



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 03:01 PM UTC

PDB ID : 1M7S / pdb_00001m7s
Title : Crystal Structure Analysis of Catalase CatF of Pseudomonas syringae
Authors : Carpena, X.; Soriano, M.; Klotz, M.G.; Duckworth, H.W.; Donald, L.J.; Melik-Adamyan, W.; Fita, I.; Loewen, P.C.
Deposited on : 2002-07-22
Resolution : 1.80 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

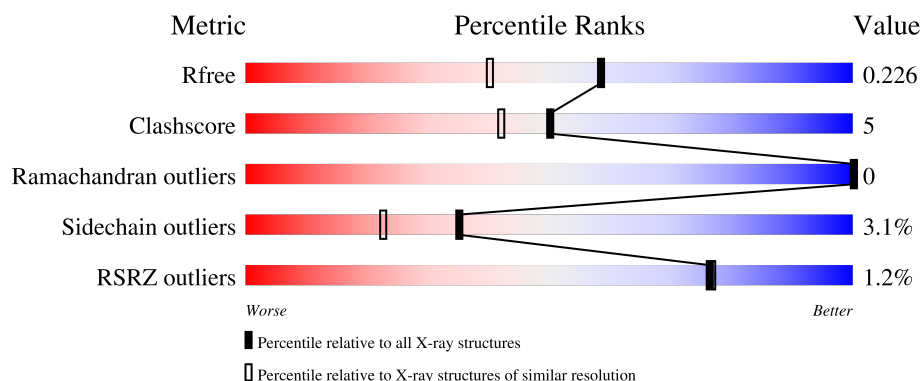
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	484	% 79% 18% .
1	B	484	2% 77% 20% .
1	C	484	% 79% 19% .
1	D	484	% 83% 14% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17561 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	0	3	0
			3820	2406	671	737	6			
1	B	483	Total	C	N	O	S	0	3	0
			3810	2401	670	733	6			
1	C	483	Total	C	N	O	S	0	3	0
			3810	2401	670	733	6			
1	D	484	Total	C	N	O	S	0	3	0
			3820	2406	671	737	6			

There are 28 discrepancies between the modelled and reference sequences:

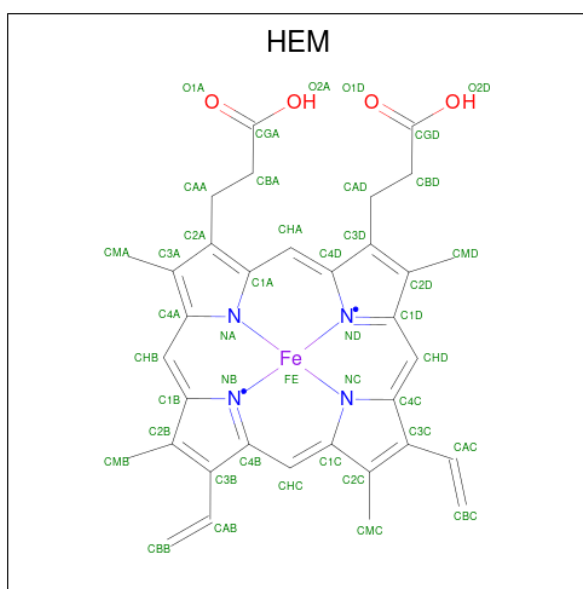
Chain	Residue	Modelled	Actual	Comment	Reference
A	369	ASN	ILE	SEE REMARK 999	UNP P46206
A	445	TYR	PHE	SEE REMARK 999	UNP P46206
A	459	LYS	ARG	SEE REMARK 999	UNP P46206
A	468	LEU	HIS	SEE REMARK 999	UNP P46206
A	478	TYR	VAL	SEE REMARK 999	UNP P46206
A	484	PRO	ARG	SEE REMARK 999	UNP P46206
A	485	ASN	HIS	SEE REMARK 999	UNP P46206
B	369	ASN	ILE	SEE REMARK 999	UNP P46206
B	445	TYR	PHE	SEE REMARK 999	UNP P46206
B	459	LYS	ARG	SEE REMARK 999	UNP P46206
B	468	LEU	HIS	SEE REMARK 999	UNP P46206
B	478	TYR	VAL	SEE REMARK 999	UNP P46206
B	484	PRO	ARG	SEE REMARK 999	UNP P46206
B	485	ASN	HIS	SEE REMARK 999	UNP P46206
C	369	ASN	ILE	SEE REMARK 999	UNP P46206
C	445	TYR	PHE	SEE REMARK 999	UNP P46206
C	459	LYS	ARG	SEE REMARK 999	UNP P46206
C	468	LEU	HIS	SEE REMARK 999	UNP P46206
C	478	TYR	VAL	SEE REMARK 999	UNP P46206
C	484	PRO	ARG	SEE REMARK 999	UNP P46206
C	485	ASN	HIS	SEE REMARK 999	UNP P46206

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Chain	Residue	Modelled	Actual	Comment	Reference
D	369	ASN	ILE	SEE REMARK 999	UNP P46206
D	445	TYR	PHE	SEE REMARK 999	UNP P46206
D	459	LYS	ARG	SEE REMARK 999	UNP P46206
D	468	LEU	HIS	SEE REMARK 999	UNP P46206
D	478	TYR	VAL	SEE REMARK 999	UNP P46206
D	484	PRO	ARG	SEE REMARK 999	UNP P46206
D	485	ASN	HIS	SEE REMARK 999	UNP P46206

- 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	C	Fe	N	O	
			43	34	1	4	4	
2	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
2	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	602	Total	O		
			602	602	0	0

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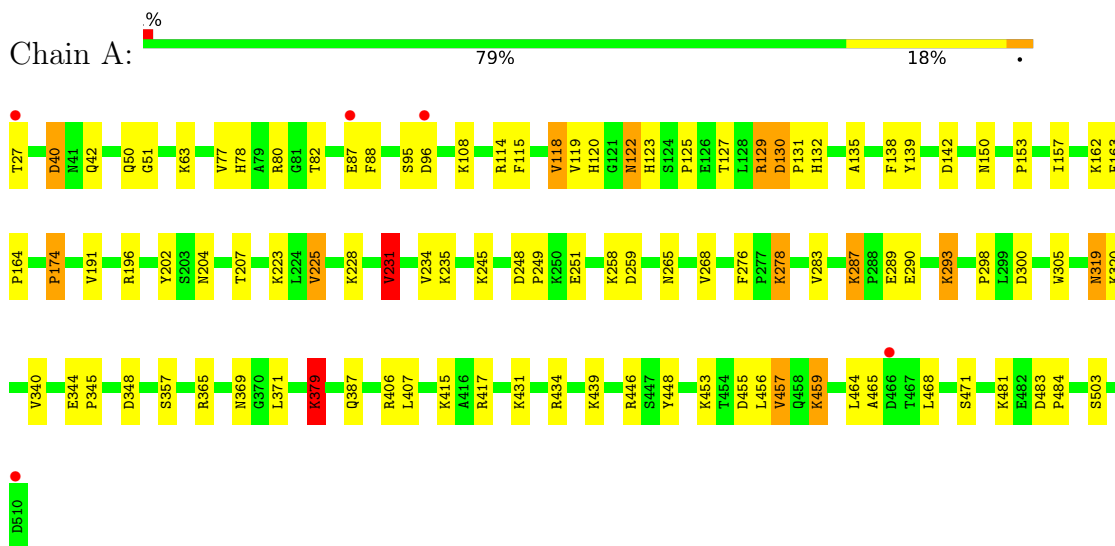
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	475	Total 475	O 475	0	0
3	C	438	Total 438	O 438	0	0
3	D	614	Total 614	O 614	0	0

