Full wwPDB X-ray Structure Validation Report (i)

Aug 8, 2023 – 04:50 PM EDT

PDB ID	:	1P7Y
Title	:	Crystal structure of the D181A variant of catalase HPII from E. coli
Authors	:	Chelikani, P.; Carpena, X.; Fita, I.; Loewen, P.C.
Deposited on	:	2003-05-06
Resolution	:	2.40 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 (i) 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 (i)) were used in the production of this report:

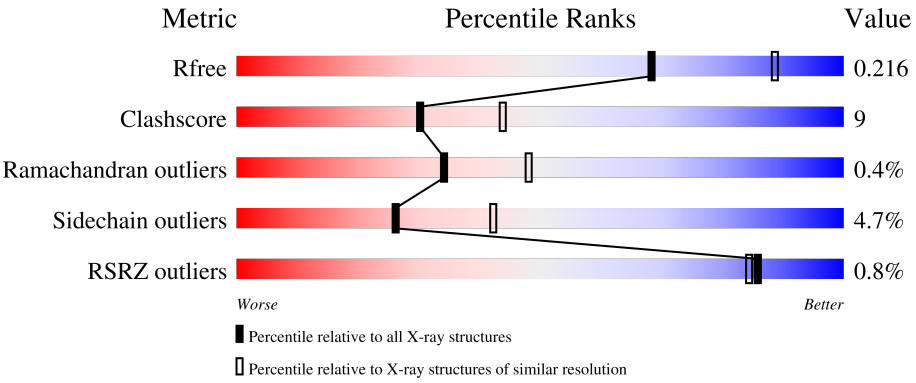
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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	74% 20%
1	B	753	68% 26%
1	C	753	72% 22%
1	D	753	70% 23%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 25927 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.

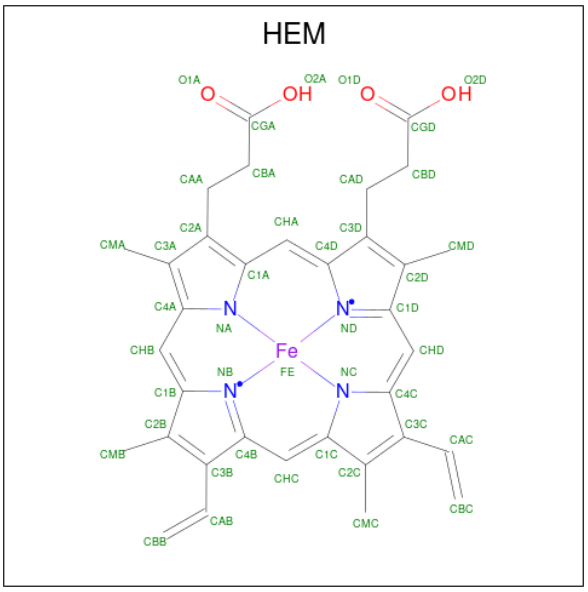
- Molecule 1 is a protein called Catalase HPII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total 5747	C 3648	N 1006	O 1081	S 12	0	1	0
1	B	727	Total 5747	C 3648	N 1006	O 1081	S 12	0	1	0
1	C	727	Total 5747	C 3648	N 1006	O 1081	S 12	0	1	0
1	D	727	Total 5747	C 3648	N 1006	O 1081	S 12	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	ALA	ASP	engineered mutation	UNP P21179
B	181	ALA	ASP	engineered mutation	UNP P21179
C	181	ALA	ASP	engineered mutation	UNP P21179
D	181	ALA	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	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is water.

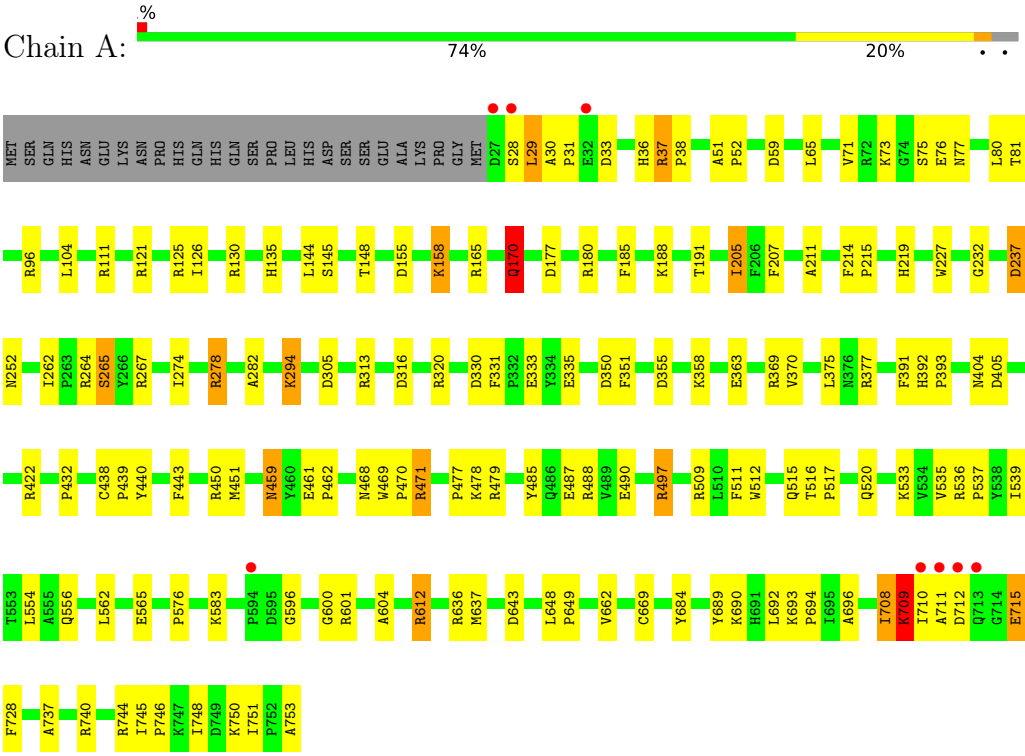
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	732	Total	O	0	0
			732	732		
3	B	641	Total	O	0	0
			641	641		
3	C	673	Total	O	0	0
			673	673		
3	D	721	Total	O	0	0
			721	721		

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.

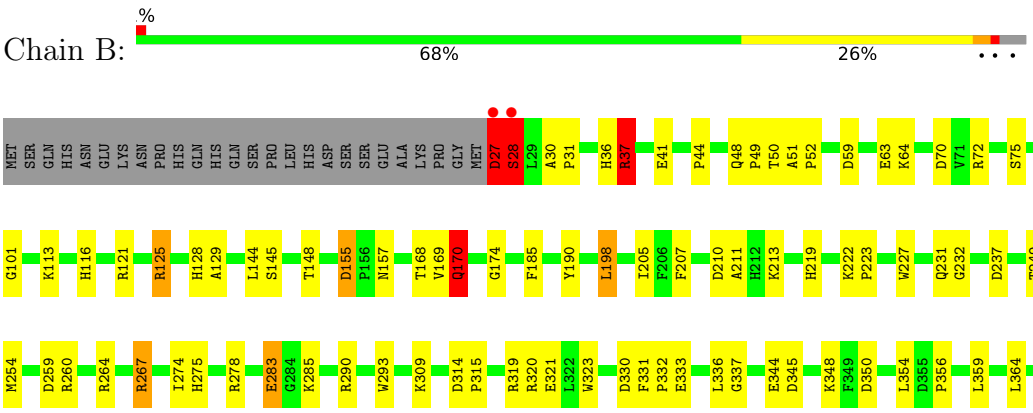
• Molecule 1: Catalase HPII

Chain A:



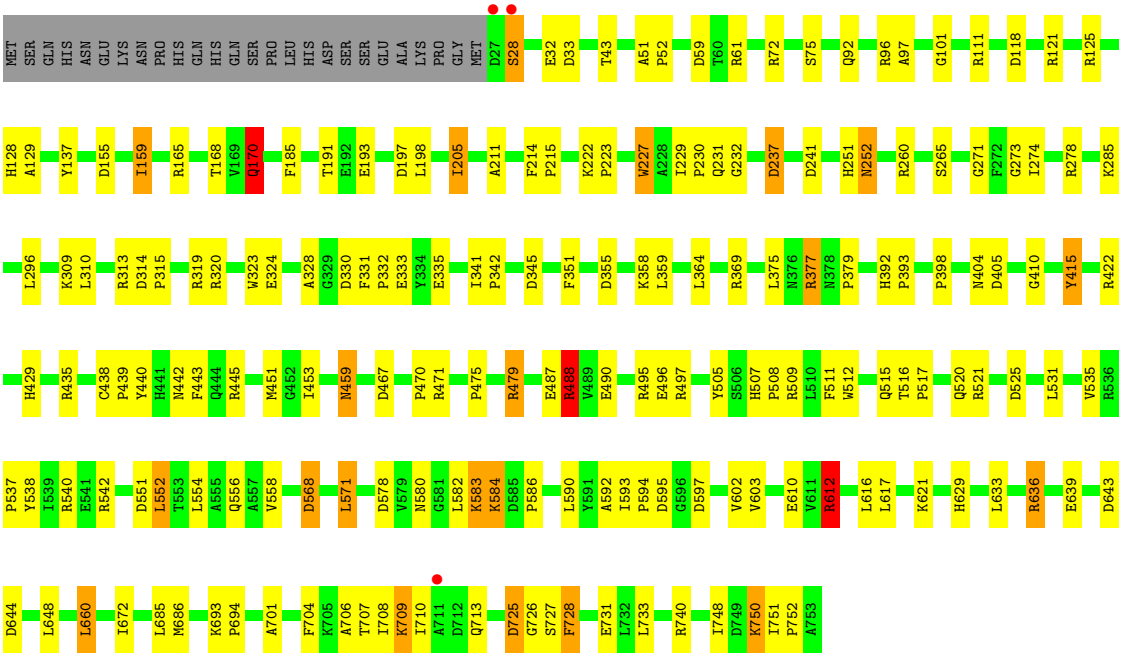
• Molecule 1: Catalase HPII

Chain B:



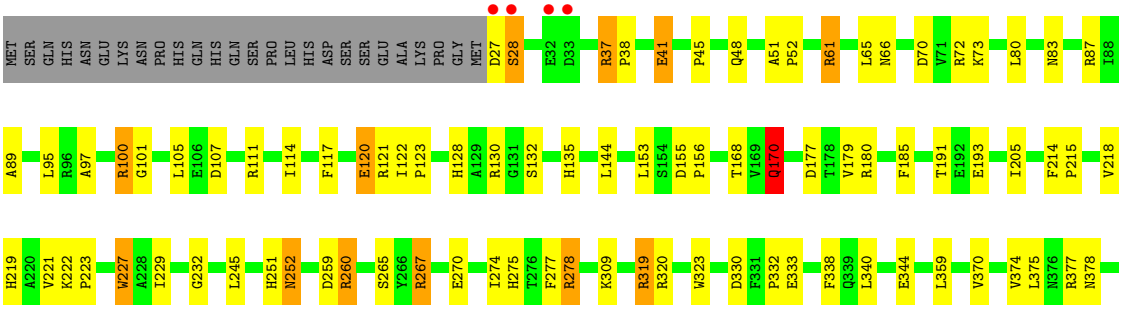
• Molecule 1: Catalase HPII

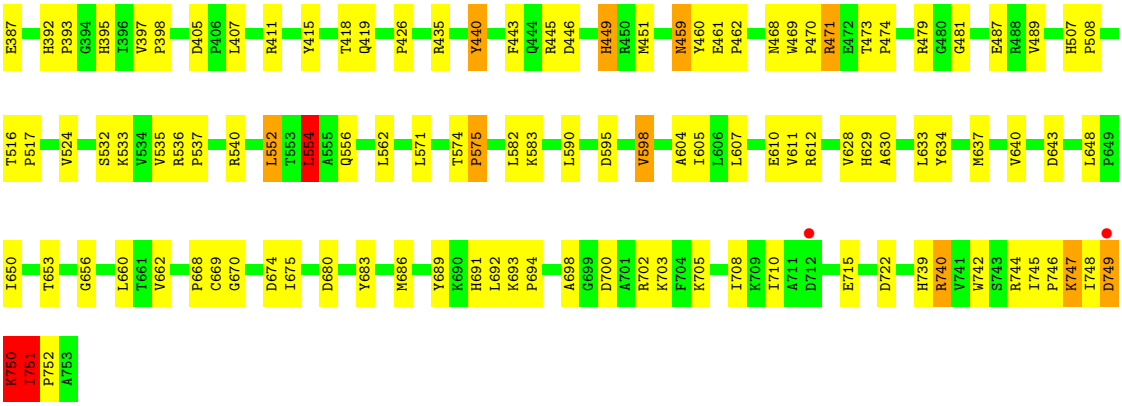
Chain C:



• Molecule 1: Catalase HPII

Chain D:




E387 H392 P393 G394 H395 I396 V397 P398 D405 P406 L407 R411 Y415 T418 Q419 P426 R435 Y440 F443 Q444 R445 D446 H449 R450 M451 N459 Y460 E461 P462 N468 W469 P470 R471 E472 T473 P474 R479 G480 G481 E487 R488 V489 H507 P508
T516 P517 V524 S532 K533 V534 V535 R536 P537 R540 L552 T553 L554 A555 Q556 L562 L571 T574 P575 L582 K583 L590 D595 V598 A604 I605 L606 L607 E610 V611 R612 V628 H629 A630 L633 Y634 M637 V640 D643 L648 P649
I650 T653 G656 L660 T661 V662 P668 C669 G670 D674 I675 D680 Y683 M686 Y689 K690 H691 L692 K693 P694 A698 G699 D700 A701 R702 K703 F704 K705 I708 K709 I710 A711 D712 E715 D722 H739 R740 V741 W742 S743 R744 I745 P746 K747 I748 D749
K750 I751 P752 A753

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.29Å 132.86Å 121.75Å 90.00° 109.40° 90.00°	Depositor
Resolution (Å)	29.80 – 2.40 17.96 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.8 (29.80-2.40) 96.9 (17.96-2.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 2.40Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.144 , 0.225 0.145 , 0.216	Depositor DCC
R_{free} test set	5332 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	16.0	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 67.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	25927	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.56	0/5908	1.44	49/8032 (0.6%)
1	B	0.55	0/5908	1.47	65/8032 (0.8%)
1	C	0.56	0/5908	1.52	58/8032 (0.7%)
1	D	0.56	0/5908	1.48	68/8032 (0.8%)
All	All	0.56	0/23632	1.48	240/32128 (0.7%)

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	C	0	1

There are no bond length outliers.

