54	108.26	113.80
1	C	155	ASP	CA-C-N	5.53	125.20	119.56
1	C	155	ASP	C-N-CA	5.53	125.20	119.56
1	B	237	ASP	N-CA-C	5.49	117.70	111.11
1	D	629	HIS	CA-CB-CG	-5.47	108.33	113.80
1	C	436	PRO	N-CA-CB	5.45	108.09	103.35
1	C	725	ASP	N-CA-CB	5.45	119.70	110.49
1	A	217	PHE	CA-CB-CG	-5.43	108.37	113.80
1	A	37	ARG	CA-C-N	5.42	125.19	119.76
1	A	37	ARG	C-N-CA	5.42	125.19	119.76
1	B	156	PRO	N-CA-CB	5.41	108.89	103.48
1	D	751	ILE	CA-C-O	5.38	127.16	119.95
1	B	224	GLU	CA-C-N	5.37	124.88	119.19
1	B	224	GLU	C-N-CA	5.37	124.88	119.19
1	D	189	PHE	CA-CB-CG	5.37	119.17	113.80
1	A	446	ASP	CA-CB-CG	5.37	117.97	112.60
1	C	424	GLY	N-CA-C	5.36	123.15	114.90
1	C	181	GLN	OE1-CD-NE2	5.34	127.94	122.60
1	D	263	PRO	N-CA-CB	5.34	107.99	103.35
1	C	398	PRO	N-CA-CB	5.34	107.99	103.19
1	B	456	ASN	CA-C-N	5.33	125.14	119.28
1	B	456	ASN	C-N-CA	5.33	125.14	119.28
1	B	37	ARG	CA-C-N	5.33	125.23	119.85
1	B	37	ARG	C-N-CA	5.33	125.23	119.85
1	B	597	ASP	CA-CB-CG	5.32	117.92	112.60
1	C	745	ILE	N-CA-CB	5.31	114.08	110.52
1	D	586	PRO	N-CA-CB	5.30	108.78	103.48
1	C	657	ALA	CA-C-N	5.30	125.59	119.92
1	C	657	ALA	C-N-CA	5.30	125.59	119.92
1	B	574	THR	CA-C-N	5.30	123.53	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	574	THR	C-N-CA	5.30	123.53	119.66
1	B	28	SER	N-CA-CB	5.30	119.44	110.49
1	B	189	PHE	CA-CB-CG	5.29	119.09	113.80
1	C	304	TRP	N-CA-C	5.29	117.46	111.11
1	D	521	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	D	246	GLN	CA-C-N	5.29	124.95	119.56
1	D	246	GLN	C-N-CA	5.29	124.95	119.56
1	D	420	ILE	CB-CA-C	-5.28	105.01	112.14
1	C	585	ASP	CA-C-N	5.26	124.92	119.56
1	C	585	ASP	C-N-CA	5.26	124.92	119.56
1	D	577	PRO	N-CA-CB	5.26	108.33	103.39
1	D	585	ASP	CA-C-N	5.25	124.92	119.56
1	D	585	ASP	C-N-CA	5.25	124.92	119.56
1	D	224	GLU	CB-CA-C	5.24	117.80	109.52
1	D	314	ASP	CA-C-N	5.21	124.93	119.82
1	D	314	ASP	C-N-CA	5.21	124.93	119.82
1	D	98	GLY	N-CA-C	-5.18	105.23	112.18
1	A	749	ASP	CA-CB-CG	-5.18	107.42	112.60
1	A	475	PRO	N-CA-CB	5.18	108.15	103.33
1	C	498	SER	CA-C-N	5.17	124.97	119.28
1	C	498	SER	C-N-CA	5.17	124.97	119.28
1	C	278	ARG	NE-CZ-NH1	-5.16	116.34	121.50
1	D	57	ALA	CA-C-N	5.16	124.96	119.28
1	D	57	ALA	C-N-CA	5.16	124.96	119.28
1	A	51	ALA	N-CA-C	5.15	114.06	108.14
1	B	51	ALA	N-CA-C	5.15	112.85	108.22
1	D	467	ASP	CA-C-O	5.15	127.19	120.81
1	D	42	PRO	N-CA-CB	5.14	107.90	103.27
1	A	170	GLN	OE1-CD-NE2	-5.14	117.46	122.60
1	D	183	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	D	182	ILE	N-CA-C	-5.12	102.99	109.80
1	B	38	PRO	N-CA-CB	5.12	108.09	103.33
1	D	265	SER	N-CA-CB	-5.11	103.63	111.56
1	C	405	ASP	CA-C-N	5.11	124.72	119.56
1	C	405	ASP	C-N-CA	5.11	124.72	119.56
1	C	593	ILE	CA-C-N	5.11	125.40	119.93
1	C	593	ILE	C-N-CA	5.11	125.40	119.93
1	A	708	ILE	CA-C-O	5.10	127.16	120.78
1	C	597	ASP	CA-CB-CG	5.09	117.69	112.60
1	A	577	PRO	N-CA-CB	5.09	108.17	103.39
1	C	348	LYS	CA-CB-CG	-5.08	103.94	114.10
1	B	342	PRO	N-CA-CB	5.08	107.77	103.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	612	ARG	NE-CZ-NH2	5.07	123.77	119.20
1	D	521	ARG	CD-NE-CZ	-5.07	117.30	124.40
1	D	342	PRO	N-CA-CB	5.07	107.76	103.35
1	A	168	THR	N-CA-C	-5.06	102.52	110.17
1	B	170	GLN	N-CA-C	5.06	117.57	111.40
1	B	217	PHE	CA-CB-CG	-5.06	108.74	113.80
1	A	57	ALA	CA-C-N	5.05	124.84	119.28
1	A	57	ALA	C-N-CA	5.05	124.84	119.28
1	A	51	ALA	N-CA-CB	-5.04	104.94	111.35
1	A	263	PRO	N-CA-CB	5.04	107.74	103.35
1	B	649	PRO	N-CA-CB	5.04	107.54	103.36
1	C	317	PHE	N-CA-C	5.04	116.46	111.07
1	D	377	ARG	NH1-CZ-NH2	5.04	125.85	119.30
1	D	41	GLU	CB-CG-CD	5.03	121.16	112.60
1	C	140	PRO	N-CA-CB	5.03	108.02	103.15
1	A	246	GLN	CA-C-N	5.02	124.68	119.56
1	A	246	GLN	C-N-CA	5.02	124.68	119.56
1	A	155	ASP	CA-CB-CG	5.02	117.62	112.60
1	D	213	LYS	CB-CG-CD	5.01	122.83	111.30
1	C	217	PHE	CA-CB-CG	-5.01	108.79	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5752	0	5585	47	0
1	B	5752	0	5585	67	0
1	C	5752	0	5585	53	0
1	D	5752	0	5585	53	0
2	A	43	0	30	1	0
2	B	43	0	30	2	0
2	C	43	0	30	1	0
2	D	43	0	30	1	0
3	A	858	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	740	0	0	6	0
3	C	782	0	0	7	0
3	D	841	0	0	8	0
All	All	26401	0	22460	200	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 4.