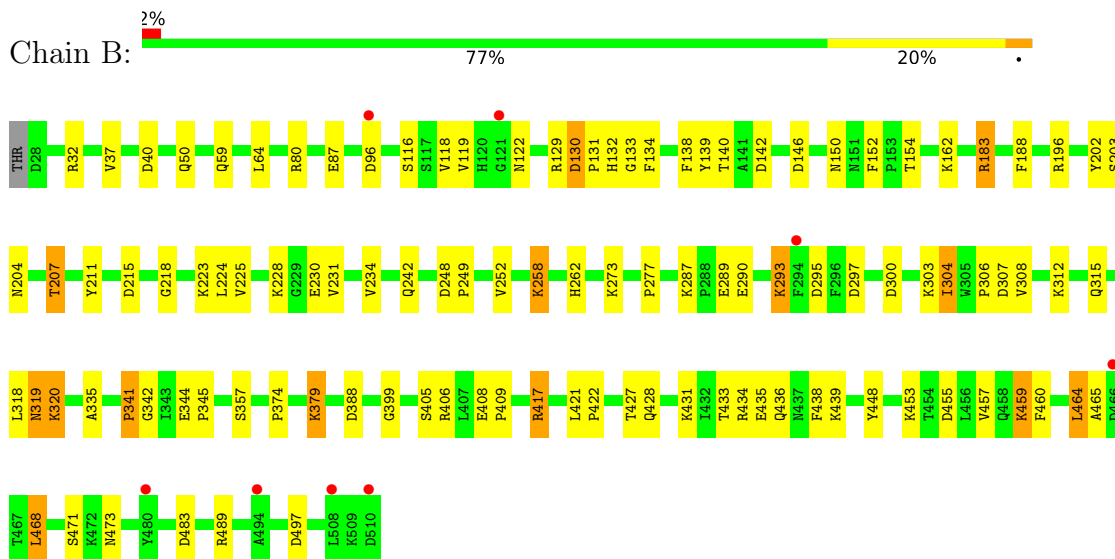
3 Residue-property plots [i](#)

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

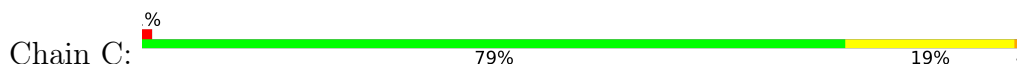
• Molecule 1: Catalase

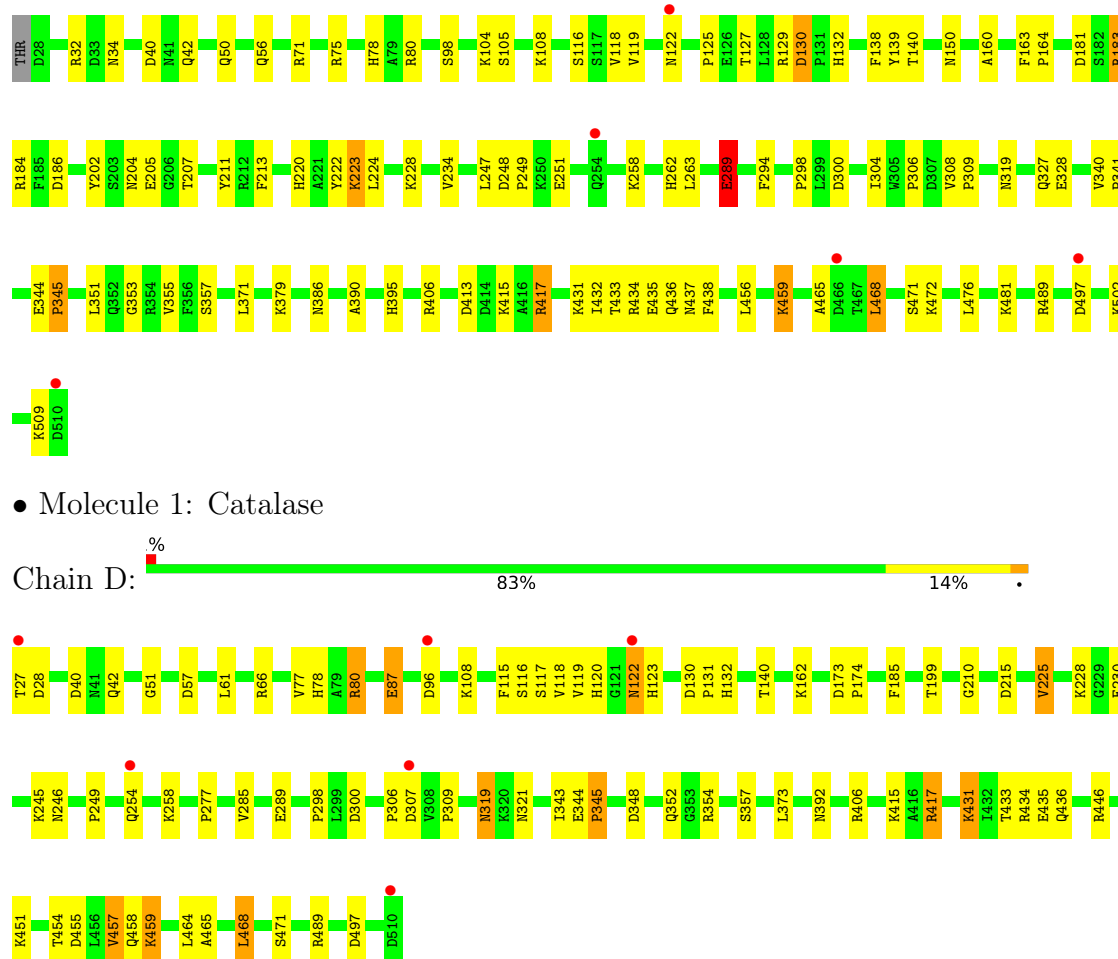


• Molecule 1: Catalase



• Molecule 1: Catalase





• Molecule 1: Catalase

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.63Å 153.87Å 109.19Å 90.00° 102.80° 90.00°	Depositor
Resolution (Å)	21.90 – 1.80 21.90 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (21.90-1.80) 97.7 (21.90-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 1.80Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.187 , 0.240 0.174 , 0.226	Depositor DCC
R_{free} test set	8773 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	12.9	Xtriage
Anisotropy	0.522	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17561	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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 [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	0.90	1/3915 (0.0%)	1.74	64/5305 (1.2%)
1	B	0.82	0/3905	1.75	65/5291 (1.2%)
1	C	0.79	0/3905	1.68	56/5291 (1.1%)
1	D	0.93	0/3915	1.71	60/5305 (1.1%)
All	All	0.86	1/15640 (0.0%)	1.72	245/21192 (1.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	77	VAL	CA-C	5.48	1.59	1.52