All (240) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	612	ARG	CD-NE-CZ	35.28	173.00	123.60
1	A	497	ARG	NE-CZ-NH1	21.94	131.27	120.30
1	D	479	ARG	CD-NE-CZ	18.44	149.41	123.60
1	B	37	ARG	NE-CZ-NH2	16.17	128.38	120.30
1	D	612	ARG	CD-NE-CZ	15.64	145.50	123.60
1	A	497	ARG	NE-CZ-NH2	-14.30	113.15	120.30
1	A	264	ARG	NE-CZ-NH2	-12.53	114.03	120.30
1	C	445	ARG	NE-CZ-NH2	-12.40	114.10	120.30
1	A	542	ARG	NE-CZ-NH2	-12.33	114.13	120.30
1	C	612	ARG	NE-CZ-NH1	11.94	126.27	120.30
1	C	121	ARG	NE-CZ-NH2	-11.75	114.42	120.30
1	D	72	ARG	NE-CZ-NH2	-11.53	114.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	320	ARG	NE-CZ-NH2	-11.51	114.54	120.30
1	C	377	ARG	NE-CZ-NH1	-11.35	114.62	120.30
1	D	471	ARG	NE-CZ-NH1	11.31	125.95	120.30
1	D	471	ARG	NE-CZ-NH2	-11.16	114.72	120.30
1	B	601	ARG	CD-NE-CZ	11.00	138.99	123.60
1	B	319	ARG	NE-CZ-NH1	-10.83	114.88	120.30
1	B	37	ARG	CD-NE-CZ	10.82	138.75	123.60
1	A	313	ARG	NE-CZ-NH2	10.66	125.63	120.30
1	A	422	ARG	NE-CZ-NH2	10.32	125.46	120.30
1	A	485	TYR	CB-CG-CD1	-10.28	114.83	121.00
1	D	121	ARG	NE-CZ-NH2	-10.25	115.17	120.30
1	D	61	ARG	NE-CZ-NH1	-10.21	115.19	120.30
1	D	61	ARG	NE-CZ-NH2	10.10	125.35	120.30
1	B	320	ARG	NE-CZ-NH2	-10.09	115.25	120.30
1	B	435	ARG	NE-CZ-NH1	10.06	125.33	120.30
1	B	121	ARG	NE-CZ-NH1	10.01	125.31	120.30
1	C	121	ARG	NE-CZ-NH1	10.01	125.31	120.30
1	C	170[A]	GLN	CA-CB-CG	9.92	135.22	113.40
1	C	170[B]	GLN	CA-CB-CG	9.92	135.22	113.40
1	B	319	ARG	NE-CZ-NH2	9.89	125.25	120.30
1	C	241	ASP	CB-CG-OD2	9.84	127.16	118.30
1	D	278	ARG	NE-CZ-NH1	-9.70	115.45	120.30
1	D	61	ARG	CD-NE-CZ	9.61	137.06	123.60
1	D	445	ARG	NE-CZ-NH1	9.49	125.05	120.30
1	D	121	ARG	NE-CZ-NH1	9.34	124.97	120.30
1	B	369	ARG	NE-CZ-NH1	9.31	124.95	120.30
1	B	37	ARG	NE-CZ-NH1	-9.23	115.69	120.30
1	C	471	ARG	NE-CZ-NH2	-9.22	115.69	120.30
1	C	445	ARG	NE-CZ-NH1	9.17	124.88	120.30
1	D	536	ARG	NE-CZ-NH2	-9.16	115.72	120.30
1	D	540	ARG	NE-CZ-NH1	9.16	124.88	120.30
1	C	121	ARG	CD-NE-CZ	9.15	136.41	123.60
1	B	260	ARG	NE-CZ-NH1	9.07	124.84	120.30
1	A	740	ARG	NE-CZ-NH2	9.03	124.81	120.30
1	C	72	ARG	NE-CZ-NH2	-8.97	115.81	120.30
1	C	509	ARG	NE-CZ-NH1	-8.92	115.84	120.30
1	D	536	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	B	369	ARG	CD-NE-CZ	8.80	135.91	123.60
1	B	125	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	A	485	TYR	CB-CG-CD2	8.69	126.22	121.00
1	C	495	ARG	NE-CZ-NH1	8.47	124.54	120.30
1	D	170[A]	GLN	CA-CB-CG	8.46	132.02	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	170[B]	GLN	CA-CB-CG	8.46	132.02	113.40
1	C	495	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	B	744	ARG	NE-CZ-NH1	8.35	124.48	120.30
1	B	278	ARG	CD-NE-CZ	8.27	135.17	123.60
1	C	726	GLY	N-CA-C	-8.21	92.58	113.10
1	B	27	ASP	CB-CG-OD1	8.14	125.63	118.30
1	B	96	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	C	422	ARG	CD-NE-CZ	8.08	134.91	123.60
1	C	725	ASP	N-CA-CB	8.06	125.11	110.60
1	A	37	ARG	NE-CZ-NH2	-7.99	116.31	120.30
1	D	177	ASP	CB-CG-OD2	7.97	125.48	118.30
1	C	319	ARG	NE-CZ-NH1	-7.92	116.34	120.30
1	D	540	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	C	165	ARG	NE-CZ-NH1	7.91	124.26	120.30
1	B	27	ASP	C-N-CA	7.91	141.47	121.70
1	C	471	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	A	377	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	D	70	ASP	CB-CG-OD1	-7.77	111.31	118.30
1	C	479	ARG	NE-CZ-NH1	7.73	124.17	120.30
1	B	121	ARG	NE-CZ-NH2	-7.71	116.44	120.30
1	C	320	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	B	290	ARG	NE-CZ-NH2	7.67	124.13	120.30
1	B	41	GLU	OE1-CD-OE2	-7.63	114.14	123.30
1	C	319	ARG	NE-CZ-NH2	7.61	124.10	120.30
1	A	471	ARG	NE-CZ-NH2	7.59	124.10	120.30
1	B	479	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	C	568	ASP	CB-CG-OD1	-7.52	111.53	118.30
1	B	445	ARG	NE-CZ-NH1	-7.47	116.56	120.30
1	B	479	ARG	NE-CZ-NH2	-7.45	116.58	120.30
1	B	28	SER	N-CA-CB	7.43	121.65	110.50
1	D	446	ASP	CB-CG-OD2	7.43	124.99	118.30
1	A	305	ASP	CB-CG-OD2	-7.40	111.64	118.30
1	C	28	SER	N-CA-CB	7.38	121.57	110.50
1	D	70	ASP	CB-CG-OD2	7.38	124.94	118.30
1	A	177	ASP	CB-CG-OD2	7.34	124.91	118.30
1	C	471	ARG	CD-NE-CZ	-7.34	113.32	123.60
1	D	680	ASP	CB-CG-OD2	7.33	124.89	118.30
1	D	170[A]	GLN	CB-CG-CD	7.30	130.59	111.60
1	D	170[B]	GLN	CB-CG-CD	7.30	130.59	111.60
1	C	313	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	C	155	ASP	CB-CG-OD2	7.24	124.82	118.30
1	D	267	ARG	NE-CZ-NH2	-7.23	116.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	33	ASP	CB-CG-OD1	7.19	124.78	118.30
1	B	59	ASP	CB-CG-OD1	-7.17	111.85	118.30
1	D	643	ASP	CB-CG-OD1	7.16	124.74	118.30
1	A	180	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	C	540	ARG	NE-CZ-NH2	7.15	123.87	120.30
1	A	278	ARG	NE-CZ-NH1	-7.14	116.73	120.30
1	B	290	ARG	N-CA-CB	7.13	123.44	110.60
1	A	450	ARG	NE-CZ-NH2	7.07	123.84	120.30
1	D	377	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	B	495	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	A	170[A]	GLN	CA-CB-CG	7.00	128.79	113.40
1	A	170[B]	GLN	CA-CB-CG	7.00	128.79	113.40
1	D	405	ASP	CB-CG-OD1	6.99	124.59	118.30
1	A	601	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	B	411	ARG	NE-CZ-NH1	6.93	123.76	120.30
1	A	87	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	D	37	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	B	744	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	B	70	ASP	CB-CG-OD2	6.85	124.47	118.30
1	A	350	ASP	CB-CA-C	6.85	124.09	110.40
1	B	283	GLU	CA-CB-CG	6.83	128.44	113.40
1	A	37	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	B	615	ASP	CB-CG-OD2	6.81	124.43	118.30
1	D	28	SER	N-CA-CB	6.81	120.71	110.50
1	D	320	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	A	479	ARG	CD-NE-CZ	6.78	133.09	123.60
1	D	479	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	D	449	HIS	CA-CB-CG	6.71	125.01	113.60
1	B	170[A]	GLN	CA-CB-CG	6.67	128.07	113.40
1	B	170[B]	GLN	CA-CB-CG	6.67	128.07	113.40
1	D	260	ARG	NE-CZ-NH1	-6.64	116.98	120.30
1	B	264	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	D	445	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	B	314	ASP	CB-CG-OD2	6.55	124.19	118.30
1	A	111	ARG	NE-CZ-NH1	-6.54	117.03	120.30
1	D	130	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	C	551	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	B	497	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	D	100	ARG	CD-NE-CZ	6.49	132.68	123.60
1	C	96	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	C	595	ASP	CA-CB-CG	6.45	127.59	113.40
1	C	118	ASP	CB-CG-OD2	6.43	124.09	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	121	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	A	350	ASP	CB-CG-OD1	-6.37	112.57	118.30
1	B	27	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	B	72	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	D	120	GLU	OE1-CD-OE2	-6.32	115.72	123.30
1	C	636	ARG	NE-CZ-NH2	-6.23	117.18	120.30
1	A	612	ARG	CD-NE-CZ	6.22	132.31	123.60
1	C	237	ASP	CB-CG-OD2	6.17	123.86	118.30
1	C	111	ARG	CD-NE-CZ	6.17	132.24	123.60
1	D	691	HIS	O-C-N	-6.14	112.87	122.70
1	C	59	ASP	CB-CG-OD1	6.13	123.81	118.30
1	A	320	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	A	165	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	B	155	ASP	CB-CG-OD1	-6.01	112.89	118.30
1	D	435	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	D	37	ARG	N-CA-CB	-6.00	99.80	110.60
1	D	612	ARG	CG-CD-NE	6.00	124.39	111.80
1	D	440	TYR	CB-CG-CD2	-5.99	117.41	121.00
1	D	319	ARG	CD-NE-CZ	5.98	131.98	123.60
1	B	401	ASP	CB-CG-OD1	-5.96	112.93	118.30
1	A	377	ARG	NH1-CZ-NH2	5.94	125.94	119.40
1	B	505	TYR	CB-CG-CD1	-5.93	117.44	121.00
1	B	575	PRO	N-CA-CB	5.89	110.37	103.30
1	B	609	ASP	CB-CG-OD2	5.89	123.61	118.30
1	B	435	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	D	435	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	B	536	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	B	96	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	B	740	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	D	387	GLU	OE1-CD-OE2	-5.85	116.28	123.30
1	D	722	ASP	CB-CG-OD1	5.83	123.54	118.30
1	A	684	TYR	CB-CG-CD1	5.82	124.49	121.00
1	D	598	VAL	N-CA-CB	-5.79	98.77	111.50
1	B	505	TYR	CB-CG-CD2	5.75	124.45	121.00
1	C	273	GLY	C-N-CA	5.73	136.03	121.70
1	A	541	GLU	CA-CB-CG	-5.73	100.79	113.40
1	D	338	PHE	CB-CG-CD2	5.72	124.80	120.80
1	D	575	PRO	N-CA-CB	5.68	110.12	103.30
1	D	674	ASP	CB-CG-OD2	5.68	123.42	118.30
1	A	669	CYS	CA-CB-SG	5.68	124.23	114.00
1	A	96	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	37	ARG	CD-NE-CZ	5.66	131.53	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	264	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	A	725	ASP	CB-CG-OD2	5.64	123.38	118.30
1	B	542	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	D	180	ARG	CD-NE-CZ	5.59	131.43	123.60
1	B	210	ASP	CB-CG-OD1	5.57	123.31	118.30
1	C	479	ARG	CD-NE-CZ	5.56	131.39	123.60
1	A	684	TYR	CB-CG-CD2	-5.56	117.67	121.00
1	D	474	PRO	N-CA-CB	5.54	109.95	103.30
1	D	595	ASP	CB-CG-OD2	5.49	123.24	118.30
1	C	355	ASP	CB-CG-OD2	5.48	123.23	118.30
1	B	479	ARG	CD-NE-CZ	5.48	131.27	123.60
1	C	355	ASP	CB-CG-OD1	-5.48	113.37	118.30
1	A	708	ILE	C-N-CA	5.46	135.34	121.70
1	B	275	HIS	CB-CA-C	-5.45	99.50	110.40
1	C	155	ASP	CB-CG-OD1	-5.45	113.40	118.30
1	B	702	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	355	ASP	CB-CG-OD1	-5.40	113.44	118.30
1	C	197	ASP	CB-CG-OD1	-5.38	113.46	118.30
1	C	345	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	170[A]	GLN	CB-CG-CD	5.37	125.56	111.60
1	A	170[B]	GLN	CB-CG-CD	5.37	125.56	111.60
1	D	41	GLU	CA-CB-CG	5.37	125.20	113.40
1	B	267	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	377	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	B	59	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	125	ARG	CD-NE-CZ	5.29	131.00	123.60
1	D	260	ARG	NE-CZ-NH2	5.28	122.94	120.30
1	C	728	PHE	CA-CB-CG	5.28	126.57	113.90
1	C	595	ASP	CB-CG-OD2	5.27	123.04	118.30
1	C	324	GLU	OE1-CD-OE2	-5.26	116.99	123.30
1	D	554	LEU	CA-CB-CG	5.25	127.36	115.30
1	D	643	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	D	45	PRO	N-CA-CB	5.24	109.59	103.30
1	C	740	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	130	ARG	CD-NE-CZ	5.21	130.89	123.60
1	B	545	ASP	CB-CG-OD2	5.20	122.98	118.30
1	D	740	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	111	ARG	CD-NE-CZ	5.18	130.86	123.60
1	D	259	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	485	TYR	CB-CG-CD1	-5.18	117.89	121.00
1	C	497	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	C	636	ARG	NE-CZ-NH1	5.18	122.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	270	GLU	OE1-CD-OE2	-5.17	117.09	123.30
1	C	488	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	A	130	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	A	636	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	D	440	TYR	CB-CG-CD1	5.12	124.07	121.00
1	D	111	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	377	ARG	CD-NE-CZ	5.09	130.73	123.60
1	D	598	VAL	CA-CB-CG1	5.09	118.53	110.90
1	D	612	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	C	709	LYS	CA-CB-CG	5.06	124.53	113.40
1	C	475	PRO	N-CA-CB	5.04	109.35	103.30
1	B	350	ASP	CB-CG-OD1	-5.03	113.77	118.30
1	C	496	GLU	N-CA-CB	-5.03	101.55	110.60
1	C	96	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	B	198	LEU	CA-CB-CG	5.01	126.83	115.30
1	B	100	ARG	CD-NE-CZ	5.01	130.62	123.60
1	B	155	ASP	CB-CG-OD2	5.01	122.81	118.30
1	B	612	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	271	GLY	Mainchain