All (200) 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:B:392[B]:HIS:ND1	1:B:415:TYR:HB2	1.16	1.49
1:A:392[B]:HIS:ND1	1:A:415:TYR:HB2	1.30	1.41
1:D:392[B]:HIS:ND1	1:D:415:TYR:HB2	1.50	1.26
1:C:392[B]:HIS:ND1	1:C:415:TYR:HB2	1.47	1.25
1:B:392[B]:HIS:ND1	1:B:415:TYR:CB	2.00	1.22
1:B:392[B]:HIS:CE1	1:B:415:TYR:HB2	1.73	1.22
1:A:392[B]:HIS:ND1	1:A:415:TYR:CB	2.17	1.08
1:A:392[B]:HIS:CE1	1:A:415:TYR:HB2	2.01	0.96
1:A:451:MET:HE2	1:C:451:MET:HE2	1.47	0.95
1:D:750:LYS:HD3	1:D:751:ILE:H	1.42	0.85
1:B:451:MET:HE2	1:D:451:MET:HE2	1.56	0.84
1:B:552:LEU:HD22	1:B:556:GLN:HG3	1.70	0.74
1:D:392[B]:HIS:CE1	1:D:415:TYR:HB2	2.24	0.73
1:B:612:ARG:HD3	1:B:670:GLY:HA2	1.70	0.73
1:A:682:ASN:HB3	1:A:707:THR:HG21	1.71	0.72
1:D:744:ARG:HA	1:D:747:LYS:HD3	1.73	0.71
1:B:710:ILE:HD13	1:B:718:ILE:HG13	1.76	0.68
1:C:392[B]:HIS:CE1	1:C:415:TYR:HB2	2.27	0.68
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.76	0.67
1:C:552:LEU:HD21	1:C:571:LEU:HD12	1.78	0.66
1:A:748:ILE:O	1:A:751:ILE:HG13	1.96	0.65
1:C:583:LYS:O	1:C:584:LYS:HB3	1.96	0.65
1:C:267:ARG:HG3	3:C:3862:HOH:O	1.98	0.65
1:D:111:ARG:HB3	3:D:3414:HOH:O	1.95	0.64
1:D:267:ARG:HG3	3:D:2871:HOH:O	1.98	0.63
1:D:27:ASP:O	1:D:28:SER:HB2	1.97	0.63
1:A:27:ASP:O	1:A:28:SER:C	2.42	0.62
1:D:552:LEU:HD11	1:D:571:LEU:HD23	1.82	0.62
1:A:28:SER:HB2	1:D:245:LEU:HD13	1.82	0.62
1:B:583:LYS:H	1:B:583:LYS:NZ	1.97	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:LYS:HA	1:A:709:LYS:HE3	1.83	0.61
1:C:392[B]:HIS:ND1	1:C:415:TYR:CB	2.43	0.61
1:C:704:PHE:O	1:C:707:THR:HG22	2.01	0.61
1:B:583:LYS:O	1:B:584:LYS:HB3	2.01	0.60
1:B:144:LEU:HD11	1:B:370:VAL:HG13	1.83	0.60
1:B:468:ASN:HD22	1:D:27:ASP:N	1.99	0.60
1:B:27:ASP:OD2	1:D:468:ASN:ND2	2.30	0.60
1:C:748:ILE:O	1:C:751:ILE:HG22	2.02	0.59
1:D:61:ARG:HH11	1:D:66:ASN:HA	1.69	0.58
1:A:144:LEU:HD11	1:A:370:VAL:HG13	1.86	0.57
1:B:267:ARG:HG3	3:B:2872:HOH:O	2.03	0.57
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.34	0.57
1:C:274:ILE:HD12	2:C:760:HEM:HMB1	1.87	0.56
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.90	0.55
1:B:521:ARG:HH21	1:B:745:ILE:HG21	1.72	0.55
1:B:51:ALA:HB1	1:B:52:PRO:HD2	1.89	0.54
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.91	0.54
1:A:36:HIS:CD2	1:A:36:HIS:H	2.25	0.53
1:B:359:LEU:H	1:B:507:HIS:HD2	1.55	0.53
1:B:521:ARG:HH21	1:B:745:ILE:HD13	1.73	0.53
1:D:359:LEU:H	1:D:507:HIS:HD2	1.56	0.53
1:C:610:GLU:OE1	1:C:643:ASP:HA	2.08	0.53
1:C:416:THR:HA	3:C:4199:HOH:O	2.08	0.53
1:A:751:ILE:O	1:A:751:ILE:HD12	2.09	0.53
1:D:222:LYS:HB3	1:D:223:PRO:HD2	1.91	0.53
1:B:392[B]:HIS:CE1	1:B:415:TYR:CB	2.68	0.52
1:B:535:VAL:O	1:B:537:PRO:HD3	2.10	0.52
1:D:274:ILE:HD12	2:D:760:HEM:HMB1	1.91	0.52
1:D:748:ILE:O	1:D:751:ILE:HG22	2.10	0.52
1:D:535:VAL:O	1:D:537:PRO:HD3	2.09	0.52
1:A:689:TYR:OH	1:A:710:ILE:HG21	2.10	0.51
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.93	0.51
1:C:578:ASP:HB2	1:C:582:LEU:O	2.09	0.51
1:B:438:CYS:HB2	1:B:439:PRO:HD2	1.91	0.51
1:D:598:VAL:HG13	1:D:628:VAL:CG2	2.41	0.51
1:B:748:ILE:O	1:B:751:ILE:HG22	2.11	0.51
1:B:521:ARG:NH2	1:B:745:ILE:HG21	2.26	0.51
1:A:222:LYS:HB3	1:A:223:PRO:HD2	1.93	0.50
1:B:578:ASP:HB3	1:B:582:LEU:O	2.11	0.50
1:C:309:LYS:HB3	1:C:660:LEU:HD21	1.93	0.50
1:B:552:LEU:HD21	1:B:571:LEU:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:745:ILE:HD13	3:C:3866:HOH:O	2.10	0.50
1:C:222:LYS:HB3	1:C:223:PRO:HD2	1.93	0.49
1:B:416:THR:HG21	3:D:3414:HOH:O	2.11	0.49
1:B:37:ARG:HD2	3:B:3832:HOH:O	2.12	0.49
1:A:583:LYS:O	1:A:584:LYS:HB3	2.12	0.49
3:B:1589:HOH:O	1:D:73:LYS:HD2	2.11	0.49
1:A:29:LEU:HD22	3:C:3355:HOH:O	2.12	0.49
1:C:443:PHE:CZ	1:C:470:PRO:HD2	2.47	0.49
1:A:278:ARG:HH12	1:A:487:GLU:CD	2.21	0.49
1:B:126:ILE:CD1	1:C:120:GLU:HB2	2.43	0.49
1:C:631:LYS:HG3	1:C:633:LEU:HD13	1.95	0.49
1:B:195:ILE:HD11	1:B:436:PRO:HA	1.95	0.49
1:A:37:ARG:HA	1:A:38:PRO:HD3	1.75	0.48
1:D:629:HIS:HD2	3:D:2510:HOH:O	1.96	0.48
1:A:612:ARG:HH11	1:A:669:CYS:CB	2.27	0.48
1:D:51:ALA:HB1	1:D:52:PRO:HD2	1.96	0.48
1:A:750:LYS:O	1:A:750:LYS:HE3	2.14	0.48
1:D:359:LEU:H	1:D:507:HIS:CD2	2.32	0.48
1:A:29:LEU:HD13	3:C:3355:HOH:O	2.13	0.48
1:A:128:HIS:HA	1:A:168:THR:O	2.14	0.48
1:A:443:PHE:CZ	1:A:470:PRO:HD2	2.48	0.48
1:C:137:TYR:HB2	1:C:159:ILE:HD13	1.96	0.48
1:B:344:GLU:H	1:B:344:GLU:CD	2.20	0.47
1:D:546:GLN:HG3	3:D:3688:HOH:O	2.13	0.47
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.30	0.47
1:D:577:PRO:HG2	3:D:4041:HOH:O	2.14	0.47
1:A:274:ILE:HD12	2:A:760:HEM:HMB1	1.96	0.47
1:D:404:ASN:O	1:D:405:ASP:C	2.57	0.47
1:A:28:SER:CB	1:D:245:LEU:HD22	2.45	0.47
1:A:335:GLU:OE1	1:A:369:ARG:HD3	2.14	0.47