All (245) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	446	ARG	NE-CZ-NH2	-15.22	105.50	119.20
1	C	32	ARG	CD-NE-CZ	13.32	143.04	124.40
1	A	379	LYS	CA-CB-CG	10.90	135.91	114.10
1	B	87	GLU	CB-CG-CD	9.64	129.00	112.60
1	C	300	ASP	CA-CB-CG	8.98	121.58	112.60
1	B	132	HIS	CA-CB-CG	-8.51	105.29	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	300	ASP	CA-CB-CG	8.51	121.11	112.60
1	D	77	VAL	CA-C-O	-8.34	113.38	121.63
1	C	130	ASP	CA-CB-CG	8.23	120.83	112.60
1	A	357	SER	N-CA-C	8.02	120.10	111.36
1	B	32	ARG	CD-NE-CZ	8.01	135.61	124.40
1	D	215	ASP	CA-CB-CG	7.80	120.40	112.60
1	B	203	SER	CA-C-O	-7.67	113.21	121.88
1	D	497	ASP	CA-CB-CG	7.63	120.23	112.60
1	B	262	HIS	CA-CB-CG	7.53	121.33	113.80
1	B	497	ASP	CA-CB-CG	7.49	120.08	112.60
1	C	138	PHE	CA-CB-CG	7.45	121.25	113.80
1	D	225	VAL	CB-CA-C	7.44	121.20	110.33
1	D	319	ASN	OD1-CG-ND2	-7.35	115.25	122.60
1	D	465	ALA	CA-C-O	-7.30	111.85	120.10
1	D	285	VAL	N-CA-C	7.27	118.29	108.11
1	A	191	VAL	CA-C-N	7.20	126.91	119.56
1	A	191	VAL	C-N-CA	7.20	126.91	119.56
1	B	130	ASP	CA-CB-CG	7.17	119.77	112.60
1	B	118	VAL	CB-CA-C	-7.12	105.66	111.71
1	D	433	THR	CA-C-O	-7.11	111.40	119.79
1	D	307	ASP	CA-C-N	-7.09	117.49	122.59
1	D	307	ASP	C-N-CA	-7.09	117.49	122.59
1	C	434	ARG	CD-NE-CZ	7.04	134.26	124.40
1	C	489	ARG	NE-CZ-NH2	6.99	125.49	119.20
1	D	319	ASN	CB-CG-ND2	6.92	126.78	116.40
1	C	289	GLU	CA-CB-CG	6.91	127.91	114.10
1	D	132	HIS	CA-CB-CG	-6.89	106.91	113.80
1	A	95	SER	CA-C-N	6.87	130.17	120.28
1	A	95	SER	C-N-CA	6.87	130.17	120.28
1	D	119	VAL	N-CA-C	6.87	117.48	110.82
1	B	32	ARG	NE-CZ-NH1	-6.81	114.69	121.50
1	A	340	VAL	N-CA-CB	-6.74	107.18	111.83
1	C	472	LYS	CA-C-O	-6.74	113.75	120.82
1	B	435	GLU	N-CA-C	6.72	118.39	111.14
1	A	365	ARG	NE-CZ-NH2	6.70	125.23	119.20
1	A	287	LYS	CA-C-N	6.69	126.95	119.32
1	A	287	LYS	C-N-CA	6.69	126.95	119.32
1	A	130	ASP	CA-CB-CG	6.68	119.28	112.60
1	D	130	ASP	CA-CB-CG	6.68	119.28	112.60
1	D	417	ARG	NE-CZ-NH2	-6.67	113.20	119.20
1	D	357	SER	N-CA-C	6.58	118.45	111.28
1	A	51	GLY	CA-C-N	6.55	126.52	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	51	GLY	C-N-CA	6.55	126.52	120.03
1	D	87	GLU	CB-CG-CD	6.55	123.73	112.60
1	D	345	PRO	CB-CA-C	-6.54	102.41	110.98
1	A	142	ASP	CA-CB-CG	6.54	119.14	112.60
1	B	405	SER	CA-C-O	-6.54	112.50	120.54
1	C	465	ALA	N-CA-C	6.53	119.22	111.33
1	B	319	ASN	OD1-CG-ND2	-6.49	116.11	122.60
1	D	300	ASP	CA-CB-CG	6.48	119.08	112.60
1	A	348	ASP	CA-CB-CG	6.47	119.07	112.60
1	C	459	LYS	CG-CD-CE	6.46	126.16	111.30
1	A	465	ALA	CA-C-N	-6.45	112.89	122.83
1	A	465	ALA	C-N-CA	-6.45	112.89	122.83
1	B	303	LYS	CA-C-O	6.45	128.07	120.66
1	C	32	ARG	NE-CZ-NH1	-6.45	115.05	121.50
1	B	215	ASP	CA-CB-CG	6.42	119.02	112.60
1	C	357	SER	N-CA-C	6.41	118.27	111.28
1	B	183	ARG	NE-CZ-NH2	-6.40	113.44	119.20
1	D	185	PHE	CA-CB-CG	-6.40	107.40	113.80
1	A	157	ILE	CA-C-O	-6.38	115.16	121.67
1	A	457	VAL	N-CA-CB	-6.38	101.87	110.54
1	B	427	THR	N-CA-C	-6.36	101.53	110.50
1	B	32	ARG	NH1-CZ-NH2	6.36	127.56	119.30
1	C	395	HIS	CA-CB-CG	-6.32	107.48	113.80
1	B	417	ARG	NE-CZ-NH2	-6.32	113.52	119.20
1	C	294	PHE	CA-CB-CG	-6.30	107.50	113.80
1	D	210	GLY	CA-C-O	-6.30	114.80	121.29
1	A	119	VAL	N-CA-C	6.29	116.93	110.82
1	B	211	TYR	CA-C-O	6.29	127.11	119.38
1	C	309	PRO	N-CA-CB	6.29	109.17	103.33
1	D	321	ASN	OD1-CG-ND2	-6.27	116.33	122.60
1	D	446	ARG	NH1-CZ-NH2	6.24	127.41	119.30
1	C	205	GLU	N-CA-C	-6.17	105.71	113.18
1	C	132	HIS	CA-CB-CG	-6.17	107.63	113.80
1	D	417	ARG	CG-CD-NE	-6.16	98.46	112.00
1	C	386	ASN	OD1-CG-ND2	-6.11	116.49	122.60
1	D	87	GLU	O-C-N	6.11	130.23	123.33
1	A	225	VAL	CB-CA-C	6.10	119.66	110.63
1	B	433	THR	CA-C-O	-6.10	112.56	120.00
1	D	465	ALA	CA-C-N	-6.09	113.54	122.86
1	D	465	ALA	C-N-CA	-6.09	113.54	122.86
1	C	71	ARG	CD-NE-CZ	6.09	132.93	124.40
1	B	118	VAL	N-CA-C	6.09	117.20	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	183	ARG	NH1-CZ-NH2	6.06	127.18	119.30
1	B	207	THR	CA-C-N	6.06	126.40	119.92
1	B	207	THR	C-N-CA	6.06	126.40	119.92
1	B	297	ASP	CA-C-N	6.05	125.75	119.82
1	B	297	ASP	C-N-CA	6.05	125.75	119.82
1	B	152	PHE	CA-CB-CG	6.02	119.82	113.80
1	B	357	SER	N-CA-C	6.02	118.64	111.71
1	B	307	ASP	CA-CB-CG	-6.02	106.58	112.60
1	D	352	GLN	CA-C-O	-6.00	114.47	120.90
1	C	345	PRO	N-CA-CB	6.00	108.91	103.33
1	D	51	GLY	CA-C-N	5.98	125.95	120.03
1	D	51	GLY	C-N-CA	5.98	125.95	120.03
1	D	230	GLU	O-C-N	5.98	129.71	122.96
1	D	306	PRO	CA-C-N	-5.97	113.17	122.67
1	D	306	PRO	C-N-CA	-5.97	113.17	122.67
1	D	348	ASP	CA-CB-CG	5.96	118.56	112.60
1	B	64	LEU	CA-C-O	-5.95	114.11	120.42
1	C	183	ARG	NE-CZ-NH2	-5.95	113.85	119.20
1	C	186	ASP	N-CA-C	-5.93	104.74	111.14
1	A	231	VAL	N-CA-CB	-5.92	99.66	111.91
1	C	207	THR	CA-C-N	5.87	126.20	119.92
1	C	207	THR	C-N-CA	5.87	126.20	119.92
1	A	132	HIS	CA-CB-CG	-5.86	107.94	113.80
1	C	116	SER	N-CA-C	5.86	117.04	108.14
1	A	118	VAL	CB-CA-C	-5.84	105.85	111.05
1	B	388	ASP	CA-CB-CG	5.84	118.44	112.60
1	C	262	HIS	CA-CB-CG	5.84	119.64	113.80
1	B	138	PHE	CA-CB-CG	5.82	119.61	113.80
1	C	150	ASN	CA-CB-CG	5.81	118.41	112.60
1	A	207	THR	CA-C-N	5.79	125.70	119.85
1	A	207	THR	C-N-CA	5.79	125.70	119.85
1	A	268	VAL	CA-C-N	5.78	126.36	119.94