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	5747	0	5583	103	1
1	B	5747	0	5583	129	1
1	C	5747	0	5583	103	0
1	D	5747	0	5583	124	0
2	A	43	0	30	6	0
2	B	43	0	30	1	0
2	C	43	0	30	3	0
2	D	43	0	30	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	732	0	0	8	0
3	B	641	0	0	19	0
3	C	673	0	0	12	0
3	D	721	0	0	7	0
All	All	25927	0	22452	426	1

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 9.

All (426) 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:D:750:LYS:HZ2	1:D:751:ILE:H	1.16	0.91
1:C:392:HIS:ND1	1:C:415:TYR:HB2	1.97	0.80
1:A:51:ALA:HB1	1:A:52:PRO:HD2	1.66	0.76
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.66	0.75
1:C:748:ILE:O	1:C:751:ILE:HG22	1.84	0.75
1:D:392:HIS:ND1	1:D:415:TYR:HB2	2.02	0.75
1:D:750:LYS:HZ2	1:D:751:ILE:N	1.85	0.74
1:A:392:HIS:ND1	1:A:415:TYR:HB2	2.02	0.74
1:C:28:SER:HA	3:C:3649:HOH:O	1.88	0.74
1:B:710:ILE:HD13	1:B:718:ILE:HG13	1.69	0.74
1:D:750:LYS:NZ	1:D:751:ILE:H	1.86	0.73
1:B:552:LEU:HD21	1:B:571:LEU:HD12	1.70	0.73
1:D:333:GLU:HG2	1:D:374:VAL:HG22	1.70	0.72
1:D:552:LEU:HD11	1:D:571:LEU:HD23	1.73	0.71
1:B:36:HIS:CD2	1:B:37:ARG:HD3	2.26	0.70
1:A:71:VAL:HG23	1:C:453:ILE:HD12	1.74	0.70
1:B:392:HIS:ND1	1:B:415:TYR:HB2	2.07	0.69
1:B:222:LYS:HB3	1:B:223:PRO:CD	2.23	0.67
1:B:521:ARG:HH21	1:B:745:ILE:HD13	1.59	0.67
1:A:214:PHE:HB3	1:A:215:PRO:HD3	1.77	0.67
1:A:637:MET:HG3	1:D:532:SER:HB2	1.77	0.67
1:A:170[B]:GLN:HG3	1:A:232:GLY:HA2	1.78	0.66
1:B:583:LYS:O	1:B:584:LYS:HB3	1.96	0.65
1:C:552:LEU:HD21	1:C:571:LEU:HD12	1.79	0.65
1:A:490:GLU:HG2	1:B:490:GLU:HG2	1.79	0.65
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.27	0.65
1:B:222:LYS:HB3	1:B:223:PRO:HD2	1.77	0.65
1:A:274:ILE:HD12	2:A:760:HEM:HBB2	1.78	0.64
1:A:565:GLU:HG3	3:A:2882:HOH:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:509:ARG:HD2	1:B:576:PRO:HD2	1.80	0.64
1:B:468:ASN:HD22	1:D:27:ASP:N	1.95	0.64
1:D:274:ILE:HD12	2:D:760:HEM:HMB1	1.80	0.64
1:B:521:ARG:NH2	1:B:745:ILE:HD13	2.13	0.63
1:C:260:ARG:HD3	1:C:590:LEU:HD21	1.80	0.63
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.12	0.63
1:B:507:HIS:N	1:B:508:PRO:HD2	2.14	0.63
1:A:144:LEU:HD11	1:A:370:VAL:HG13	1.79	0.62
1:C:438:CYS:HB2	1:C:439:PRO:HD2	1.81	0.62
1:C:610:GLU:OE1	1:C:643:ASP:HA	2.00	0.62
1:A:708:ILE:O	1:A:710:ILE:HG22	1.98	0.62
1:D:170[B]:GLN:HG3	1:D:232:GLY:HA2	1.81	0.62
1:B:606:LEU:HB2	1:B:667:VAL:HG22	1.82	0.62
1:C:435:ARG:HD3	3:C:2182:HOH:O	1.99	0.62
1:B:596:GLY:HA3	3:B:3195:HOH:O	2.00	0.61
1:D:122:ILE:HB	1:D:123:PRO:HD2	1.81	0.61
1:D:443:PHE:CZ	1:D:470:PRO:HD2	2.35	0.61
1:C:310:LEU:HD13	1:C:660:LEU:HB3	1.82	0.61
1:D:629:HIS:HD2	3:D:2554:HOH:O	1.83	0.60
1:C:578:ASP:HB2	1:C:582:LEU:O	2.00	0.60
1:C:507:HIS:N	1:C:508:PRO:HD2	2.16	0.60
1:C:617:LEU:HD12	3:C:3230:HOH:O	2.02	0.60
1:D:689:TYR:HA	1:D:744:ARG:NH1	2.17	0.60
1:D:459:ASN:HD22	1:D:459:ASN:H	1.49	0.60
3:B:1354:HOH:O	1:D:193:GLU:HG2	2.02	0.60
1:A:274:ILE:HD12	2:A:760:HEM:HMB1	1.84	0.59
1:D:359:LEU:H	1:D:507:HIS:CD2	2.20	0.59
1:C:704:PHE:O	1:C:707:THR:HG22	2.02	0.59
1:A:211:ALA:CB	1:A:410:GLY:HA3	2.33	0.59
1:B:583:LYS:H	1:B:583:LYS:CE	2.15	0.59
1:A:36:HIS:CD2	1:A:36:HIS:H	2.20	0.58
1:A:443:PHE:CZ	1:A:470:PRO:HD2	2.38	0.58
1:C:751:ILE:HB	3:C:3367:HOH:O	2.03	0.58
1:B:640:VAL:HG13	1:B:650:ILE:HD11	1.85	0.58
1:D:65:LEU:HD21	1:D:135:HIS:CG	2.38	0.58
1:B:321:GLU:HG3	3:B:2921:HOH:O	2.02	0.58
1:D:51:ALA:HB1	1:D:52:PRO:HD2	1.86	0.57
1:D:744:ARG:HA	1:D:747:LYS:HD3	1.85	0.57
1:C:552:LEU:HD22	1:C:556:GLN:HG3	1.86	0.57
1:B:682:ASN:HB3	1:B:707:THR:HG21	1.87	0.57
1:C:251:HIS:CE1	1:C:507:HIS:HB3	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:552:LEU:O	1:B:552:LEU:HD22	2.05	0.56
1:B:604:ALA:HB1	1:B:633:LEU:HD22	1.87	0.56
1:D:640:VAL:HG13	1:D:650:ILE:HD11	1.87	0.56
1:D:598:VAL:HG13	1:D:628:VAL:CG2	2.36	0.56
1:B:155:ASP:OD1	3:B:4138:HOH:O	2.17	0.56
1:D:535:VAL:O	1:D:537:PRO:HD3	2.05	0.56
1:A:28:SER:HB2	1:D:245:LEU:HD22	1.88	0.56
1:B:719:VAL:HG13	1:B:731:GLU:OE2	2.05	0.56
1:D:516:THR:HB	1:D:517:PRO:HD2	1.88	0.56
1:C:535:VAL:O	1:C:537:PRO:HD3	2.06	0.56
1:C:443:PHE:CZ	1:C:470:PRO:HD2	2.41	0.56
1:D:516:THR:HB	1:D:517:PRO:CD	2.36	0.56
1:D:700:ASP:HB3	1:D:703:LYS:HE2	1.88	0.56
1:B:556:GLN:HG2	1:B:566:LEU:HD23	1.88	0.55
1:C:205:ILE:HD13	1:C:205:ILE:H	1.72	0.55
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.21	0.55
1:D:683:TYR:CD2	1:D:686:MET:HE2	2.41	0.55
1:A:438:CYS:HB2	1:A:439:PRO:CD	2.37	0.55
1:C:274:ILE:HD12	2:C:760:HEM:HMB1	1.89	0.55
1:D:144:LEU:HD12	1:D:153:LEU:HD13	1.89	0.55
1:D:144:LEU:HD11	1:D:370:VAL:HG13	1.89	0.55
1:D:392:HIS:CE1	1:D:415:TYR:HB2	2.41	0.55
1:A:469:TRP:CE3	1:A:471:ARG:HG3	2.42	0.55
1:A:748:ILE:O	1:A:751:ILE:HG13	2.07	0.55
1:B:231:GLN:HB2	3:C:1859:HOH:O	2.07	0.55
1:B:745:ILE:O	1:B:748:ILE:HG12	2.07	0.54
1:D:692:LEU:HB2	1:D:740:ARG:HB3	1.89	0.54
1:A:126:ILE:CD1	1:D:120:GLU:HB2	2.37	0.54
1:B:364:LEU:HD11	1:B:580:ASN:HB2	1.89	0.54
1:D:683:TYR:HD2	1:D:686:MET:HE2	1.72	0.54
1:C:359:LEU:C	1:C:359:LEU:HD12	2.28	0.54
1:D:61:ARG:HH11	1:D:66:ASN:HA	1.72	0.54
1:A:294:LYS:NZ	3:A:2213:HOH:O	2.40	0.54
1:B:27:ASP:OD2	1:D:468:ASN:ND2	2.37	0.54
1:B:477:PRO:HD2	3:B:1270:HOH:O	2.06	0.54
1:C:51:ALA:HB1	1:C:52:PRO:HD2	1.89	0.54
1:B:552:LEU:HD22	1:B:556:GLN:HG3	1.89	0.54
1:C:170[B]:GLN:HG3	1:C:232:GLY:HA2	1.90	0.54
1:B:583:LYS:H	1:B:583:LYS:NZ	2.05	0.54
1:D:750:LYS:CD	1:D:751:ILE:H	2.21	0.54
1:D:267:ARG:HG3	3:D:2920:HOH:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:760:HEM:HBB2	2:A:760:HEM:HMB1	1.89	0.53
1:B:211:ALA:CB	1:B:410:GLY:HA3	2.38	0.53
1:B:634:TYR:O	1:B:653:THR:HA	2.07	0.53
1:C:193:GLU:OE1	1:C:479:ARG:HD3	2.08	0.53
2:C:760:HEM:CMC	2:C:760:HEM:HBC2	2.38	0.53
1:B:207:PHE:O	1:B:249:THR:HA	2.09	0.53
1:B:669:CYS:SG	1:B:670:GLY:N	2.80	0.53
1:B:274:ILE:HD12	2:B:760:HEM:HMB1	1.91	0.52
1:D:397:VAL:HB	1:D:398:PRO:HD2	1.91	0.52
1:B:213:LYS:HD3	1:C:92:GLN:HA	1.91	0.52
1:B:556:GLN:HA	1:B:566:LEU:HD21	1.90	0.52
2:C:760:HEM:HBC2	2:C:760:HEM:HMC1	1.91	0.52
1:A:369:ARG:HG2	1:A:369:ARG:HH21	1.75	0.52
1:D:745:ILE:HB	1:D:746:PRO:HD3	1.90	0.52
1:A:51:ALA:HB1	1:A:52:PRO:CD	2.37	0.52
1:B:521:ARG:NH2	1:B:745:ILE:HG21	2.24	0.52
1:A:351:PHE:HB2	1:A:358:LYS:HG3	1.91	0.52
1:C:211:ALA:CB	1:C:410:GLY:HA3	2.39	0.52
1:A:392:HIS:ND1	1:A:393:PRO:HD2	2.25	0.52
1:B:612:ARG:HD2	1:B:670:GLY:HA2	1.92	0.52
1:A:468:ASN:O	1:A:471:ARG:HG2	2.10	0.52
1:C:629:HIS:HD2	3:C:2129:HOH:O	1.93	0.52