1:B:222:LYS:HB3	1:B:223:PRO:HD2	1.97	0.47
1:A:395:HIS:HE1	3:A:4187:HOH:O	1.98	0.46
1:B:745:ILE:O	1:B:748:ILE:HG12	2.14	0.46
1:C:626:LYS:HG3	1:C:733:LEU:HG	1.95	0.46
1:A:612:ARG:HE	1:A:669:CYS:HB3	1.80	0.46
1:D:583:LYS:O	1:D:584:LYS:HB3	2.16	0.46
1:C:751:ILE:HG13	1:C:752:PRO:HD2	1.98	0.46
1:A:711:ALA:HB3	3:A:4038:HOH:O	2.16	0.45
1:B:36:HIS:H	1:B:36:HIS:HD1	1.63	0.45
1:B:119:HIS:CE1	1:D:420:ILE:HG21	2.52	0.45
1:B:459:ASN:H	1:B:459:ASN:HD22	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:521:ARG:NH2	1:B:745:ILE:HD13	2.31	0.45
1:B:274:ILE:HD12	2:B:760:HEM:HMB1	1.98	0.45
1:A:120:GLU:HB2	1:D:126:ILE:CD1	2.46	0.45
1:B:251:HIS:CE1	1:B:507:HIS:HB3	2.52	0.45
1:D:128:HIS:HA	1:D:168:THR:O	2.17	0.45
1:D:443:PHE:CZ	1:D:470:PRO:HD2	2.52	0.45
1:D:578:ASP:HB3	1:D:582:LEU:O	2.16	0.45
1:B:507:HIS:N	1:B:508:PRO:CD	2.80	0.45
1:A:126:ILE:CD1	1:D:120:GLU:HB2	2.47	0.44
1:D:37:ARG:HA	1:D:38:PRO:HD3	1.85	0.44
1:B:128:HIS:HA	1:B:168:THR:O	2.17	0.44
1:D:574:THR:HG22	3:D:2568:HOH:O	2.16	0.44
1:A:696:ALA:HB1	1:A:728:PHE:CZ	2.52	0.44
1:B:521:ARG:HD3	3:B:3992:HOH:O	2.17	0.44
1:A:38:PRO:HG2	1:A:51:ALA:HB2	1.99	0.44
1:B:359:LEU:H	1:B:507:HIS:CD2	2.33	0.44
1:A:690:LYS:HG3	1:A:751:ILE:HD11	1.98	0.44
1:B:426:PRO:HB2	1:D:116:HIS:CD2	2.53	0.44
1:C:552:LEU:HD22	1:C:556:GLN:HG3	1.99	0.44
1:C:438:CYS:HB2	1:C:439:PRO:HD2	1.99	0.44
1:A:461:GLU:HA	1:A:462:PRO:C	2.42	0.44
1:C:251:HIS:CE1	1:C:507:HIS:HB3	2.53	0.44
1:D:516:THR:HB	1:D:517:PRO:HD2	2.00	0.44
1:D:41:GLU:CD	1:D:42:PRO:HD2	2.43	0.43
1:A:126:ILE:HD11	1:D:120:GLU:HB2	2.00	0.43
1:B:278:ARG:HH22	1:B:487:GLU:CD	2.27	0.43
1:B:411:ARG:HG2	2:B:760:HEM:C2C	2.53	0.43
1:D:144:LEU:HD11	1:D:370:VAL:HG13	2.00	0.43
1:A:426:PRO:HB2	1:C:116:HIS:CD2	2.53	0.43
1:B:603:VAL:HG11	1:B:666:ILE:HD12	2.00	0.43
1:B:120:GLU:HB2	1:C:126:ILE:CD1	2.49	0.43
1:D:703:LYS:HE2	3:D:3690:HOH:O	2.18	0.43
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.34	0.43
1:B:420:ILE:HG21	1:D:119:HIS:CE1	2.53	0.43
1:B:710:ILE:CD1	1:B:718:ILE:HG13	2.46	0.43
1:B:392[B]:HIS:ND1	1:B:415:TYR:HB3	2.16	0.43
1:B:682:ASN:HB3	1:B:707:THR:HG21	2.00	0.43
1:C:359:LEU:H	1:C:507:HIS:CD2	2.37	0.43
1:C:392[A]:HIS:ND1	1:C:393:PRO:HD2	2.34	0.43
1:C:618:ALA:HB1	1:C:725:ASP:HB2	2.01	0.43
1:C:359:LEU:H	1:C:507:HIS:HD2	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:359:LEU:HD12	1:C:359:LEU:C	2.44	0.42
1:D:461:GLU:HA	1:D:462:PRO:C	2.43	0.42
1:D:211:ALA:CB	1:D:410:GLY:HA3	2.49	0.42
1:C:195:ILE:HD11	1:C:436:PRO:HA	2.02	0.42
1:C:207:PHE:O	1:C:249:THR:HA	2.19	0.42
1:B:267:ARG:HG2	1:B:332:PRO:HB3	2.01	0.42
1:A:612:ARG:HH11	1:A:669:CYS:HB2	1.84	0.42
1:B:331:PHE:HA	1:B:332:PRO:HD3	1.92	0.42
1:B:669:CYS:SG	1:B:670:GLY:N	2.93	0.42
1:C:128:HIS:HA	1:C:168:THR:O	2.19	0.42
1:B:461:GLU:HA	1:B:462:PRO:C	2.45	0.42
1:C:516:THR:HB	1:C:517:PRO:HD2	2.02	0.42
1:B:207:PHE:O	1:B:249:THR:HA	2.20	0.42
1:B:498:SER:HA	1:B:499:PRO:HD3	1.93	0.42
1:C:48:GLN:NE2	3:C:4048:HOH:O	2.53	0.42
1:D:521:ARG:HH11	1:D:521:ARG:HD3	1.65	0.42
1:B:552:LEU:CD2	1:B:556:GLN:HG3	2.45	0.41
1:C:610:GLU:O	1:C:610:GLU:HG3	2.20	0.41
1:D:602:VAL:HG13	1:D:662:VAL:HA	2.01	0.41
1:A:251:HIS:CE1	1:A:507:HIS:HB3	2.55	0.41
1:A:378:ASN:HB3	1:A:379:PRO:HD2	2.02	0.41
1:B:27:ASP:HB3	3:B:3519:HOH:O	2.20	0.41
1:B:416:THR:HA	3:B:4196:HOH:O	2.19	0.41
1:C:745:ILE:N	1:C:746:PRO:HD2	2.35	0.41
1:A:119:HIS:CE1	1:C:420:ILE:HG21	2.56	0.41
1:B:37:ARG:HA	1:B:38:PRO:HD3	1.88	0.41
1:B:443:PHE:CZ	1:B:470:PRO:HD2	2.55	0.41
1:A:457:PRO:HG2	1:C:37:ARG:HH21	1.86	0.41
1:C:76:GLU:O	1:C:77:ASN:HB2	2.19	0.41
1:C:155:ASP:HA	1:C:156:PRO:HD2	1.93	0.41
1:C:461:GLU:HA	1:C:462:PRO:C	2.46	0.41
1:D:61:ARG:NH1	1:D:66:ASN:HA	2.33	0.41
1:D:750:LYS:HD3	1:D:751:ILE:N	2.22	0.40
1:A:512:TRP:CH2	1:A:520:GLN:HB3	2.56	0.40
1:C:507:HIS:N	1:C:508:PRO:CD	2.83	0.40
1:D:593:ILE:HA	1:D:594:PRO:HD2	1.94	0.40
1:A:97:ALA:O	1:A:101:GLY:HA3	2.22	0.40
1:B:144:LEU:HD11	1:B:370:VAL:CG1	2.50	0.40
1:B:364:LEU:HD11	1:B:580:ASN:HB2	2.04	0.40
1:C:678:ASN:HB3	1:C:681:ALA:HB3	2.03	0.40
1:B:116:HIS:CD2	1:D:426:PRO:HB2	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:LYS:HB3	1:C:223:PRO:CD	2.51	0.40
1:C:507:HIS:N	1:C:508:PRO:HD2	2.36	0.40
1:C:747:LYS:HE2	3:C:3968:HOH:O	2.21	0.40
1:A:211:ALA:CB	1:A:410:GLY:HA3	2.52	0.40
1:A:404:ASN:O	1:A:405:ASP:C	2.64	0.40
1:B:507:HIS:N	1:B:508:PRO:HD2	2.36	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	726/753 (96%)	705 (97%)	17 (2%)	4 (1%)	21	8
1	B	726/753 (96%)	710 (98%)	12 (2%)	4 (1%)	21	8
1	C	726/753 (96%)	710 (98%)	14 (2%)	2 (0%)	36	21
1	D	726/753 (96%)	708 (98%)	14 (2%)	4 (1%)	21	8
All	All	2904/3012 (96%)	2833 (98%)	57 (2%)	14 (0%)	24	10