1	A	268	VAL	C-N-CA	5.78	126.36	119.94
1	B	146	ASP	CA-CB-CG	5.78	118.38	112.60
1	B	134	PHE	CA-CB-CG	5.76	119.56	113.80
1	C	328	GLU	CA-C-N	5.75	127.98	120.28
1	C	328	GLU	C-N-CA	5.75	127.98	120.28
1	A	434	ARG	CA-C-O	-5.74	114.16	120.30
1	A	259	ASP	CA-C-O	-5.72	113.04	120.25
1	A	77	VAL	O-C-N	5.71	129.47	123.02
1	B	293	LYS	N-CA-C	5.71	117.31	111.14
1	A	129	ARG	NE-CZ-NH1	5.70	127.20	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	188	PHE	CA-CB-CG	5.69	119.49	113.80
1	B	457	VAL	N-CA-C	5.68	116.41	110.62
1	A	196	ARG	CD-NE-CZ	5.67	132.34	124.40
1	D	373	LEU	CA-C-N	5.66	126.91	119.84
1	D	373	LEU	C-N-CA	5.66	126.91	119.84
1	C	417	ARG	CD-NE-CZ	-5.66	116.48	124.40
1	C	456	LEU	CA-C-O	5.66	126.95	120.90
1	A	114	ARG	NE-CZ-NH2	-5.64	114.13	119.20
1	C	308	VAL	CA-C-N	5.63	125.54	119.85
1	C	308	VAL	C-N-CA	5.63	125.54	119.85
1	C	390	ALA	O-C-N	5.63	129.79	122.87
1	B	119	VAL	N-CA-C	5.63	117.13	111.00
1	B	315	GLN	CA-C-N	-5.62	114.79	122.93
1	B	315	GLN	C-N-CA	-5.62	114.79	122.93
1	D	120	HIS	CA-CB-CG	-5.61	108.19	113.80
1	A	77	VAL	CA-C-O	-5.61	116.08	121.63
1	A	265	ASN	OD1-CG-ND2	5.59	128.19	122.60
1	D	446	ARG	NE-CZ-NH1	5.58	127.08	121.50
1	C	456	LEU	O-C-N	-5.58	116.28	122.09
1	B	483	ASP	CA-C-N	5.57	125.93	119.47
1	B	483	ASP	C-N-CA	5.57	125.93	119.47
1	D	80	ARG	NE-CZ-NH2	5.57	124.21	119.20
1	C	213	PHE	CA-CB-CG	-5.56	108.24	113.80
1	A	456	LEU	O-C-N	-5.56	116.35	122.07
1	A	446	ARG	CD-NE-CZ	5.54	132.16	124.40
1	C	437	ASN	OD1-CG-ND2	5.53	128.13	122.60
1	A	369	ASN	CA-CB-CG	-5.52	107.08	112.60
1	A	150	ASN	OD1-CG-ND2	-5.52	117.08	122.60
1	A	88	PHE	O-C-N	5.51	130.40	123.23
1	A	276	PHE	CA-C-O	5.50	124.93	119.49
1	D	115	PHE	CA-C-N	-5.48	111.89	122.09
1	D	115	PHE	C-N-CA	-5.48	111.89	122.09
1	D	131	PRO	N-CA-C	-5.48	103.19	111.41
1	A	387	GLN	N-CA-C	5.48	116.30	108.74
1	D	246	ASN	OD1-CG-ND2	5.47	128.07	122.60
1	A	115	PHE	CA-C-O	-5.47	114.83	121.28
1	D	354	ARG	CD-NE-CZ	-5.47	116.75	124.40
1	D	122[A]	ASN	CA-C-O	-5.46	112.54	119.31
1	D	122[B]	ASN	CA-C-O	-5.46	112.54	119.31
1	C	476	LEU	CA-C-O	-5.46	114.64	120.42
1	D	173	ASP	CA-C-N	5.46	125.07	119.56
1	D	173	ASP	C-N-CA	5.46	125.07	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	PHE	CA-CB-CG	5.45	119.25	113.80
1	B	218	GLY	CA-C-N	5.45	131.78	121.97
1	B	218	GLY	C-N-CA	5.45	131.78	121.97
1	B	335	ALA	CA-C-N	5.44	125.11	119.56
1	B	335	ALA	C-N-CA	5.44	125.11	119.56
1	A	125	PRO	N-CA-CB	5.42	108.15	103.27
1	C	119	VAL	N-CA-C	5.42	116.90	111.00
1	B	308	VAL	CA-C-N	5.39	125.86	120.14
1	B	308	VAL	C-N-CA	5.39	125.86	120.14
1	B	183	ARG	NH1-CZ-NH2	5.39	126.31	119.30
1	A	459	LYS	CG-CD-CE	5.39	123.70	111.30
1	A	300	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	131	PRO	N-CA-C	-5.36	103.37	111.41
1	C	125	PRO	N-CA-CB	5.36	108.09	103.27
1	D	343	ILE	CA-C-O	5.35	125.55	120.25
1	D	277	PRO	N-CA-CB	5.34	108.33	103.15
1	A	120	HIS	CA-CB-CG	-5.33	108.47	113.80
1	A	153	PRO	CA-C-O	5.31	125.59	118.90
1	A	82	THR	CA-C-O	-5.31	113.75	120.28
1	C	433	THR	CA-C-N	-5.31	115.94	122.84
1	C	433	THR	C-N-CA	-5.31	115.94	122.84
1	C	222	TYR	CA-C-N	-5.30	115.62	123.05
1	C	222	TYR	C-N-CA	-5.30	115.62	123.05
1	C	56	GLN	OE1-CD-NE2	-5.30	117.30	122.60
1	C	223	LYS	CA-CB-CG	5.30	124.69	114.10
1	C	497	ASP	CA-CB-CG	5.29	117.89	112.60
1	D	298	PRO	N-CA-CB	5.25	108.73	103.48
1	C	298	PRO	N-CA-CB	5.25	108.55	103.51
1	C	417	ARG	CA-C-O	-5.25	115.99	121.55
1	A	483	ASP	CA-C-N	5.25	125.05	119.28
1	A	483	ASP	C-N-CA	5.25	125.05	119.28
1	C	327	GLN	O-C-N	5.24	127.68	122.12
1	D	116	SER	CA-C-O	-5.24	115.67	121.28
1	A	80	ARG	NE-CZ-NH1	-5.24	116.27	121.50
1	B	465	ALA	N-CA-C	5.24	120.01	111.37
1	B	439	LYS	N-CA-C	5.22	116.65	111.07
1	B	489	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	D	66	ARG	NE-CZ-NH1	5.21	126.71	121.50
1	B	473	ASN	OD1-CG-ND2	5.21	127.81	122.60
1	A	142	ASP	CB-CA-C	-5.20	101.93	110.72
1	B	116	SER	N-CA-C	5.20	116.18	108.60
1	A	481	LYS	CA-C-N	5.19	127.19	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	481	LYS	C-N-CA	5.19	127.19	120.44
1	C	247	LEU	CA-C-O	-5.19	115.04	120.80
1	B	319	ASN	N-CA-CB	-5.15	104.07	111.54
1	B	408	GLU	O-C-N	-5.15	116.74	121.37
1	D	174	PRO	N-CA-CB	5.13	108.44	103.51
1	C	258	LYS	CB-CA-C	-5.13	100.76	109.38
1	B	434	ARG	CD-NE-CZ	5.11	131.55	124.40
1	A	293	LYS	N-CA-CB	-5.11	101.91	110.39
1	B	304	ILE	N-CA-CB	5.11	117.89	112.07
1	B	459	LYS	CA-CB-CG	-5.11	103.89	114.10
1	C	75	ARG	CD-NE-CZ	5.10	131.55	124.40
1	D	392	ASN	CA-CB-CG	-5.10	107.50	112.60
1	A	40	ASP	CA-CB-CG	5.10	117.70	112.60
1	C	34	ASN	N-CA-CB	5.09	118.23	110.44
1	B	242	GLN	CA-C-O	5.08	125.37	119.32
1	D	199	THR	O-C-N	-5.08	116.73	122.12
1	B	438	PHE	N-CA-CB	-5.06	103.86	110.59
1	A	63	LYS	CA-C-O	-5.06	115.19	120.55
1	D	309	PRO	N-CA-CB	5.03	107.73	103.35
1	C	34	ASN	O-C-N	5.03	129.31	122.37
1	B	342	GLY	N-CA-C	-5.03	108.04	114.37
1	D	434	ARG	CA-C-O	-5.02	114.97	120.70
1	B	341	PRO	N-CA-CB	5.02	107.79	103.27
1	B	142	ASP	CA-CB-CG	5.02	117.62	112.60
1	D	433	THR	N-CA-C	5.02	118.56	112.23
1	A	174	PRO	N-CA-CB	5.02	108.33	103.51
1	B	428	GLN	OE1-CD-NE2	-5.02	117.58	122.60
1	A	114	ARG	NE-CZ-NH1	5.00	126.50	121.50
1	A	298	PRO	N-CA-CB	5.00	108.48	103.48