1:D:742:TRP:O	1:D:745:ILE:HG13	2.10	0.52
1:C:438:CYS:HB2	1:C:439:PRO:CD	2.39	0.51
1:C:516:THR:HB	1:C:517:PRO:HD2	1.93	0.51
1:D:260:ARG:HD3	1:D:590:LEU:HD21	1.92	0.51
1:B:631:LYS:HE2	3:B:3446:HOH:O	2.10	0.51
1:C:512:TRP:CZ3	1:C:554:LEU:HD13	2.45	0.51
1:B:507:HIS:N	1:B:508:PRO:CD	2.73	0.51
1:B:535:VAL:O	1:B:537:PRO:HD3	2.11	0.51
1:C:341:ILE:HG22	1:C:342:PRO:O	2.11	0.51
1:A:392:HIS:CE1	1:A:415:TYR:HB2	2.45	0.51
1:C:364:LEU:HD11	1:C:580:ASN:HB2	1.93	0.51
1:A:31:PRO:HB2	1:A:33:ASP:OD1	2.10	0.51
1:A:604:ALA:HB2	1:A:662:VAL:HG11	1.92	0.51
1:C:592:ALA:O	1:C:594:PRO:HD3	2.10	0.51
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.94	0.51
1:D:507:HIS:N	1:D:508:PRO:HD2	2.25	0.51
1:C:538:TYR:O	1:C:542:ARG:HG3	2.11	0.51
1:D:634:TYR:O	1:D:653:THR:HA	2.11	0.51
1:D:61:ARG:NH1	1:D:66:ASN:HA	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:HIS:ND1	1:B:393:PRO:HD2	2.25	0.50
1:A:411:ARG:HG2	2:A:760:HEM:C2C	2.45	0.50
1:B:521:ARG:HH21	1:B:745:ILE:HG21	1.75	0.50
1:C:552:LEU:HD22	1:C:552:LEU:O	2.10	0.50
1:D:359:LEU:H	1:D:507:HIS:HD2	1.58	0.50
1:B:459:ASN:HD22	1:B:460:TYR:HD2	1.59	0.50
1:A:404:ASN:O	1:A:405:ASP:C	2.48	0.50
1:C:214:PHE:HB3	1:C:215:PRO:HD3	1.93	0.50
1:C:296:LEU:HD12	1:C:333:GLU:HB3	1.94	0.50
1:A:28:SER:CB	1:D:245:LEU:HD22	2.42	0.50
1:A:562:LEU:HA	1:D:637:MET:HB2	1.94	0.50
1:C:636:ARG:NH2	1:C:639:GLU:O	2.45	0.50
1:D:605:ILE:HD12	1:D:630:ALA:HB1	1.93	0.50
1:B:157:ASN:HB2	3:B:4138:HOH:O	2.12	0.50
1:B:116:HIS:CD2	1:D:426:PRO:HB2	2.47	0.49
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.27	0.49
1:B:456:ASN:HB2	3:B:2326:HOH:O	2.12	0.49
1:A:278:ARG:HH12	1:A:487:GLU:CD	2.16	0.49
1:B:207:PHE:CD2	1:B:252:ASN:HB3	2.47	0.49
1:B:378:ASN:HB3	1:B:379:PRO:HD2	1.94	0.49
1:C:542:ARG:NH2	3:C:1922:HOH:O	2.45	0.49
1:A:516:THR:HB	1:A:517:PRO:HD2	1.93	0.49
1:C:296:LEU:HD12	1:C:333:GLU:CB	2.43	0.49
1:A:488:ARG:NE	1:A:490:GLU:OE2	2.34	0.49
1:A:745:ILE:N	1:A:746:PRO:HD2	2.28	0.49
1:D:97:ALA:O	1:D:101:GLY:HA3	2.13	0.49
1:D:751:ILE:HD13	1:D:752:PRO:HD2	1.94	0.49
1:B:344:GLU:CD	1:B:344:GLU:H	2.14	0.49
1:C:505:TYR:HA	1:C:508:PRO:HG2	1.93	0.49
1:C:727:SER:HA	3:C:3714:HOH:O	2.12	0.49
1:C:516:THR:O	1:C:520:GLN:HG3	2.13	0.48
1:D:708:ILE:HG13	1:D:710:ILE:HG12	1.94	0.48
1:D:750:LYS:HZ2	1:D:750:LYS:HB2	1.76	0.48
1:C:222:LYS:HB3	1:C:223:PRO:CD	2.43	0.48
1:A:65:LEU:HD21	1:A:135:HIS:CG	2.49	0.48
1:A:188:LYS:HB2	1:A:391:PHE:CE1	2.48	0.48
1:A:438:CYS:HB2	1:A:439:PRO:HD2	1.93	0.48
1:B:36:HIS:NE2	1:B:37:ARG:HD3	2.29	0.48
1:C:351:PHE:HB2	1:C:358:LYS:HG3	1.95	0.48
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.95	0.48
1:C:125:ARG:HB2	1:C:129:ALA:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:507:HIS:N	1:C:508:PRO:CD	2.76	0.48
1:C:404:ASN:O	1:C:405:ASP:C	2.49	0.48
1:A:265:SER:OG	1:A:267:ARG:HB2	2.13	0.48
1:B:174:GLY:O	1:C:231:GLN:HG2	2.13	0.48
1:D:122:ILE:HB	1:D:123:PRO:CD	2.44	0.48
1:A:709:LYS:HE3	1:A:709:LYS:HA	1.96	0.48
1:B:128:HIS:HA	1:B:168:THR:O	2.14	0.48
1:B:745:ILE:HB	1:B:746:PRO:HD3	1.95	0.48
1:C:323:TRP:CZ3	1:C:379:PRO:HD2	2.48	0.48
1:C:335:GLU:OE2	1:C:369:ARG:NH2	2.47	0.48
1:C:621:LYS:NZ	3:C:4070:HOH:O	2.45	0.48
1:B:392:HIS:CE1	1:B:415:TYR:HB2	2.48	0.48
1:C:392:HIS:CG	1:C:415:TYR:HB2	2.49	0.48
1:B:333:GLU:HG2	1:B:374:VAL:HG22	1.96	0.47
1:D:607:LEU:HD22	1:D:611:VAL:HG21	1.96	0.47
1:A:71:VAL:CG2	1:C:453:ILE:HD12	2.44	0.47
1:B:612:ARG:O	1:B:614:ALA:N	2.47	0.47
1:C:392:HIS:CE1	1:C:415:TYR:HB2	2.49	0.47
1:B:748:ILE:O	1:B:751:ILE:HG22	2.14	0.47
1:B:145:SER:HA	1:B:148:THR:O	2.15	0.47
1:C:516:THR:HB	1:C:517:PRO:CD	2.44	0.47
1:C:643:ASP:OD1	1:C:644:ASP:N	2.47	0.47
1:D:95:LEU:HB3	1:D:107:ASP:HB2	1.96	0.47
1:A:237:ASP:OD2	1:A:536:ARG:HG3	2.13	0.47
1:B:359:LEU:H	1:B:507:HIS:HD2	1.62	0.47
1:B:443:PHE:CZ	1:B:470:PRO:HD2	2.49	0.47
1:D:227:TRP:CE3	1:D:229:ILE:HD12	2.48	0.47
1:A:30:ALA:HB1	1:A:31:PRO:HD2	1.97	0.47
1:C:128:HIS:HA	1:C:168:THR:O	2.14	0.47
1:D:309:LYS:HB3	1:D:660:LEU:HD11	1.97	0.47
1:B:461:GLU:HA	1:B:462:PRO:C	2.35	0.47
1:D:323:TRP:CH2	1:D:378:ASN:HB3	2.50	0.47
1:D:583:LYS:HB2	1:D:583:LYS:NZ	2.30	0.47
1:C:610:GLU:HG3	1:C:610:GLU:O	2.15	0.46
1:C:728:PHE:O	1:C:731:GLU:HB2	2.15	0.46
1:B:267:ARG:HG3	3:B:2921:HOH:O	2.15	0.46
1:B:345:ASP:OD1	1:B:348:LYS:NZ	2.42	0.46
1:C:229:ILE:HG23	1:C:230:PRO:HA	1.98	0.46
1:D:392:HIS:ND1	1:D:393:PRO:HD2	2.31	0.46
1:A:83:ASN:HB3	1:C:429:HIS:CD2	2.50	0.46
1:A:461:GLU:HA	1:A:462:PRO:C	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:693:LYS:HA	1:A:694:PRO:HD3	1.81	0.46
1:B:717:GLY:HA3	1:B:741:VAL:HG11	1.97	0.46
1:D:37:ARG:HA	1:D:38:PRO:HD2	1.76	0.46
1:D:710:ILE:HG23	1:D:715:GLU:HG2	1.98	0.46
1:C:612:ARG:HA	1:C:643:ASP:OD2	2.15	0.46
1:D:418:THR:HG23	1:D:419:GLN:HG3	1.98	0.46
1:A:414:SER:HB2	1:D:114:ILE:HG21	1.98	0.46
1:A:689:TYR:OH	1:A:715:GLU:OE2	2.30	0.46
1:B:113:LYS:HD2	3:B:1609:HOH:O	2.16	0.46
1:A:516:THR:O	1:A:520:GLN:HG3	2.16	0.46
1:A:696:ALA:HB1	1:A:728:PHE:CZ	2.50	0.46
1:B:563:GLY:HA2	3:B:1767:HOH:O	2.15	0.46
1:B:252:ASN:HD22	1:B:252:ASN:HA	1.55	0.46
1:B:631:LYS:HG3	1:B:633:LEU:HD13	1.97	0.46
1:C:97:ALA:O	1:C:101:GLY:HA3	2.15	0.46
1:C:751:ILE:HG13	1:C:752:PRO:HD2	1.98	0.46
1:A:516:THR:HB	1:A:517:PRO:CD	2.46	0.46
1:B:251:HIS:CE1	1:B:507:HIS:HB3	2.50	0.46
1:B:616:LEU:HD23	1:B:616:LEU:HA	1.87	0.46
1:C:43:THR:O	1:C:328:ALA:HA	2.16	0.46
1:C:252:ASN:HD22	1:C:252:ASN:HA	1.58	0.46
1:C:672:ILE:HD12	1:C:701:ALA:HA	1.97	0.46
1:D:155:ASP:HA	1:D:156:PRO:HD2	1.81	0.46
1:D:607:LEU:O	1:D:675:ILE:HD13	2.16	0.46
1:A:363:GLU:HG2	3:A:2160:HOH:O	2.16	0.45
1:A:596:GLY:HA3	1:A:737:ALA:O	2.16	0.45
1:B:709:LYS:HA	1:B:709:LYS:HD2	1.67	0.45
3:B:1439:HOH:O	1:C:231:GLN:HB2	2.16	0.45
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.99	0.45
1:C:602:VAL:HG12	1:C:603:VAL:N	2.31	0.45
1:D:556:GLN:NE2	3:D:3773:HOH:O	2.50	0.45
1:B:470:PRO:HB2	1:D:80:LEU:HA	1.96	0.45
1:B:593:ILE:HA	1:B:594:PRO:HD2	1.65	0.45
1:C:750:LYS:N	1:C:750:LYS:HE2	2.32	0.45
1:B:331:PHE:HA	1:B:332:PRO:HD3	1.83	0.45
1:C:525:ASP:HB3	3:C:3259:HOH:O	2.16	0.45
1:C:554:LEU:O	1:C:558:VAL:HG23	2.17	0.45
1:A:316:ASP:HB3	1:D:229:ILE:HG12	1.99	0.45
1:D:252:ASN:HD22	1:D:252:ASN:HA	1.53	0.45
1:D:278:ARG:HH12	1:D:487:GLU:CD	2.20	0.45
1:B:44:PRO:HB3	1:B:629:HIS:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:259:ASP:OD1	1:B:522:HIS:ND1	2.47	0.45
1:A:207:PHE:O	1:A:249:THR:HA	2.17	0.45
1:A:262:ILE:HG13	1:A:262:ILE:O	2.17	0.45