All (14) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
1	A	75	SER
1	C	584	LYS
1	C	75	SER
1	B	75	SER
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	613/636 (96%)	595 (97%)	18 (3%)	37	14
1	B	613/636 (96%)	590 (96%)	23 (4%)	29	7
1	C	613/636 (96%)	585 (95%)	28 (5%)	24	5
1	D	613/636 (96%)	584 (95%)	29 (5%)	23	5
All	All	2452/2544 (96%)	2354 (96%)	98 (4%)	29	7

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	73	LYS
1	A	191	THR
1	A	205	ILE
1	A	213	LYS
1	A	252	ASN
1	A	294	LYS
1	A	369	ARG
1	A	375	LEU
1	A	392[A]	HIS
1	A	392[B]	HIS
1	A	440	TYR
1	A	459	ASN
1	A	552	LEU
1	A	707	THR
1	A	709	LYS

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Mol	Chain	Res	Type
1	A	712	ASP
1	A	750	LYS
1	B	27	ASP
1	B	37	ARG
1	B	191	THR
1	B	205	ILE
1	B	213	LYS
1	B	252	ASN
1	B	344	GLU
1	B	375	LEU
1	B	392[A]	HIS
1	B	392[B]	HIS
1	B	440	TYR
1	B	459	ASN
1	B	552	LEU
1	B	562	LEU
1	B	565	GLU
1	B	568	ASP
1	B	571	LEU
1	B	583	LYS
1	B	610	GLU
1	B	633	LEU
1	B	703	LYS
1	B	709	LYS
1	B	751	ILE
1	C	159	ILE
1	C	191	THR
1	C	205	ILE
1	C	213	LYS
1	C	252	ASN
1	C	285	LYS
1	C	375	LEU
1	C	377	ARG
1	C	392[A]	HIS
1	C	392[B]	HIS
1	C	415	TYR
1	C	440	TYR
1	C	459	ASN
1	C	478	LYS
1	C	488	ARG
1	C	521	ARG
1	C	531	LEU

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Mol	Chain	Res	Type
1	C	568	ASP
1	C	571	LEU
1	C	584	LYS
1	C	606	LEU
1	C	616	LEU
1	C	633	LEU
1	C	648	LEU
1	C	660	LEU
1	C	685	LEU
1	C	733	LEU
1	C	750	LYS
1	D	41	GLU
1	D	48	GLN
1	D	73	LYS
1	D	191	THR
1	D	205	ILE
1	D	213	LYS
1	D	252	ASN
1	D	340	LEU
1	D	344	GLU
1	D	375	LEU
1	D	392[A]	HIS
1	D	392[B]	HIS
1	D	415	TYR
1	D	440	TYR
1	D	459	ASN
1	D	490	GLU
1	D	552	LEU
1	D	554	LEU
1	D	574	THR
1	D	582	LEU
1	D	598	VAL
1	D	616	LEU
1	D	633	LEU
1	D	648	LEU
1	D	713	GLN
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 (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	252	ASN
1	A	459	ASN
1	B	157	ASN
1	B	181	GLN
1	B	252	ASN
1	B	459	ASN
1	B	507	HIS
1	B	629	HIS
1	C	181	GLN
1	C	252	ASN
1	C	449	HIS
1	C	459	ASN
1	C	507	HIS
1	C	546	GLN
1	C	556	GLN
1	C	572	ASN
1	C	629	HIS
1	C	671	ASN
1	D	48	GLN
1	D	77	ASN
1	D	252	ASN
1	D	459	ASN
1	D	507	HIS
1	D	629	HIS
1	D	671	ASN
1	D	713	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	D	760	1	50,50,50	1.33	9 (18%)	67,82,82	0.97	3 (4%)
2	HEM	C	760	1	50,50,50	1.34	7 (14%)	67,82,82	1.02	4 (5%)
2	HEM	B	760	1	50,50,50	1.40	11 (22%)	67,82,82	1.13	5 (7%)
2	HEM	A	760	1	50,50,50	1.32	8 (16%)	67,82,82	1.08	5 (7%)

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	D	760	1	-	2/14/54/54	-
2	HEM	C	760	1	-	2/14/54/54	-
2	HEM	B	760	1	-	4/14/54/54	-
2	HEM	A	760	1	-	4/14/54/54	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	760	HEM	CAB-C3B	3.06	1.55	1.47
2	B	760	HEM	FE-ND	3.05	2.04	1.94
2	D	760	HEM	FE-ND	2.86	2.03	1.94
2	D	760	HEM	FE-NA	2.83	2.04	1.95
2	C	760	HEM	FE-NB	2.76	2.03	1.94
2	A	760	HEM	FE-ND	2.69	2.03	1.94
2	C	760	HEM	FE-ND	2.63	2.03	1.94
2	B	760	HEM	CAC-C3C	2.63	1.54	1.47
2	D	760	HEM	CAC-C3C	2.60	1.54	1.47
2	B	760	HEM	CAB-C3B	2.59	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	760	HEM	FE-NA	2.58	2.03	1.95
2	D	760	HEM	CAB-C3B	2.58	1.54	1.47
2	A	760	HEM	CAC-C3C	2.57	1.54	1.47
2	A	760	HEM	CAB-C3B	2.56	1.54	1.47
2	C	760	HEM	CAC-C3C	2.55	1.54	1.47
2	B	760	HEM	FE-NB	2.52	2.02	1.94
2	A	760	HEM	FE-NA	2.52	2.03	1.95
2	A	760	HEM	FE-NB	2.45	2.02	1.94
2	D	760	HEM	FE-NB	2.42	2.02	1.94
2	D	760	HEM	CMA-C3A	2.41	1.55	1.50
2	C	760	HEM	FE-NA	2.41	2.03	1.95
2	A	760	HEM	FE-NC	2.35	2.02	1.95
2	B	760	HEM	FE-NC	2.33	2.02	1.95
2	A	760	HEM	CMD-C2D	2.32	1.55	1.50
2	B	760	HEM	C2A-C3A	-2.31	1.32	1.38
2	B	760	HEM	CMB-C2B	2.31	1.55	1.50
2	D	760	HEM	CMC-C2C	2.27	1.55	1.50
2	D	760	HEM	CMD-C2D	2.19	1.55	1.50
2	C	760	HEM	CMA-C3A	2.17	1.55	1.50
2	D	760	HEM	CMB-C2B	2.14	1.55	1.50
2	A	760	HEM	CMB-C2B	2.13	1.55	1.50
2	B	760	HEM	CMA-C3A	2.11	1.55	1.50
2	B	760	HEM	CMC-C2C	2.10	1.55	1.50
2	B	760	HEM	CMD-C2D	2.08	1.55	1.50
2	C	760	HEM	CMD-C2D	2.07	1.55	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	760	HEM	O2D-CGD-O1D	3.12	131.34	123.33
2	A	760	HEM	O1D-CGD-CBD	-3.09	113.30	123.09
2	C	760	HEM	O1D-CGD-CBD	-2.92	113.84	123.09
2	B	760	HEM	O1D-CGD-CBD	-2.90	113.89	123.09
2	B	760	HEM	O2A-CGA-O1A	2.84	130.63	123.33
2	D	760	HEM	O2A-CGA-O1A	2.79	130.51	123.33
2	B	760	HEM	O1A-CGA-CBA	-2.73	114.42	123.09
2	C	760	HEM	O1A-CGA-CBA	-2.65	114.70	123.09
2	B	760	HEM	CAA-CBA-CGA	-2.50	107.03	113.67
2	D	760	HEM	O1A-CGA-CBA	-2.45	115.32	123.09
2	A	760	HEM	O2A-CGA-O1A	2.44	129.61	123.33
2	C	760	HEM	O2A-CGA-O1A	2.35	129.37	123.33
2	D	760	HEM	CAA-CBA-CGA	-2.34	107.45	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	760	HEM	CMA-C3A-C2A	2.21	130.31	125.62
2	A	760	HEM	O1A-CGA-CBA	-2.16	116.25	123.09
2	C	760	HEM	CAA-CBA-CGA	-2.07	108.18	113.67
2	A	760	HEM	CAA-CBA-CGA	-2.03	108.29	113.67