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123[A]	HIS	Mainchain
1	D	123[B]	HIS	Mainchain

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	3820	0	3732	47	0
1	B	3810	0	3723	52	0
1	C	3810	0	3723	43	0
1	D	3820	0	3732	31	0
2	A	43	0	30	2	0
2	B	43	0	30	0	0
2	C	43	0	30	0	0
2	D	43	0	30	0	0
3	A	602	0	0	13	0
3	B	475	0	0	11	0
3	C	438	0	0	9	0
3	D	614	0	0	8	0
All	All	17561	0	15030	161	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (161) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ARG:NH2	1:A:459:LYS:HD2	1.74	1.00
1:A:249:PRO:HG3	1:A:459:LYS:HD3	1.48	0.94
1:A:407:LEU:HD21	1:B:468:LEU:HD22	1.48	0.94
1:C:249:PRO:HG3	1:C:459:LYS:HD3	1.53	0.91
1:C:129:ARG:NH2	1:C:459:LYS:HD2	1.89	0.87
1:A:204:ASN:OD1	1:A:459:LYS:NZ	2.10	0.85
1:A:129:ARG:HH22	1:A:459:LYS:HD2	1.40	0.84
1:B:249:PRO:HG3	1:B:459:LYS:HD2	1.61	0.83
1:D:468:LEU:HD23	3:D:1279:HOH:O	1.79	0.83
1:B:248:ASP:HB2	1:B:249:PRO:HD2	1.64	0.80
1:C:202:TYR:O	1:C:459:LYS:HE3	1.82	0.79
1:A:468:LEU:HD23	3:A:1283:HOH:O	1.82	0.78
1:C:468:LEU:HD11	1:D:406:ARG:HD2	1.65	0.77
1:A:468:LEU:HD13	3:A:2289:HOH:O	1.85	0.75
1:D:468:LEU:HD21	1:D:471:SER:OG	1.87	0.75
1:A:87:GLU:OE2	1:A:108:LYS:HG2	1.88	0.73
1:D:245:LYS:HE3	3:D:2730:HOH:O	1.87	0.73
1:C:129:ARG:HH22	1:C:459:LYS:HD2	1.53	0.72
1:B:468:LEU:HD23	3:B:1872:HOH:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:LEU:HD21	1:A:471:SER:OG	1.91	0.71
1:D:468:LEU:HD13	3:D:2543:HOH:O	1.92	0.70
1:A:406:ARG:HD2	1:B:468:LEU:HD11	1.73	0.69
1:A:468:LEU:HD11	1:B:406:ARG:HD2	1.73	0.69
1:A:468:LEU:CD1	1:A:471:SER:H	2.06	0.67
1:B:204:ASN:OD1	1:B:459:LYS:NZ	2.28	0.66
1:D:468:LEU:HD11	1:D:471:SER:H	1.60	0.65
1:C:406:ARG:HD2	1:D:468:LEU:HD11	1.79	0.65
1:C:468:LEU:HD23	3:C:2178:HOH:O	1.95	0.65
1:A:468:LEU:HD11	1:A:471:SER:H	1.62	0.63
1:B:468:LEU:HD21	1:B:471:SER:OG	1.99	0.63
1:B:129:ARG:NH2	1:B:459:LYS:HE3	2.14	0.63
1:B:249:PRO:HG3	1:B:459:LYS:CD	2.29	0.63
1:B:154:THR:HG21	1:B:196:ARG:HD3	1.81	0.62
1:C:468:LEU:HD21	1:C:471:SER:OG	1.99	0.61
1:D:468:LEU:CD1	1:D:471:SER:H	2.13	0.61
1:A:278:LYS:HE3	3:A:2622:HOH:O	2.02	0.60
1:A:249:PRO:CG	1:A:459:LYS:HD3	2.28	0.60
1:A:289:GLU:H	1:A:289:GLU:CD	2.10	0.60
1:B:320:LYS:HD2	3:B:2814:HOH:O	2.00	0.59
1:C:163:PHE:HB3	1:C:164:PRO:HD3	1.83	0.59
1:C:204:ASN:OD1	1:C:459:LYS:NZ	2.23	0.59
1:B:59:GLN:HB3	3:B:2644:HOH:O	2.03	0.59
1:C:224:LEU:HD12	1:C:234:VAL:HG21	1.85	0.59
1:C:431:LYS:HD2	1:C:432:ILE:O	2.02	0.59
1:A:27:THR:HG21	3:C:2240:HOH:O	2.03	0.58
1:B:290:GLU:HA	1:B:293:LYS:HD2	1.86	0.57
1:D:78:HIS:CE1	1:D:118:VAL:HG22	2.40	0.57
1:B:409:PRO:O	1:D:27:THR:HG21	2.05	0.57
1:A:344:GLU:HB3	1:A:345:PRO:HD2	1.86	0.57
1:C:78:HIS:CE1	1:C:118:VAL:HG22	2.41	0.56
1:A:135:ALA:N	3:A:3059:HOH:O	2.39	0.56
1:B:224:LEU:HD12	1:B:234:VAL:HG21	1.87	0.55
1:B:80:ARG:HD3	1:B:122[B]:ASN:O	2.06	0.55
1:B:139:TYR:HB3	1:B:379:LYS:HG3	1.88	0.55
1:C:98:SER:HB2	1:C:224:LEU:HB3	1.88	0.54
1:B:40:ASP:OD2	1:D:417:ARG:NH2	2.40	0.54
1:B:202:TYR:O	1:B:459:LYS:HE2	2.07	0.54
1:A:202:TYR:O	1:A:459:LYS:HE2	2.09	0.53
1:B:287:LYS:HB2	1:B:290:GLU:HG3	1.90	0.53
1:B:277:PRO:HD2	1:B:318:LEU:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:ASP:OD1	1:C:415:LYS:HG2	2.07	0.53
1:B:417:ARG:NH2	1:D:40:ASP:OD2	2.41	0.53
1:D:80:ARG:HD3	1:D:122[A]:ASN:O	2.08	0.53
1:C:248:ASP:HB2	1:C:249:PRO:HD2	1.90	0.53
1:C:344:GLU:HB3	1:C:345:PRO:HD2	1.91	0.52
1:A:78:HIS:CE1	1:A:118:VAL:HG22	2.45	0.52
1:B:133:GLY:HA2	1:B:150:ASN:OD1	2.10	0.52
1:A:287:LYS:HB2	1:A:290:GLU:HG3	1.91	0.52
1:A:448:TYR:O	1:A:453:LYS:NZ	2.43	0.52
1:B:129:ARG:HH22	1:B:459:LYS:HE3	1.73	0.52
1:B:223:LYS:HG2	1:B:231:VAL:HG13	1.91	0.52
1:C:468:LEU:HG	1:C:468:LEU:O	2.08	0.51
1:A:455:ASP:HB3	1:A:459:LYS:NZ	2.25	0.51
1:D:454:THR:HG22	3:D:2503:HOH:O	2.11	0.51
1:A:202:TYR:O	1:A:459:LYS:CE	2.58	0.51
1:A:162:LYS:HD3	1:D:42:GLN:HA	1.93	0.51
1:C:289:GLU:HG3	3:C:2320:HOH:O	2.10	0.51
1:B:162:LYS:HD3	1:C:42:GLN:HA	1.92	0.50
1:D:254:GLN:HG2	3:D:2793:HOH:O	2.12	0.50
1:C:481:LYS:NZ	3:C:2272:HOH:O	2.28	0.50
1:A:139:TYR:HB3	1:A:379:LYS:HG2	1.92	0.50