1:A:552:LEU:O	1:A:556:GLN:HG3	2.17	0.45
1:A:241:ASP:HB2	1:A:539:ILE:HD13	1.98	0.45
1:A:612:ARG:HA	1:A:643:ASP:OD2	2.16	0.45
1:A:725:ASP:H	1:A:728:PHE:HB3	1.82	0.44
1:A:751:ILE:HD12	1:A:751:ILE:O	2.16	0.44
1:B:170[B]:GLN:HG3	1:B:232:GLY:HA2	1.99	0.44
1:D:87:ARG:HB3	3:D:2379:HOH:O	2.17	0.44
1:A:692:LEU:HD21	1:A:748:ILE:HD13	2.00	0.44
1:D:750:LYS:HD3	1:D:751:ILE:N	2.31	0.44
1:A:637:MET:CG	1:D:532:SER:HB2	2.45	0.44
3:A:1392:HOH:O	1:D:100:ARG:HG3	2.16	0.44
1:D:407:LEU:O	1:D:411:ARG:HG3	2.18	0.44
1:D:461:GLU:HB2	1:D:462:PRO:HA	1.99	0.44
1:A:708:ILE:O	1:A:710:ILE:N	2.51	0.44
1:C:552:LEU:HD21	1:C:571:LEU:CD1	2.46	0.44
1:D:604:ALA:HB2	1:D:662:VAL:HG11	1.99	0.44
1:B:369:ARG:HG2	3:B:2639:HOH:O	2.16	0.44
1:B:692:LEU:O	1:B:741:VAL:HG23	2.18	0.44
1:B:720:GLU:O	1:B:721:ALA:HB2	2.17	0.44
1:D:745:ILE:O	1:D:748:ILE:HG12	2.17	0.44
1:A:689:TYR:OH	1:A:710:ILE:HG21	2.18	0.44
1:C:586:PRO:HB2	1:C:593:ILE:HD11	2.00	0.44
1:D:748:ILE:O	1:D:749:ASP:C	2.56	0.44
1:A:81:THR:O	1:C:442:ASN:HB3	2.18	0.44
1:A:512:TRP:CZ3	1:A:554:LEU:HD13	2.52	0.44
1:A:535:VAL:O	1:A:537:PRO:HD3	2.18	0.44
1:A:282:ALA:HB1	1:A:477:PRO:HB3	1.99	0.44
1:A:331:PHE:O	1:A:333:GLU:HG3	2.18	0.44
1:B:438:CYS:HB2	1:B:439:PRO:HD2	1.98	0.44
1:D:469:TRP:CE3	1:D:471:ARG:HG3	2.53	0.44
1:A:751:ILE:HD13	1:A:753:ALA:HB3	2.00	0.43
1:D:524:VAL:HG22	1:D:554:LEU:HD23	2.00	0.43
1:B:462:PRO:HA	1:B:468:ASN:OD1	2.19	0.43
1:D:750:LYS:HD3	1:D:751:ILE:H	1.82	0.43
1:A:451:MET:HG3	1:C:451:MET:HE1	1.99	0.43
1:B:686:MET:SD	1:B:707:THR:HG22	2.58	0.43
1:D:473:THR:O	1:D:481:GLY:HA3	2.18	0.43
1:B:97:ALA:O	1:B:101:GLY:HA3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:ILE:HD13	1:A:205:ILE:H	1.83	0.43
1:A:690:LYS:HG3	1:A:751:ILE:HD11	1.99	0.43
1:A:126:ILE:HD13	1:D:117:PHE:O	2.19	0.43
1:A:533:LYS:NZ	1:D:656:GLY:O	2.47	0.43
1:B:211:ALA:HB3	1:B:410:GLY:HA3	2.00	0.43
1:B:323:TRP:CH2	1:B:378:ASN:HB3	2.54	0.43
1:C:583:LYS:O	1:C:584:LYS:HB3	2.19	0.43
1:B:128:HIS:CE1	1:B:169:VAL:HG22	2.53	0.43
1:B:629:HIS:HD2	3:B:1708:HOH:O	2.01	0.43
1:B:144:LEU:HD11	1:B:370:VAL:HG13	2.01	0.43
1:D:179:VAL:HA	3:D:1743:HOH:O	2.19	0.43
1:D:574:THR:OG1	1:D:575:PRO:HD2	2.19	0.43
1:A:86:VAL:HG13	1:C:398:PRO:HD3	2.01	0.43
1:A:369:ARG:NH2	3:A:1391:HOH:O	2.51	0.43
1:B:27:ASP:HB3	3:B:3571:HOH:O	2.19	0.43
1:B:561:ASN:HB3	3:B:3136:HOH:O	2.19	0.43
1:D:459:ASN:HD22	1:D:459:ASN:N	2.12	0.43
1:D:750:LYS:O	1:D:751:ILE:O	2.37	0.43
1:A:29:LEU:HB3	1:C:467:ASP:OD1	2.19	0.42
1:A:710:ILE:HG13	1:A:711:ALA:N	2.34	0.42
1:B:30:ALA:HB1	1:B:31:PRO:HD2	2.01	0.42
1:B:416:THR:HG23	3:B:3659:HOH:O	2.19	0.42
1:C:512:TRP:CH2	1:C:520:GLN:HB3	2.54	0.42
1:A:478:LYS:HE3	3:A:3779:HOH:O	2.19	0.42
1:A:509:ARG:HD2	1:A:576:PRO:HD2	2.00	0.42
1:B:27:ASP:HB3	1:B:28:SER:H	1.36	0.42
1:B:125:ARG:HB2	1:B:129:ALA:HA	2.01	0.42
1:B:451:MET:HG3	1:D:451:MET:HE1	2.01	0.42
1:D:668:PRO:HA	1:D:698:ALA:HB3	2.01	0.42
1:A:104:LEU:HB3	3:C:1175:HOH:O	2.18	0.42
1:A:612:ARG:HH22	1:A:723:SER:HB3	1.84	0.42
1:A:689:TYR:HA	1:A:744:ARG:NH1	2.34	0.42
1:B:617:LEU:HA	3:B:3762:HOH:O	2.18	0.42
1:C:331:PHE:HA	1:C:332:PRO:HD3	1.85	0.42
1:C:511:PHE:O	1:C:515:GLN:HG2	2.19	0.42
1:D:128:HIS:HA	1:D:168:THR:O	2.18	0.42
1:B:536:ARG:HB3	1:B:538:TYR:CE2	2.54	0.42
1:B:556:GLN:HG2	1:B:566:LEU:CD2	2.48	0.42
1:D:214:PHE:HB3	1:D:215:PRO:HD3	2.00	0.42
1:D:693:LYS:HA	1:D:694:PRO:HD3	1.84	0.42
1:A:145:SER:HA	1:A:148:THR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:PHE:O	1:A:515:GLN:HG2	2.19	0.42
1:B:558:VAL:O	1:B:562:LEU:HD22	2.18	0.42
1:C:314:ASP:HA	1:C:315:PRO:HD2	1.88	0.42
1:C:488:ARG:HE	1:C:488:ARG:HB2	1.46	0.42
1:D:275:HIS:HB2	1:D:277:PHE:CE2	2.54	0.42
1:B:473:THR:O	1:D:89:ALA:HA	2.20	0.42
1:A:335:GLU:OE1	1:A:369:ARG:HD3	2.19	0.42
1:B:48:GLN:HB3	1:B:49:PRO:HD2	2.01	0.42
1:B:354:LEU:O	1:B:356:PRO:HD3	2.20	0.42
1:B:605:ILE:HG21	1:B:616:LEU:HD21	2.01	0.42
1:B:631:LYS:HG3	1:B:633:LEU:CD1	2.50	0.42
1:C:584:LYS:HB2	1:C:584:LYS:NZ	2.34	0.42
1:D:222:LYS:HB3	1:D:223:PRO:CD	2.50	0.42
1:A:76:GLU:O	1:A:77:ASN:HB2	2.19	0.41
1:A:648:LEU:HA	1:A:649:PRO:HD2	1.91	0.41
1:B:469:TRP:CH2	1:B:471:ARG:HD2	2.55	0.41
1:C:359:LEU:H	1:C:507:HIS:HD2	1.67	0.41
1:A:637:MET:HB2	1:D:562:LEU:HA	2.02	0.41
1:B:309:LYS:HD3	1:C:309:LYS:HE3	2.01	0.41
1:B:672:ILE:HG22	1:B:676:ALA:HB2	2.02	0.41
1:D:702:ARG:O	1:D:705:LYS:HG3	2.20	0.41
1:A:497:ARG:HG2	3:A:1076:HOH:O	2.21	0.41
1:B:678:ASN:OD1	1:B:680:ASP:HB2	2.20	0.41
1:C:490:GLU:HA	1:D:489:VAL:O	2.21	0.41
1:A:583:LYS:HB2	3:A:2913:HOH:O	2.20	0.41
1:B:222:LYS:CB	1:B:223:PRO:CD	2.91	0.41
1:D:574:THR:HG22	3:D:2614:HOH:O	2.20	0.41
1:B:293:TRP:CZ3	1:B:336:LEU:HB2	2.56	0.41
1:D:411:ARG:HG2	2:D:760:HEM:C2C	2.55	0.41
1:D:459:ASN:H	1:D:459:ASN:ND2	2.17	0.41
1:B:413:PHE:HB2	1:D:105:LEU:HD11	2.02	0.41
1:C:686:MET:CB	1:C:751:ILE:HD11	2.50	0.41
1:A:745:ILE:O	1:A:748:ILE:HG12	2.21	0.41
1:B:50:THR:HG21	1:C:227:TRP:CZ3	2.56	0.41
1:D:132:SER:OG	1:D:319:ARG:HG3	2.20	0.41
1:D:392:HIS:HA	1:D:393:PRO:HD2	1.90	0.41
1:A:330:ASP:OD1	1:A:600:GLY:HA2	2.21	0.41
1:D:443:PHE:CE2	1:D:470:PRO:HD2	2.56	0.41
1:B:51:ALA:HB1	1:B:52:PRO:HD2	2.02	0.41
1:B:602:VAL:HG12	1:B:603:VAL:N	2.36	0.41
1:C:278:ARG:HH12	1:C:487:GLU:CD	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:693:LYS:HA	1:C:694:PRO:HD3	1.94	0.41
1:D:48:GLN:HE21	1:D:48:GLN:HB3	1.64	0.41
1:D:459:ASN:HD22	1:D:460:TYR:HD2	1.69	0.41
1:D:533:LYS:NZ	3:D:3941:HOH:O	2.38	0.41
1:B:253:VAL:O	1:B:254:MET:C	2.60	0.41
1:B:323:TRP:CZ3	1:B:379:PRO:HD2	2.56	0.41
1:D:392:HIS:HB3	1:D:395:HIS:CE1	2.56	0.41
1:B:643:ASP:OD1	1:B:644:ASP:N	2.54	0.40
1:D:251:HIS:CE1	1:D:507:HIS:HB3	2.55	0.40
1:D:267:ARG:HG2	1:D:332:PRO:HB3	2.02	0.40
1:D:392:HIS:CG	1:D:415:TYR:HB2	2.56	0.40
1:D:739:HIS:CD2	1:D:740:ARG:HG2	2.56	0.40
1:B:64:LYS:HE2	1:B:190:TYR:CZ	2.56	0.40
1:C:227:TRP:CE2	1:C:229:ILE:HB	2.56	0.40
1:A:80:LEU:HD12	1:C:442:ASN:HA	2.02	0.40
1:A:155:ASP:HB3	1:A:158:LYS:HB2	2.03	0.40
1:B:337:GLY:HA2	1:B:368:GLN:O	2.20	0.40
1:C:706:ALA:HB3	3:C:3263:HOH:O	2.20	0.40
1:B:429:HIS:CG	1:D:83:ASN:HB3	2.56	0.40
1:B:449:HIS:HB2	1:D:449:HIS:CE1	2.56	0.40
1:D:218:VAL:HA	1:D:221:VAL:HG12	2.03	0.40
1:D:669:CYS:SG	1:D:670:GLY:N	2.93	0.40
1:A:37:ARG:HA	1:A:38:PRO:HD3	1.93	0.40
1:A:274:ILE:HD12	2:A:760:HEM:CBB	2.50	0.40
2:A:760:HEM:HBB2	2:A:760:HEM:CMB	2.51	0.40
1:B:476:GLY:HA3	3:B:1270:HOH:O	2.22	0.40
1:C:392:HIS:ND1	1:C:393:PRO:HD2	2.36	0.40
1:C:392:HIS:HA	1:C:393:PRO:HD2	1.94	0.40