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	760	HEM	CAA-CBA-CGA-O2A
2	D	760	HEM	CAA-CBA-CGA-O1A
2	B	760	HEM	CAA-CBA-CGA-O1A
2	A	760	HEM	CAA-CBA-CGA-O1A
2	A	760	HEM	CAA-CBA-CGA-O2A
2	C	760	HEM	CAA-CBA-CGA-O2A
2	D	760	HEM	CAA-CBA-CGA-O2A
2	C	760	HEM	CAA-CBA-CGA-O1A
2	A	760	HEM	CAD-CBD-CGD-O1D
2	A	760	HEM	CAD-CBD-CGD-O2D
2	B	760	HEM	CAD-CBD-CGD-O2D
2	B	760	HEM	CAD-CBD-CGD-O1D

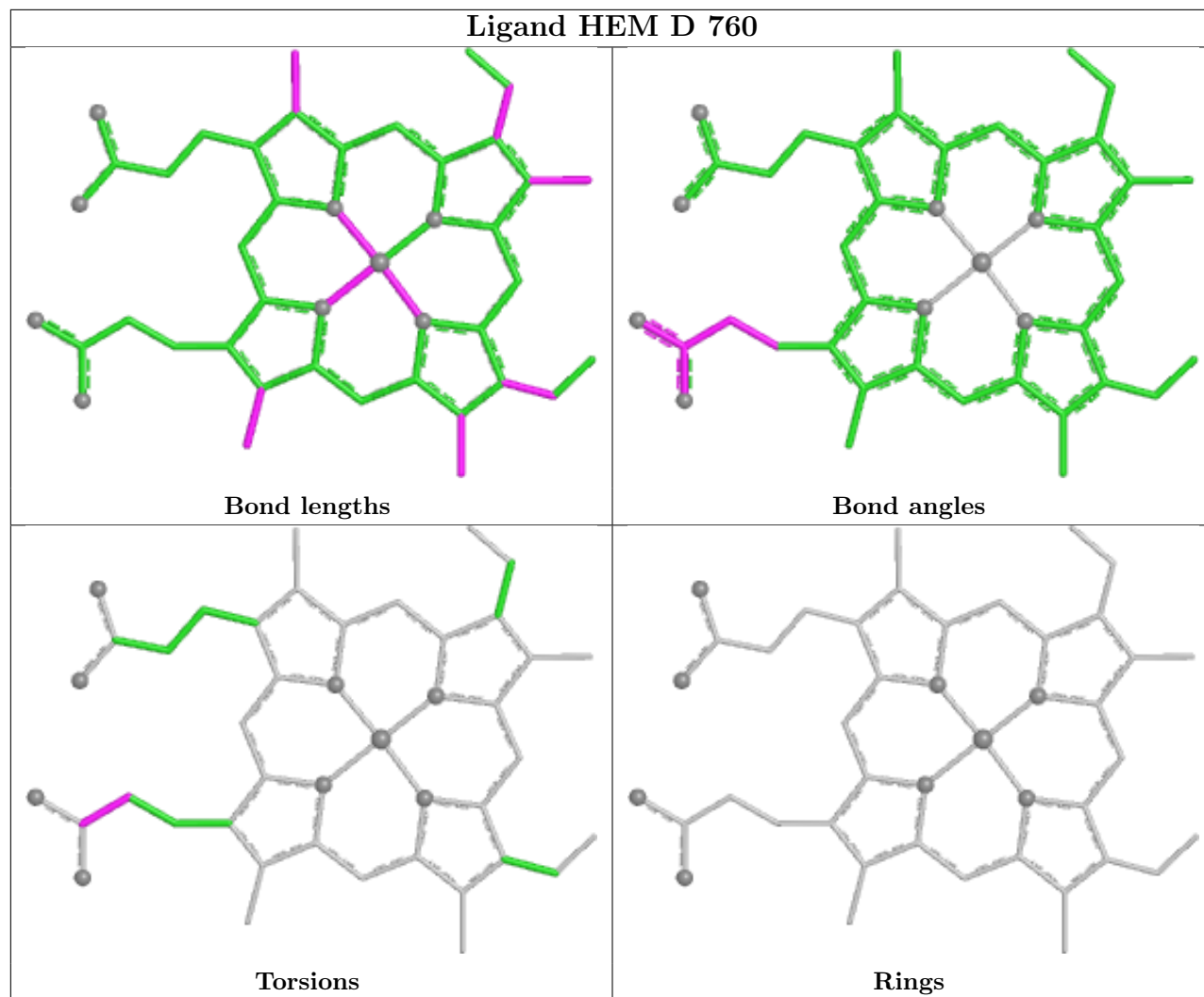
There are no ring outliers.