3:B:2232:HOH:O	1:D:27:THR:HG22	2.12	0.50
1:C:355:VAL:HB	3:C:2917:HOH:O	2.10	0.50
1:C:211:TYR:CE1	1:C:263:LEU:HD13	2.47	0.49
2:A:600:HEM:HMA2	3:A:3059:HOH:O	2.12	0.49
1:B:468:LEU:CD1	1:B:471:SER:H	2.24	0.49
1:D:455:ASP:O	1:D:459:LYS:HG2	2.12	0.49
1:C:139:TYR:HB3	1:C:379:LYS:HG2	1.95	0.49
1:B:304:ILE:O	1:B:306:PRO:HD3	2.13	0.49
1:D:122[B]:ASN:HB2	3:D:1685:HOH:O	2.12	0.49
1:D:458:GLN:HB3	1:D:459:LYS:HE2	1.95	0.49
1:A:42:GLN:HA	1:D:162:LYS:HD3	1.94	0.48
1:B:183:ARG:HD3	3:B:1133:HOH:O	2.12	0.48
1:B:448:TYR:O	1:B:453:LYS:NZ	2.46	0.48
1:C:122[B]:ASN:H	1:C:122[B]:ASN:HD22	1.59	0.48
1:C:160:ALA:CB	1:C:353:GLY:HA3	2.43	0.48
1:A:122[A]:ASN:HB3	3:A:3126:HOH:O	2.11	0.48
1:C:509:LYS:HD3	3:C:2510:HOH:O	2.14	0.47
1:C:438:PHE:CD1	1:C:481:LYS:HG2	2.50	0.47
1:D:57:ASP:O	1:D:61:LEU:HD23	2.15	0.47
1:C:80:ARG:HD3	1:C:122[A]:ASN:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:457:VAL:HG11	1:D:489:ARG:HB3	1.96	0.46
1:A:417:ARG:NH2	1:C:40:ASP:OD2	2.49	0.46
1:A:455:ASP:HB3	1:A:459:LYS:HZ3	1.81	0.46
1:C:248:ASP:OD2	1:C:251:GLU:HG3	2.15	0.46
1:B:421:LEU:HA	1:B:422:PRO:HD3	1.84	0.46
1:B:207:THR:HG21	1:B:252:VAL:HG21	1.97	0.46
1:B:50:GLN:HG2	3:B:2549:HOH:O	2.16	0.46
1:D:78:HIS:HA	1:D:117:SER:O	2.16	0.46
1:B:122[A]:ASN:HB2	3:B:3127:HOH:O	2.17	0.45
1:C:502:LYS:HE2	3:C:2647:HOH:O	2.15	0.45
1:D:249:PRO:HG2	1:D:459:LYS:HE3	1.99	0.45
1:D:27:THR:HG22	1:D:28:ASP:N	2.32	0.45
1:C:181:ASP:O	1:C:184:ARG:HG2	2.16	0.45
1:C:371:LEU:HD22	3:C:2054:HOH:O	2.16	0.45
1:B:130:ASP:HB3	1:B:131:PRO:O	2.17	0.45
1:A:174:PRO:HG2	1:B:399:GLY:HA2	1.98	0.45
1:A:248:ASP:OD2	1:A:251:GLU:HG3	2.17	0.45
1:B:37:VAL:HG22	3:D:1053:HOH:O	2.18	0.44
1:C:104:LYS:O	1:C:105:SER:C	2.60	0.44
1:A:223:LYS:HG3	1:A:231:VAL:HG13	1.97	0.44
1:A:234:VAL:HG13	1:A:283:VAL:HB	1.99	0.44
1:A:371:LEU:HD13	3:A:2998:HOH:O	2.17	0.44
1:B:468:LEU:HD11	1:B:471:SER:H	1.81	0.44
1:B:273:LYS:HA	1:B:273:LYS:HD3	1.73	0.43
1:C:183:ARG:HD3	3:C:1011:HOH:O	2.18	0.43
1:B:139:TYR:HB3	1:B:379:LYS:CG	2.47	0.43
1:B:460:PHE:O	1:B:464:LEU:HB2	2.18	0.43
1:D:344:GLU:HB3	1:D:345:PRO:HD2	1.99	0.43
3:B:2393:HOH:O	1:D:27:THR:HG21	2.17	0.43
1:A:50:GLN:HG2	3:A:2821:HOH:O	2.19	0.43
1:A:163:PHE:HB3	1:A:164:PRO:HD3	2.01	0.43
1:B:455:ASP:O	1:B:459:LYS:HD3	2.18	0.43
1:D:87:GLU:OE2	1:D:108:LYS:HG2	2.18	0.43
1:A:319:ASN:C	1:A:319:ASN:HD22	2.26	0.42
1:C:223:LYS:HG3	1:C:344:GLU:HB2	2.00	0.42
1:B:228:LYS:HZ3	1:B:230:GLU:CD	2.27	0.42
1:B:228:LYS:NZ	1:B:230:GLU:OE2	2.52	0.42
1:C:340:VAL:HB	1:C:341:PRO:HD2	2.00	0.42
1:D:431:LYS:HB2	1:D:431:LYS:NZ	2.34	0.42
1:A:503:SER:HB2	3:A:3043:HOH:O	2.18	0.42
1:C:220:HIS:CD2	1:C:351:LEU:HD13	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:PRO:HG3	3:A:2988:HOH:O	2.19	0.42
3:B:2127:HOH:O	1:C:50:GLN:HG3	2.19	0.42
1:A:40:ASP:OD2	1:C:417:ARG:NH2	2.54	0.41
1:B:223:LYS:CG	1:B:231:VAL:HG13	2.51	0.41
1:C:304:ILE:O	1:C:306:PRO:HD3	2.20	0.41
1:A:235:LYS:HE3	1:A:305:TRP:NE1	2.35	0.41
1:B:344:GLU:HB3	1:B:345:PRO:HD2	2.02	0.41
1:A:245:LYS:HE3	1:A:245:LYS:HB2	1.82	0.41
1:A:439:LYS:NZ	3:A:2655:HOH:O	2.53	0.41
1:B:295:ASP:OD2	1:B:436:GLN:NE2	2.53	0.41
1:A:379:LYS:NZ	3:A:2669:HOH:O	2.53	0.41
1:A:468:LEU:HD11	1:A:471:SER:N	2.34	0.40
1:B:431:LYS:HG2	3:B:2023:HOH:O	2.21	0.40
1:D:435:GLU:O	1:D:436:GLN:C	2.64	0.40
1:B:224:LEU:CD1	1:B:234:VAL:HG21	2.51	0.40
1:B:341:PRO:HG3	3:D:2185:HOH:O	2.21	0.40
2:A:600:HEM:CMA	3:A:3059:HOH:O	2.68	0.40
1:B:258:LYS:HB2	3:B:2093:HOH:O	2.21	0.40
1:C:435:GLU:O	1:C:436:GLN:C	2.63	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	485/484 (100%)	472 (97%)	13 (3%)	0	100	100
1	B	484/484 (100%)	468 (97%)	16 (3%)	0	100	100
1	C	484/484 (100%)	476 (98%)	8 (2%)	0	100	100
1	D	485/484 (100%)	473 (98%)	12 (2%)	0	100	100
All	All	1938/1936 (100%)	1889 (98%)	49 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	414/414 (100%)	396 (96%)	18 (4%)	26	13
1	B	412/414 (100%)	400 (97%)	12 (3%)	37	25
1	C	412/414 (100%)	404 (98%)	8 (2%)	50	41
1	D	414/414 (100%)	400 (97%)	14 (3%)	32	20
All	All	1652/1656 (100%)	1600 (97%)	52 (3%)	35	23