All (1) 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)
1:A:59:ASP:OD1	1:B:369:ARG:NH1[2_646]	2.14	0.06

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%)	697 (96%)	27 (4%)	2 (0%)	41	55
1	B	726/753 (96%)	691 (95%)	29 (4%)	6 (1%)	19	29
1	C	726/753 (96%)	697 (96%)	28 (4%)	1 (0%)	51	68
1	D	726/753 (96%)	694 (96%)	29 (4%)	3 (0%)	34	48
All	All	2904/3012 (96%)	2779 (96%)	113 (4%)	12 (0%)	34	48

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	709	LYS
1	B	28	SER
1	B	613	SER
1	D	28	SER
1	D	750	LYS
1	D	751	ILE
1	A	75	SER
1	B	584	LYS
1	C	75	SER
1	B	75	SER
1	B	725	ASP
1	B	594	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	612/635 (96%)	591 (97%)	21 (3%)	37	56
1	B	612/635 (96%)	579 (95%)	33 (5%)	22	36
1	C	612/635 (96%)	573 (94%)	39 (6%)	17	28
1	D	612/635 (96%)	587 (96%)	25 (4%)	30	48
All	All	2448/2540 (96%)	2330 (95%)	118 (5%)	26	41

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	73	LYS
1	A	158	LYS
1	A	170[A]	GLN
1	A	170[B]	GLN
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	265	SER
1	A	294	LYS
1	A	375	LEU
1	A	432	PRO
1	A	440	TYR
1	A	459	ASN
1	A	709	LYS
1	A	712	ASP
1	A	715	GLU
1	A	750	LYS
1	B	27	ASP
1	B	28	SER
1	B	37	ARG
1	B	63	GLU
1	B	170[A]	GLN
1	B	170[B]	GLN
1	B	185	PHE
1	B	198	LEU
1	B	205	ILE
1	B	227	TRP
1	B	237	ASP
1	B	252	ASN

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Mol	Chain	Res	Type
1	B	283	GLU
1	B	285	LYS
1	B	315	PRO
1	B	372	LYS
1	B	375	LEU
1	B	377	ARG
1	B	440	TYR
1	B	459	ASN
1	B	461	GLU
1	B	552	LEU
1	B	560	LYS
1	B	562	LEU
1	B	565	GLU
1	B	568	ASP
1	B	571	LEU
1	B	583	LYS
1	B	612	ARG
1	B	633	LEU
1	B	639	GLU
1	B	749	ASP
1	B	751	ILE
1	C	32	GLU
1	C	61	ARG
1	C	159	ILE
1	C	170[A]	GLN
1	C	170[B]	GLN
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	285	LYS
1	C	375	LEU
1	C	377	ARG
1	C	415	TYR
1	C	440	TYR
1	C	459	ASN
1	C	488	ARG
1	C	521	ARG

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Mol	Chain	Res	Type
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	612	ARG
1	C	616	LEU
1	C	633	LEU
1	C	648	LEU
1	C	660	LEU
1	C	685	LEU
1	C	709	LYS
1	C	713	GLN
1	C	725	ASP
1	C	733	LEU
1	C	750	LYS
1	D	41	GLU
1	D	73	LYS
1	D	170[A]	GLN
1	D	170[B]	GLN
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	340	LEU
1	D	344	GLU
1	D	375	LEU
1	D	440	TYR
1	D	459	ASN
1	D	552	LEU
1	D	554	LEU
1	D	582	LEU
1	D	610	GLU
1	D	633	LEU
1	D	648	LEU
1	D	747	LYS
1	D	749	ASP
1	D	750	LYS

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Mol	Chain	Res	Type
1	D	751	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) 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	A	713	GLN
1	B	252	ASN
1	B	459	ASN
1	B	507	HIS
1	B	629	HIS
1	C	252	ASN
1	C	368	GLN
1	C	459	ASN
1	C	507	HIS
1	C	556	GLN
1	C	572	ASN
1	C	629	HIS
1	C	671	ASN
1	D	48	GLN
1	D	252	ASN
1	D	368	GLN
1	D	459	ASN
1	D	507	HIS
1	D	546	GLN
1	D	572	ASN
1	D	629	HIS
1	D	671	ASN

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	41,50,50	1.42	3 (7%)	45,82,82	1.60	10 (22%)
2	HEM	A	760	1	41,50,50	1.55	6 (14%)	45,82,82	1.07	2 (4%)
2	HEM	D	760	1	41,50,50	1.40	3 (7%)	45,82,82	1.34	7 (15%)
2	HEM	C	760	1	41,50,50	1.43	4 (9%)	45,82,82	1.42	6 (13%)

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	-	2/12/54/54	-
2	HEM	A	760	1	-	2/12/54/54	-
2	HEM	D	760	1	-	2/12/54/54	-
2	HEM	C	760	1	-	4/12/54/54	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	760	HEM	C3C-C2C	-5.12	1.33	1.40
2	B	760	HEM	C3C-C2C	-4.85	1.33	1.40
2	D	760	HEM	C3C-C2C	-4.81	1.33	1.40
2	C	760	HEM	C3C-C2C	-4.39	1.34	1.40
2	A	760	HEM	C3C-CAC	3.56	1.55	1.47
2	C	760	HEM	C3C-CAC	3.30	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	760	HEM	C3C-CAC	2.66	1.53	1.47
2	D	760	HEM	C3C-CAC	2.66	1.53	1.47
2	B	760	HEM	CAB-C3B	2.43	1.54	1.47
2	A	760	HEM	CMB-C2B	2.42	1.55	1.50
2	D	760	HEM	CAB-C3B	2.39	1.54	1.47
2	C	760	HEM	CAB-C3B	2.39	1.54	1.47
2	A	760	HEM	CAB-C3B	2.25	1.53	1.47
2	C	760	HEM	C3D-C2D	-2.07	1.32	1.36
2	A	760	HEM	C3B-C2B	-2.06	1.33	1.37
2	A	760	HEM	C1B-NB	-2.05	1.36	1.40

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	760	HEM	CMA-C3A-C4A	-4.07	122.22	128.46
2	B	760	HEM	CBA-CAA-C2A	3.86	119.20	112.62
2	B	760	HEM	CMA-C3A-C4A	-3.55	123.01	128.46
2	D	760	HEM	CBA-CAA-C2A	3.45	118.51	112.62
2	B	760	HEM	CMC-C2C-C3C	3.42	131.08	124.68
2	B	760	HEM	C4C-CHD-C1D	3.15	126.72	122.56
2	D	760	HEM	CMA-C3A-C4A	-3.02	123.82	128.46
2	C	760	HEM	CMA-C3A-C2A	2.94	130.49	124.94
2	D	760	HEM	O2A-CGA-O1A	2.91	130.56	123.30
2	D	760	HEM	O1A-CGA-CBA	-2.89	113.81	123.08
2	A	760	HEM	CMA-C3A-C4A	-2.63	124.43	128.46
2	B	760	HEM	CMD-C2D-C1D	-2.61	121.07	125.04
2	B	760	HEM	C4B-CHC-C1C	2.49	125.85	122.56
2	D	760	HEM	C4C-CHD-C1D	2.48	125.83	122.56
2	C	760	HEM	CMC-C2C-C3C	2.44	129.24	124.68
2	C	760	HEM	C4C-CHD-C1D	2.39	125.71	122.56
2	A	760	HEM	O1A-CGA-CBA	-2.35	115.54	123.08
2	D	760	HEM	CHC-C4B-NB	2.21	126.83	124.43
2	B	760	HEM	CMD-C2D-C3D	2.18	132.05	126.12
2	B	760	HEM	CBB-CAB-C3B	-2.12	117.06	127.62
2	C	760	HEM	O1D-CGD-CBD	-2.12	116.28	123.08
2	B	760	HEM	C4D-ND-C1D	2.10	107.24	105.07
2	C	760	HEM	O1A-CGA-CBA	-2.09	116.38	123.08
2	D	760	HEM	CMA-C3A-C2A	2.08	128.86	124.94
2	B	760	HEM	CMA-C3A-C2A	2.02	128.75	124.94

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	760	HEM	C2B-C3B-CAB-CBB
2	C	760	HEM	C4B-C3B-CAB-CBB
2	B	760	HEM	CAA-CBA-CGA-O2A
2	A	760	HEM	CAA-CBA-CGA-O1A
2	B	760	HEM	CAA-CBA-CGA-O1A
2	C	760	HEM	CAA-CBA-CGA-O1A
2	C	760	HEM	CAA-CBA-CGA-O2A
2	D	760	HEM	CAA-CBA-CGA-O2A
2	A	760	HEM	CAA-CBA-CGA-O2A
2	D	760	HEM	CAA-CBA-CGA-O1A

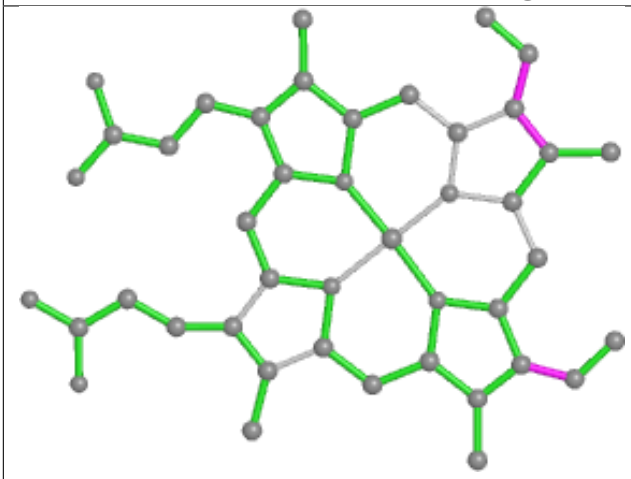
There are no ring outliers.

4 monomers are involved in 12 short contacts:

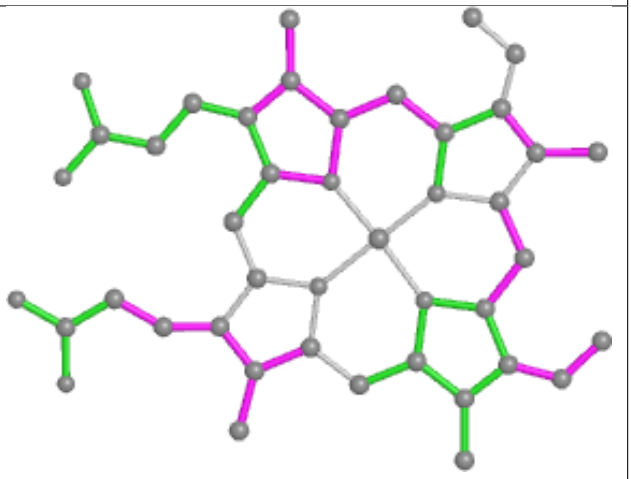
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	760	HEM	1	0
2	A	760	HEM	6	0
2	D	760	HEM	2	0
2	C	760	HEM	3	0