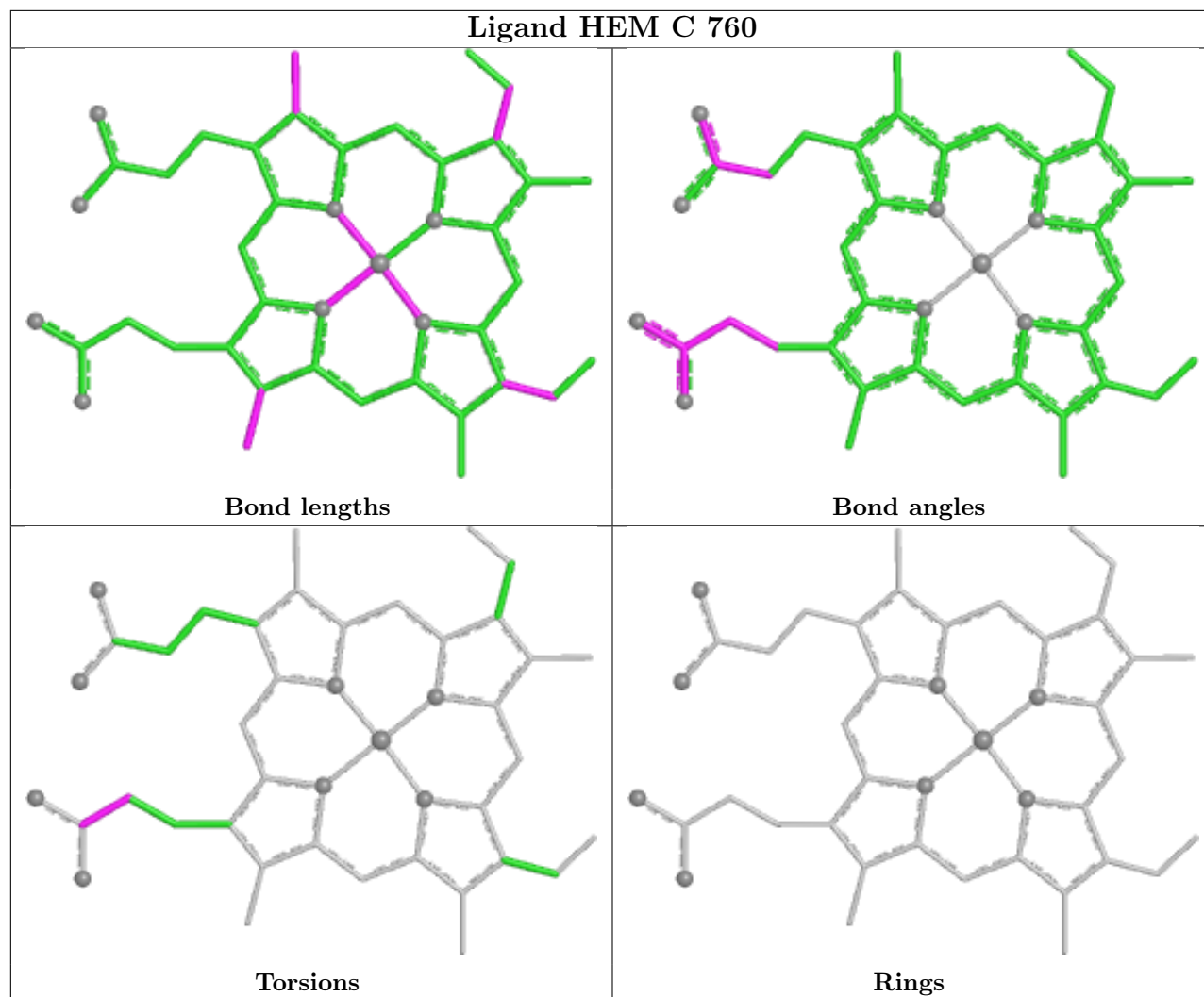
4 monomers are involved in 5 short contacts:

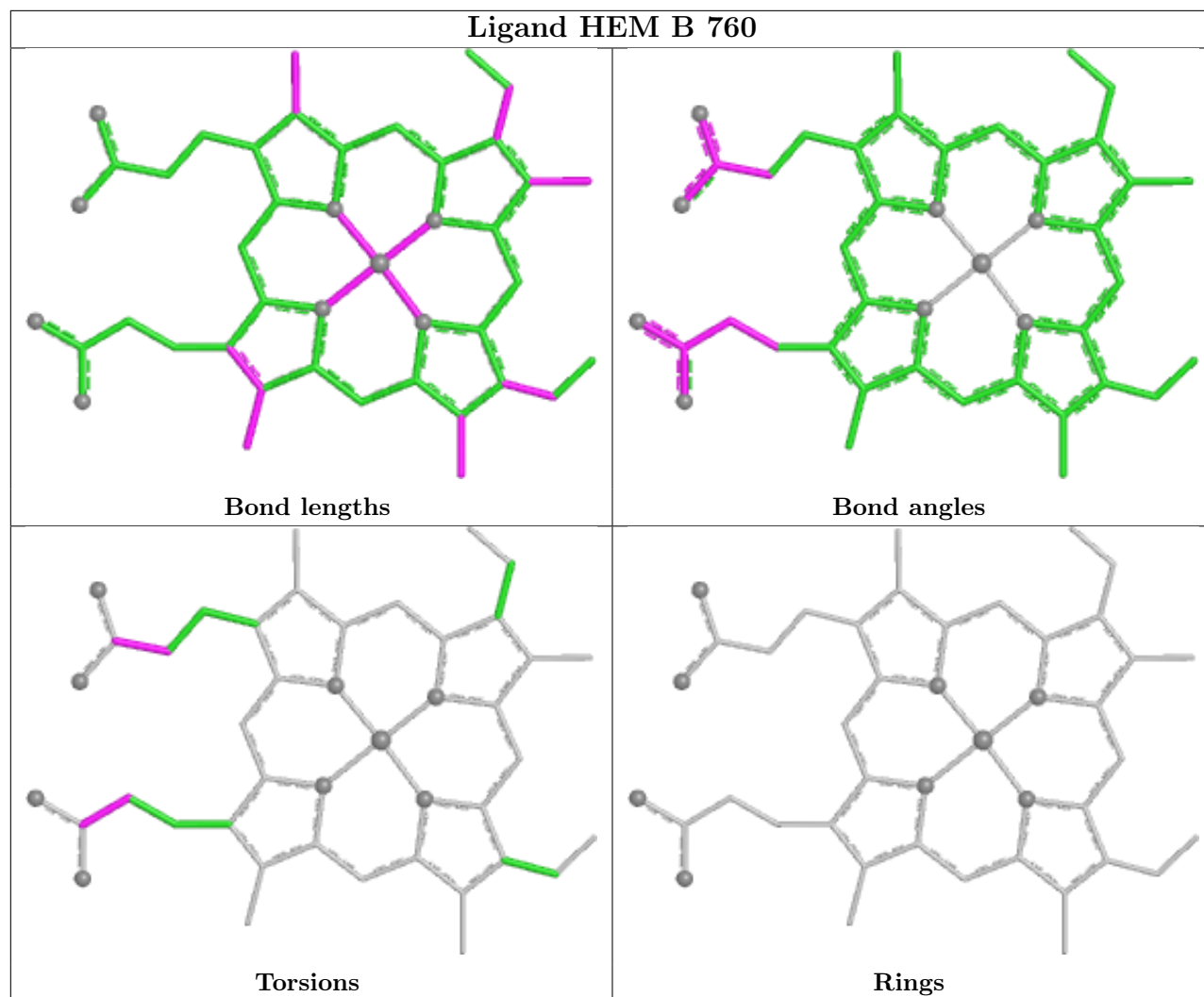
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	760	HEM	1	0
2	C	760	HEM	1	0
2	B	760	HEM	2	0
2	A	760	HEM	1	0