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	ASP
1	A	122[A]	ASN
1	A	122[B]	ASN
1	A	127	THR
1	A	130	ASP
1	A	225	VAL
1	A	228	LYS
1	A	231	VAL
1	A	258	LYS
1	A	278	LYS
1	A	293	LYS
1	A	319	ASN
1	A	320	LYS
1	A	379	LYS
1	A	415	LYS
1	A	431	LYS
1	A	457	VAL
1	A	464	LEU
1	B	96	ASP
1	B	140	THR
1	B	225	VAL
1	B	258	LYS

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Mol	Chain	Res	Type
1	B	289	GLU
1	B	312	LYS
1	B	319	ASN
1	B	320	LYS
1	B	374	PRO
1	B	379	LYS
1	B	464	LEU
1	B	468	LEU
1	C	108	LYS
1	C	127	THR
1	C	130	ASP
1	C	140	THR
1	C	228	LYS
1	C	289	GLU
1	C	319	ASN
1	C	468	LEU
1	D	96	ASP
1	D	140	THR
1	D	225	VAL
1	D	228	LYS
1	D	258	LYS
1	D	289	GLU
1	D	319	ASN
1	D	415	LYS
1	D	431	LYS
1	D	451	LYS
1	D	457	VAL
1	D	459	LYS
1	D	464	LEU
1	D	468	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	GLN
1	A	315	GLN
1	A	319	ASN
1	A	428	GLN
1	B	43	ASN
1	C	43	ASN
1	C	319	ASN
1	C	485	ASN