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

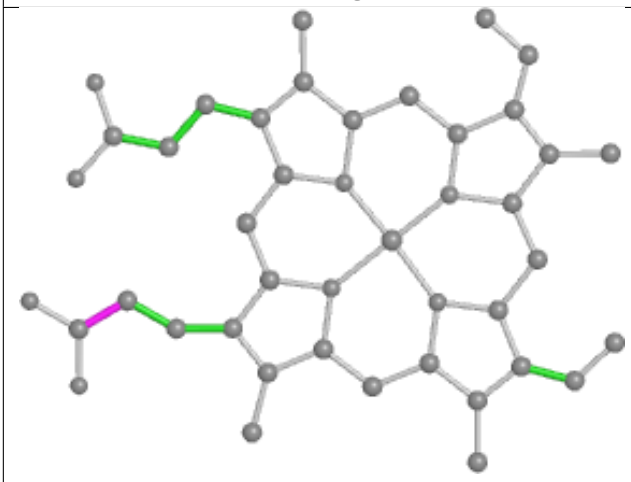
Ligand HEM B 760



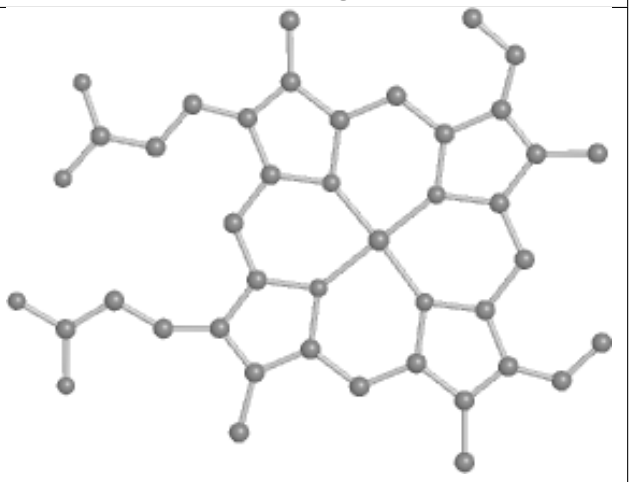
Bond lengths



Bond angles

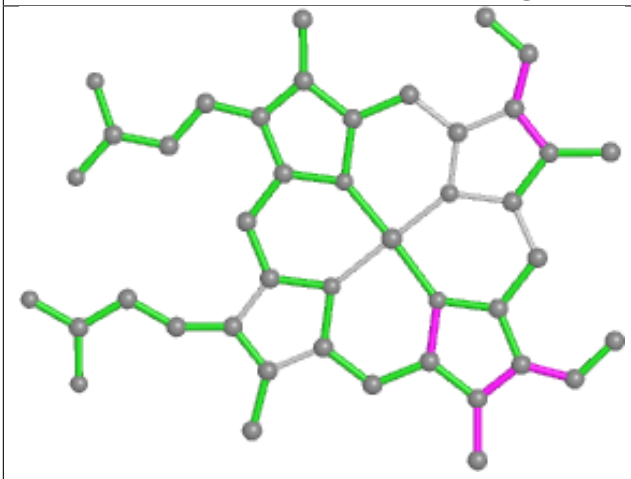


Torsions

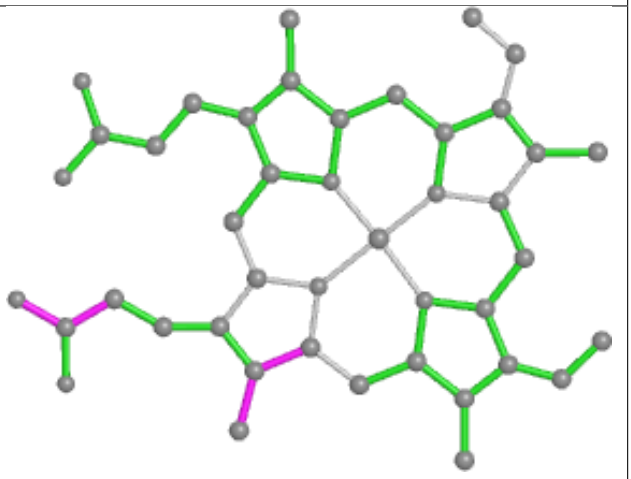


Rings

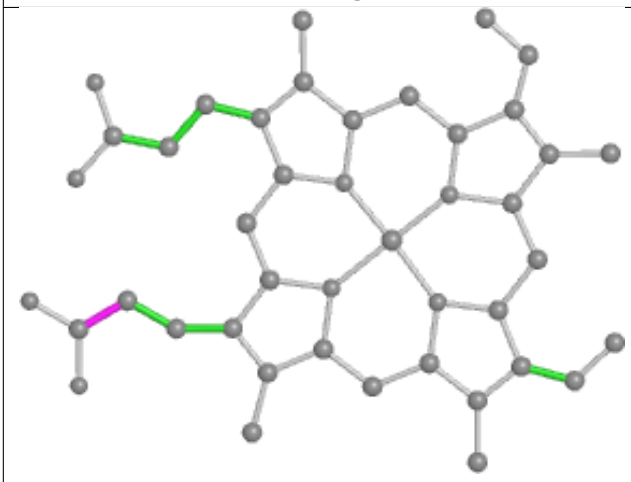
Ligand HEM A 760



Bond lengths



Bond angles



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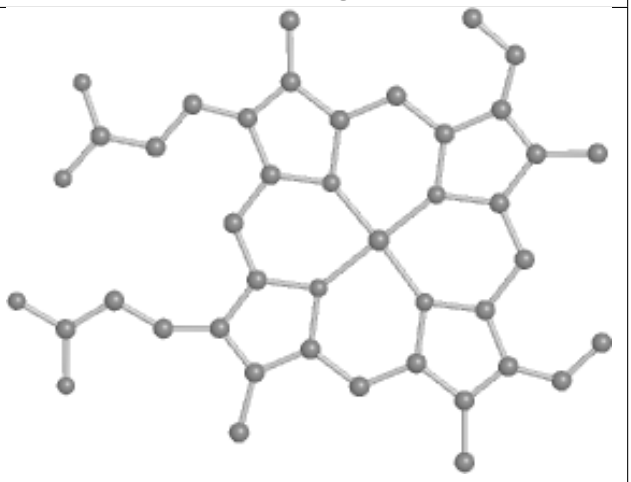
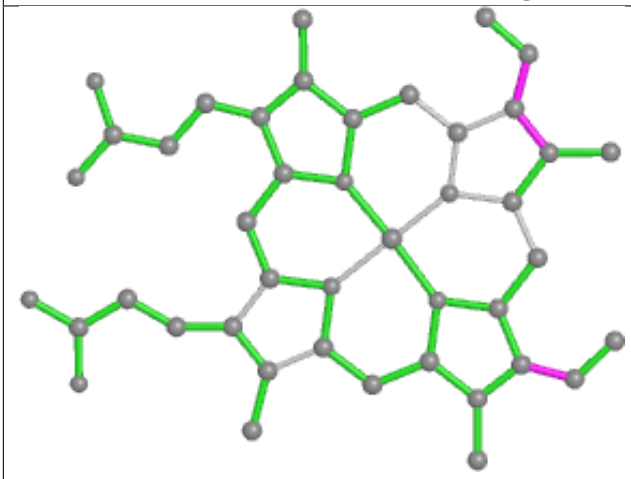
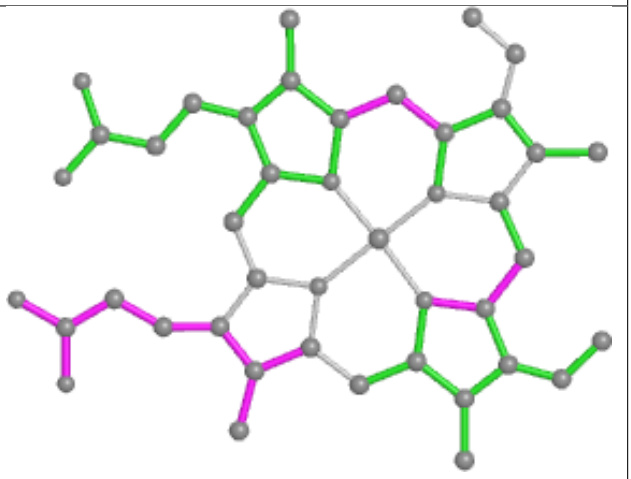


Rings

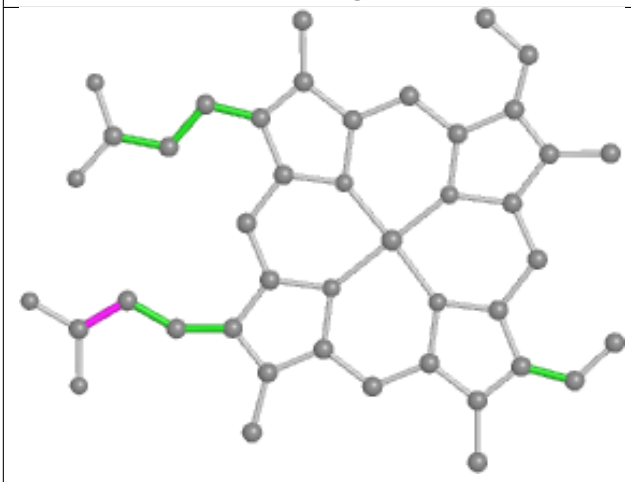
Ligand HEM D 760



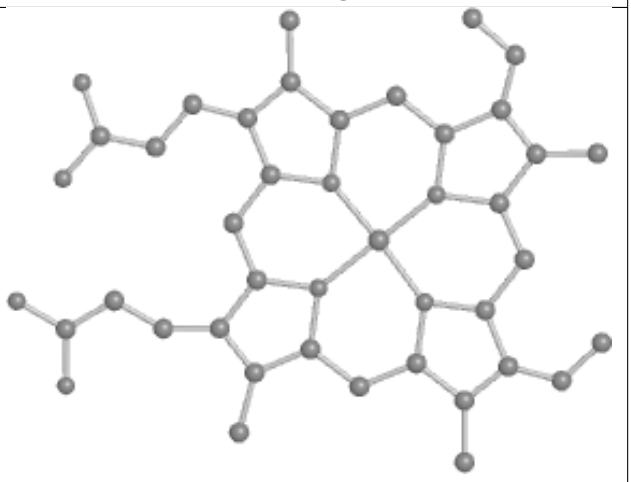
Bond lengths



Bond angles

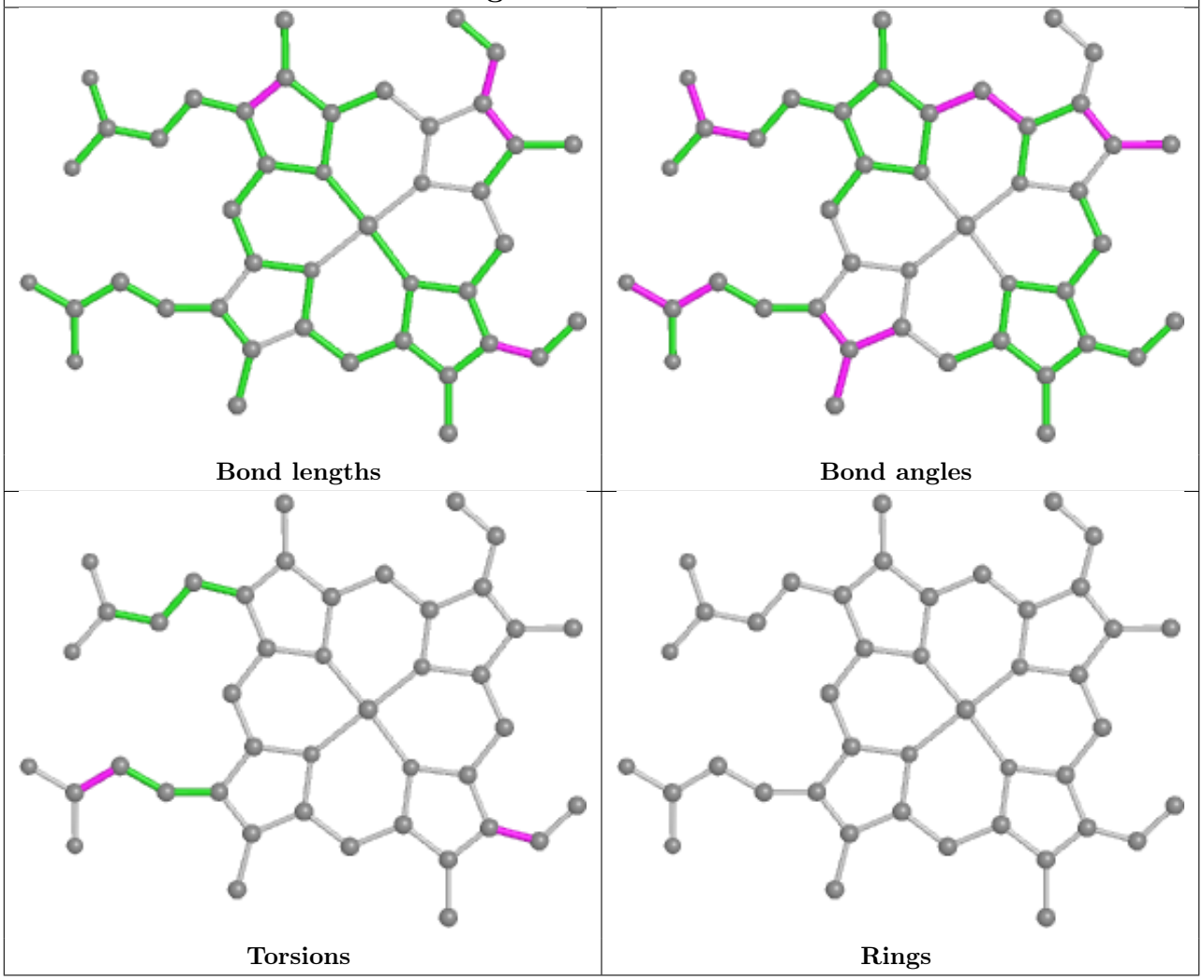


Torsions



Rings

Ligand HEM C 760



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^{th} 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%)	-0.83	8 (1%)	80	79	13, 23, 43, 70	1 (0%)
1	B	727/753 (96%)	-0.75	6 (0%)	86	84	14, 24, 48, 66	1 (0%)
1	C	727/753 (96%)	-0.79	3 (0%)	92	91	15, 24, 47, 64	1 (0%)
1	D	727/753 (96%)	-0.81	6 (0%)	86	84	15, 23, 44, 64	1 (0%)
All	All	2908/3012 (96%)	-0.80	23 (0%)	86	84	13, 23, 46, 70	4 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	ASP	7.4
1	C	27	ASP	4.8
1	A	28	SER	4.7
1	A	711	ALA	4.3
1	D	27	ASP	4.1
1	C	28	SER	4.1
1	B	27	ASP	3.3
1	D	749	ASP	2.9
1	A	32	GLU	2.8
1	D	28	SER	2.7
1	A	712	ASP	2.5
1	D	712	ASP	2.4
1	D	33	ASP	2.3
1	B	726	GLY	2.2
1	B	750	LYS	2.2
1	D	32	GLU	2.2
1	B	711	ALA	2.1
1	B	28	SER	2.1
1	A	594	PRO	2.1
1	C	711	ALA	2.1
1	A	710	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	713	GLN	2.0
1	A	713	GLN	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)