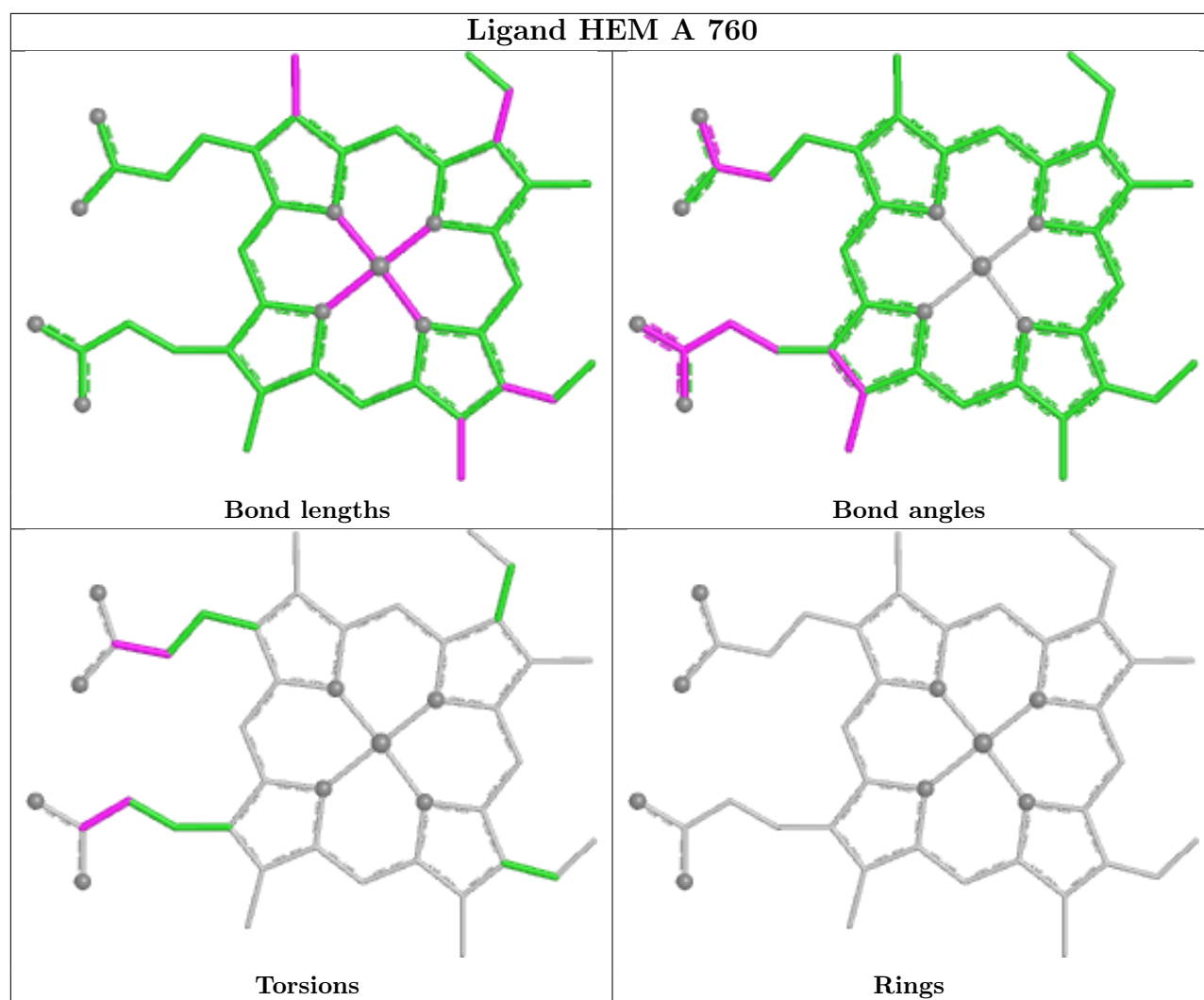
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	727/753 (96%)	-0.20	14 (1%) 66 71	10, 16, 31, 54	1 (0%)
1	B	727/753 (96%)	-0.03	19 (2%) 57 62	10, 18, 38, 48	1 (0%)
1	C	727/753 (96%)	-0.06	16 (2%) 62 68	10, 18, 38, 47	1 (0%)
1	D	727/753 (96%)	-0.17	16 (2%) 62 68	9, 16, 31, 50	1 (0%)
All	All	2908/3012 (96%)	-0.11	65 (2%) 62 68	9, 17, 36, 54	4 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	28	SER	8.3
1	A	27	ASP	6.3
1	D	27	ASP	5.1
1	A	711	ALA	5.1
1	B	27	ASP	4.5
1	C	27	ASP	4.5
1	D	28	SER	4.3
1	A	710	ILE	4.2
1	C	726	GLY	4.0
1	C	724	ALA	3.6
1	A	712	ASP	3.6
1	A	751	ILE	3.5
1	D	750	LYS	3.4
1	A	29	LEU	3.3
1	D	710	ILE	3.2
1	A	724	ALA	3.2
1	A	713	GLN	3.1
1	D	595	ASP	3.1
1	B	642	ALA	3.0
1	A	749	ASP	3.0
1	B	37	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	725	ASP	2.9
1	C	28	SER	2.8
1	D	749	ASP	2.8
1	B	724	ALA	2.8
1	B	710	ILE	2.8
1	C	751	ILE	2.8
1	D	748	ILE	2.7
1	D	596	GLY	2.7
1	C	753	ALA	2.7
1	B	721	ALA	2.6
1	C	703	LYS	2.6
1	C	449	HIS	2.5
1	D	711	ALA	2.5
1	C	676	ALA	2.5
1	B	753	ALA	2.5
1	A	750	LYS	2.5
1	D	751	ILE	2.5
1	D	29	LEU	2.4
1	B	578	ASP	2.3
1	C	669	CYS	2.3
1	D	61	ARG	2.3
1	B	670	GLY	2.3
1	B	596	GLY	2.3
1	B	751	ILE	2.3
1	C	710	ILE	2.3
1	A	709	LYS	2.2
1	A	707	THR	2.2
1	C	673	ALA	2.2
1	D	707	THR	2.2
1	C	712	ASP	2.2
1	D	712	ASP	2.2
1	B	750	LYS	2.2
1	B	28	SER	2.2
1	A	706	ALA	2.1
1	B	583	LYS	2.1
1	B	709	LYS	2.1
1	B	568	ASP	2.1
1	C	595	ASP	2.1
1	B	609	ASP	2.1
1	C	596	GLY	2.0
1	B	701	ALA	2.0
1	D	713	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	612	ARG	2.0
1	B	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

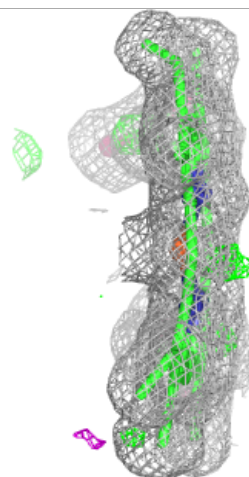
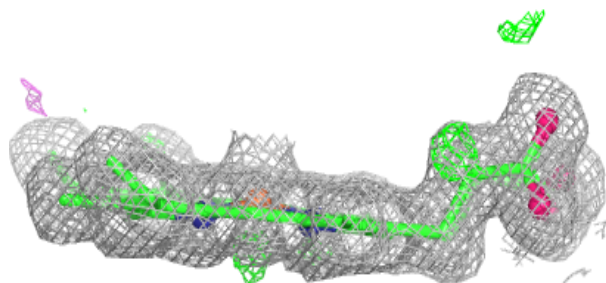
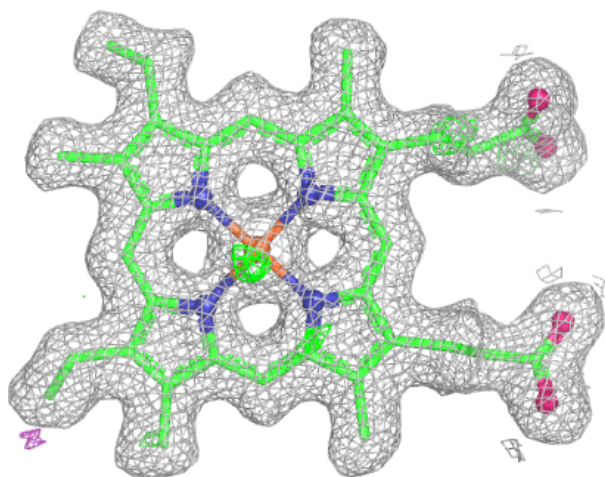
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	A	760	43/43	0.99	0.04	9,10,12,12	0
2	HEM	B	760	43/43	0.99	0.04	10,12,13,15	0
2	HEM	C	760	43/43	0.99	0.04	10,11,13,14	0
2	HEM	D	760	43/43	0.99	0.04	9,11,12,13	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.