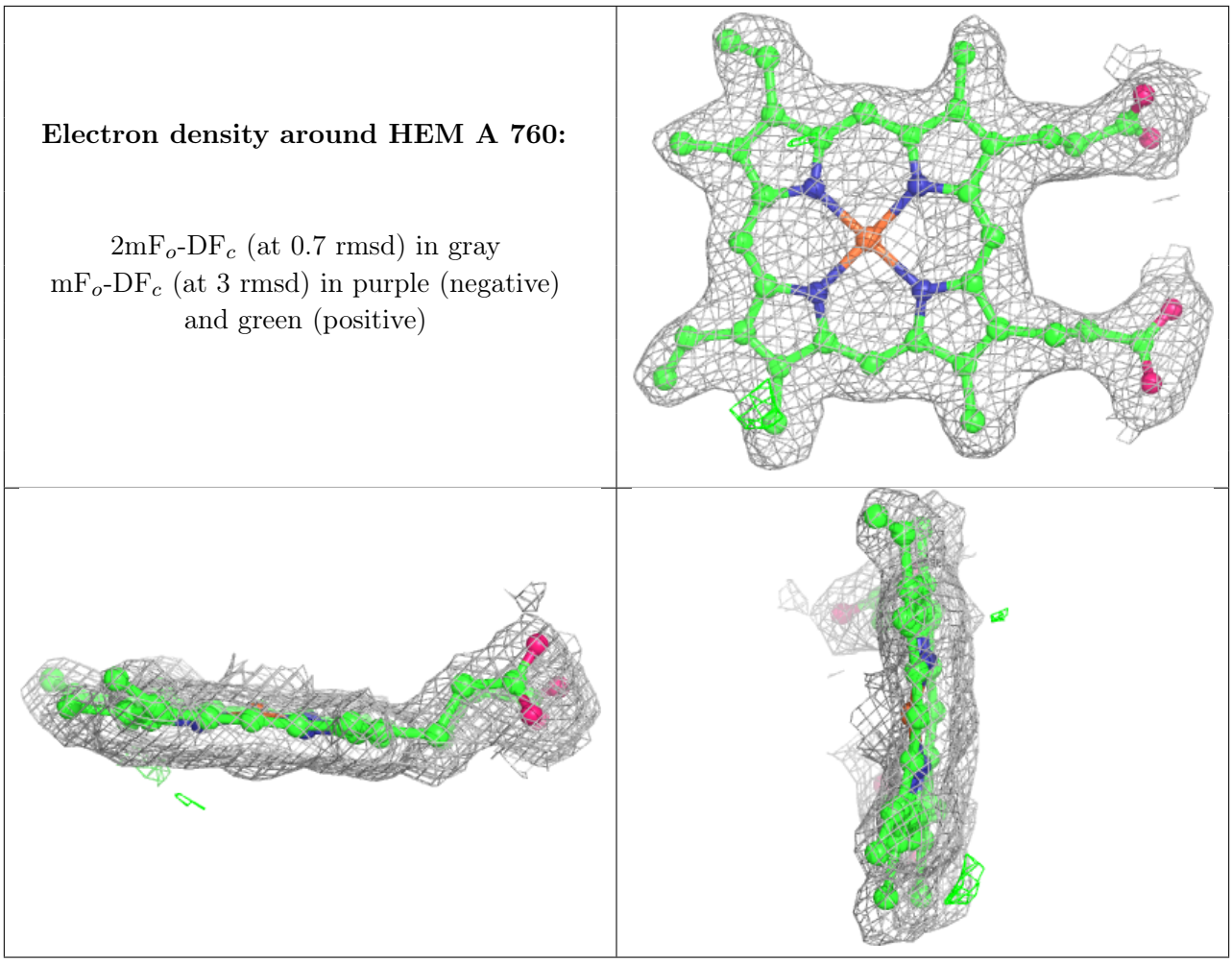
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEM	A	760	43/43	0.98	0.08	14,18,20,21	0
2	HEM	B	760	43/43	0.98	0.09	15,17,19,20	0
2	HEM	C	760	43/43	0.98	0.08	18,19,22,23	0
2	HEM	D	760	43/43	0.98	0.09	14,16,19,21	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.

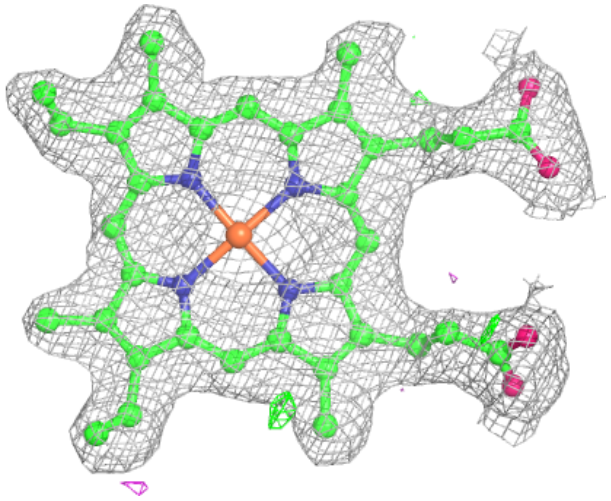
Electron density around HEM A 760:

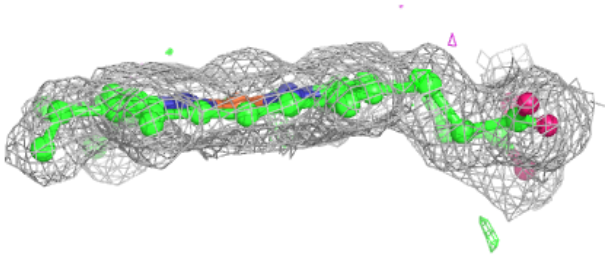
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

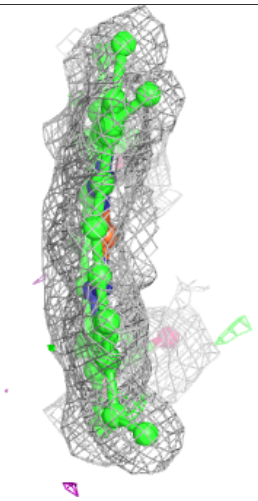


Electron density around HEM B 760:

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

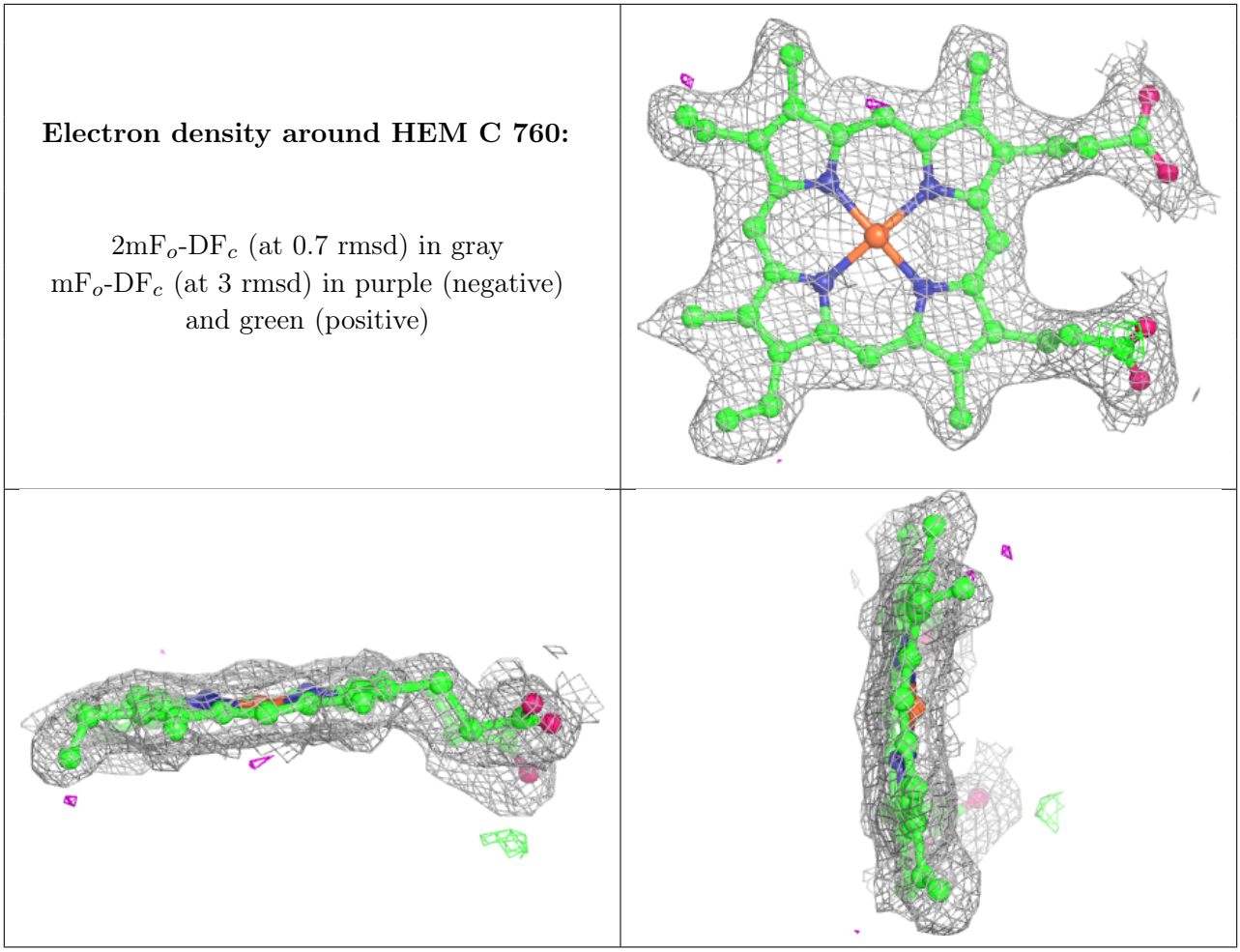






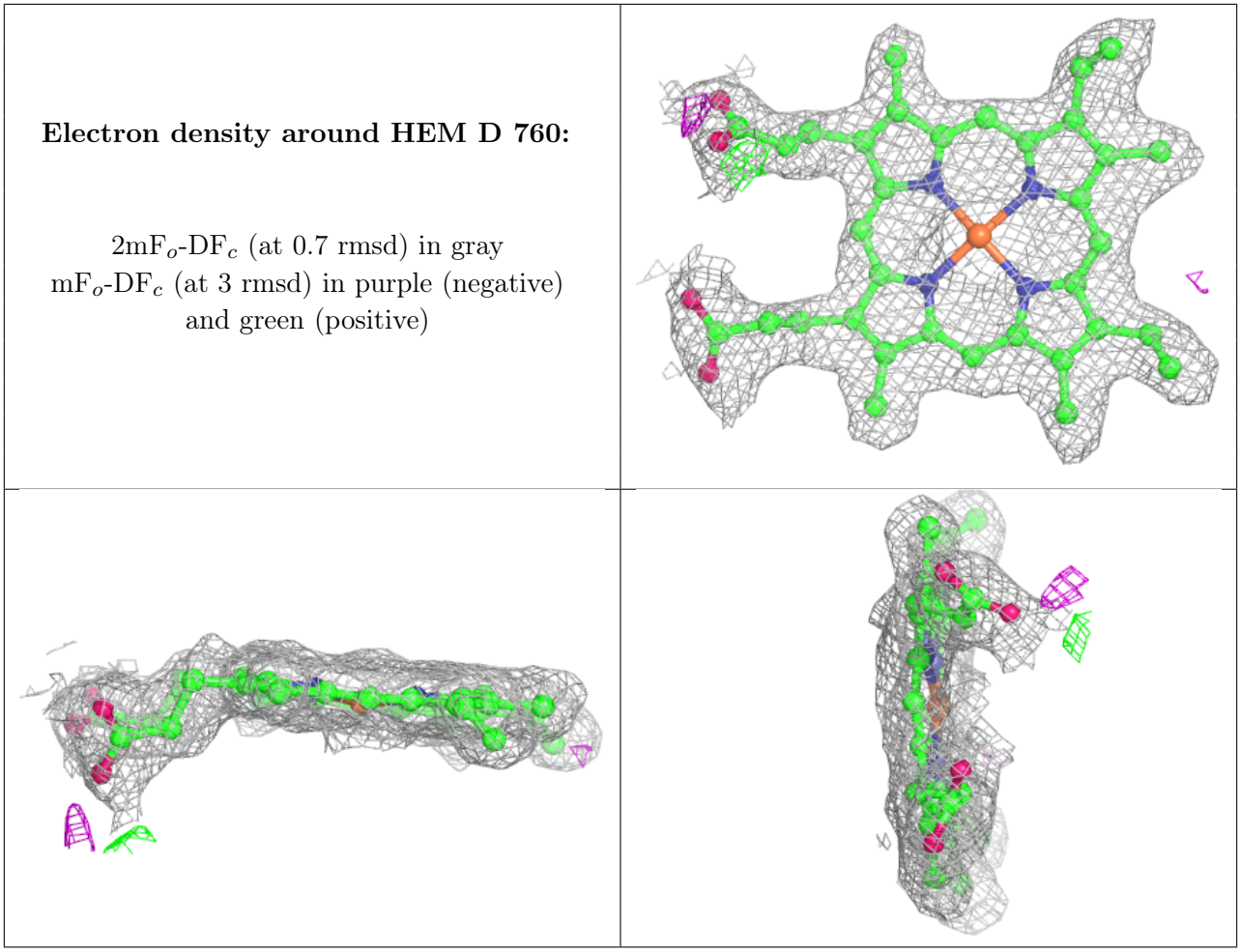
Electron density around HEM C 760:

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



Electron density around HEM D 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.