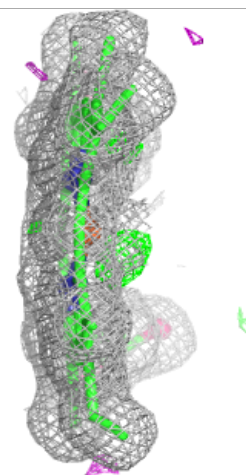
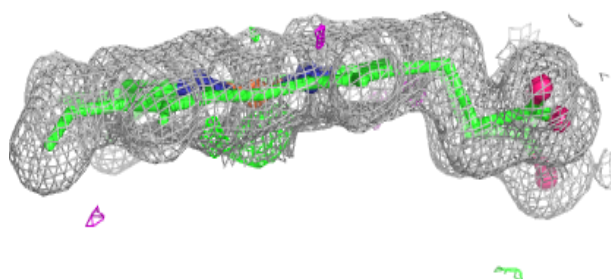
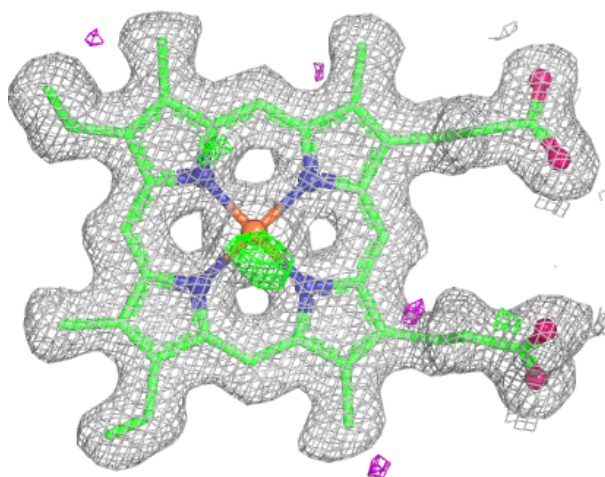
Electron density around HEM A 760:

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



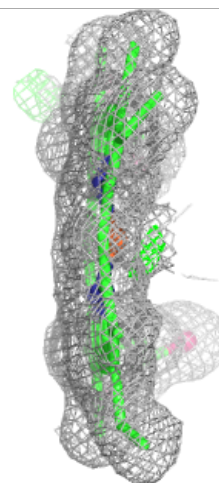
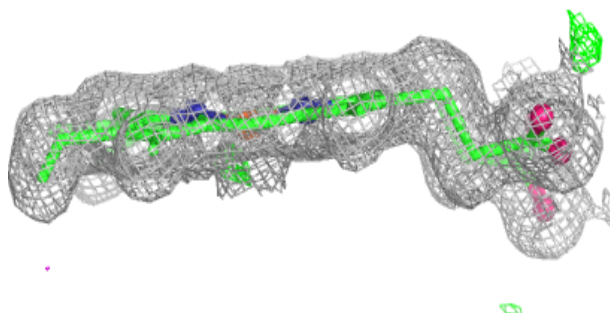
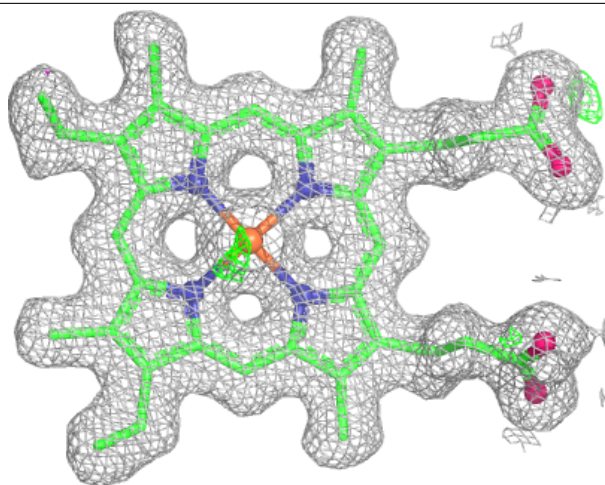
Electron density around HEM B 760:

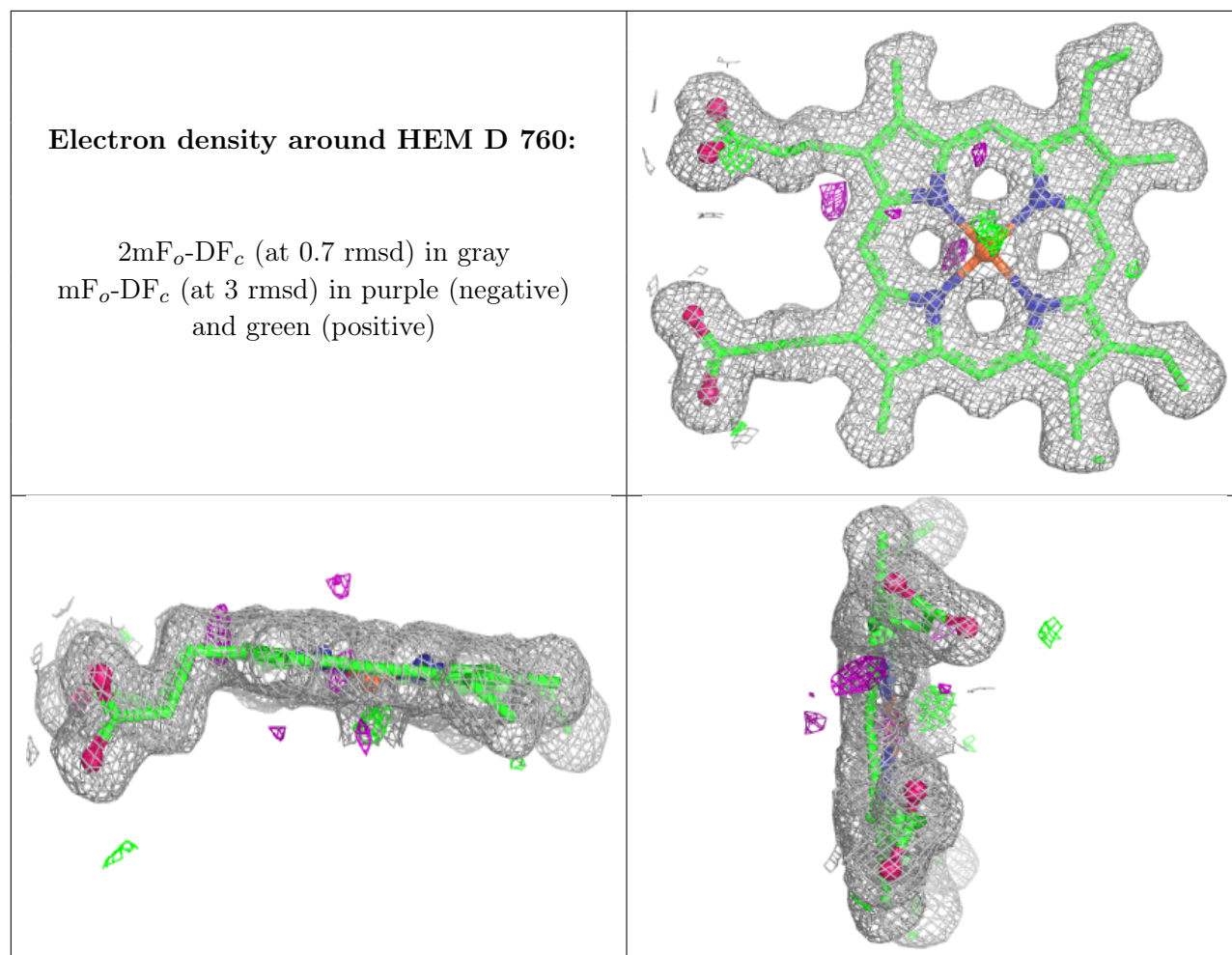
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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 ⓘ

There are no such residues in this entry.