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Mol	Chain	Res	Type
1	D	43	ASN
1	D	256	GLN
1	D	315	GLN
1	D	319	ASN
1	D	369	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 oligosaccharides 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	A	600	1,3	50,50,50	1.43	10 (20%)	67,82,82	1.28	5 (7%)
2	HEM	B	600	1,3	50,50,50	1.37	7 (14%)	67,82,82	1.07	4 (5%)
2	HEM	C	600	1,3	50,50,50	1.25	7 (14%)	67,82,82	1.14	6 (8%)
2	HEM	D	600	1,3	50,50,50	1.32	7 (14%)	67,82,82	1.02	3 (4%)

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	A	600	1,3	-	4/14/54/54	-
2	HEM	B	600	1,3	-	2/14/54/54	-
2	HEM	C	600	1,3	-	2/14/54/54	-
2	HEM	D	600	1,3	-	2/14/54/54	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	HEM	FE-ND	3.20	2.04	1.94
2	C	600	HEM	FE-ND	2.86	2.03	1.94
2	C	600	HEM	FE-NB	2.79	2.03	1.94
2	D	600	HEM	FE-NB	2.77	2.03	1.94
2	D	600	HEM	FE-ND	2.75	2.03	1.94
2	A	600	HEM	CAC-C3C	2.70	1.54	1.47
2	B	600	HEM	CAB-C3B	2.67	1.54	1.47
2	C	600	HEM	CAC-C3C	2.67	1.54	1.47
2	B	600	HEM	FE-NB	2.66	2.03	1.94
2	C	600	HEM	CAB-C3B	2.64	1.54	1.47
2	D	600	HEM	FE-NC	2.53	2.03	1.95
2	B	600	HEM	CAC-C3C	2.53	1.54	1.47
2	A	600	HEM	FE-NB	2.50	2.02	1.94
2	D	600	HEM	CAB-C3B	2.47	1.54	1.47
2	A	600	HEM	FE-NA	2.47	2.03	1.95
2	B	600	HEM	C4D-ND	-2.45	1.36	1.40
2	B	600	HEM	CMC-C2C	2.43	1.55	1.50
2	A	600	HEM	CMC-C2C	2.40	1.55	1.50
2	B	600	HEM	CMA-C3A	2.24	1.55	1.50
2	A	600	HEM	CAB-C3B	2.23	1.53	1.47
2	A	600	HEM	CBA-CGA	2.20	1.55	1.50
2	D	600	HEM	CAC-C3C	2.18	1.53	1.47
2	A	600	HEM	FE-ND	2.15	2.01	1.94
2	A	600	HEM	FE-NC	2.14	2.02	1.95
2	C	600	HEM	CAD-C3D	2.11	1.56	1.51
2	D	600	HEM	CMB-C2B	2.07	1.55	1.50
2	C	600	HEM	CMB-C2B	2.07	1.55	1.50
2	D	600	HEM	CMD-C2D	2.06	1.55	1.50
2	C	600	HEM	C2A-C3A	-2.06	1.33	1.38
2	A	600	HEM	C1A-C2A	2.06	1.48	1.44
2	A	600	HEM	C2A-C3A	-2.02	1.33	1.38

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	HEM	O2A-CGA-O1A	4.25	134.26	123.33
2	A	600	HEM	O1A-CGA-CBA	-3.23	112.86	123.09
2	D	600	HEM	CHC-C1C-NC	2.88	127.59	124.45
2	A	600	HEM	O2D-CGD-CBD	2.80	122.85	114.00
2	A	600	HEM	CHD-C1D-ND	2.80	127.44	124.42
2	C	600	HEM	CHD-C1D-ND	2.67	127.30	124.42
2	B	600	HEM	C4D-ND-C1D	2.59	108.28	105.21
2	B	600	HEM	O1A-CGA-CBA	-2.56	114.99	123.09
2	C	600	HEM	CMA-C3A-C2A	2.49	130.91	125.62
2	C	600	HEM	CMA-C3A-C4A	-2.49	121.63	125.42
2	C	600	HEM	C4D-ND-C1D	2.37	108.01	105.21
2	B	600	HEM	CBC-CAC-C3C	-2.30	116.02	127.53
2	A	600	HEM	O1D-CGD-CBD	-2.30	115.79	123.09
2	B	600	HEM	CHD-C1D-ND	2.29	126.89	124.42
2	D	600	HEM	O1D-CGD-CBD	-2.22	116.05	123.09
2	C	600	HEM	O1A-CGA-CBA	-2.21	116.09	123.09
2	C	600	HEM	C1B-NB-C4B	2.16	107.76	105.21
2	D	600	HEM	C2A-C1A-NA	-2.08	107.84	110.15

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	HEM	CAA-CBA-CGA-O2A
2	A	600	HEM	CAA-CBA-CGA-O1A
2	B	600	HEM	CAA-CBA-CGA-O1A
2	C	600	HEM	CAA-CBA-CGA-O1A
2	D	600	HEM	CAA-CBA-CGA-O2A
2	C	600	HEM	CAA-CBA-CGA-O2A
2	B	600	HEM	CAA-CBA-CGA-O2A
2	D	600	HEM	CAA-CBA-CGA-O1A
2	A	600	HEM	CAD-CBD-CGD-O2D
2	A	600	HEM	CAD-CBD-CGD-O1D

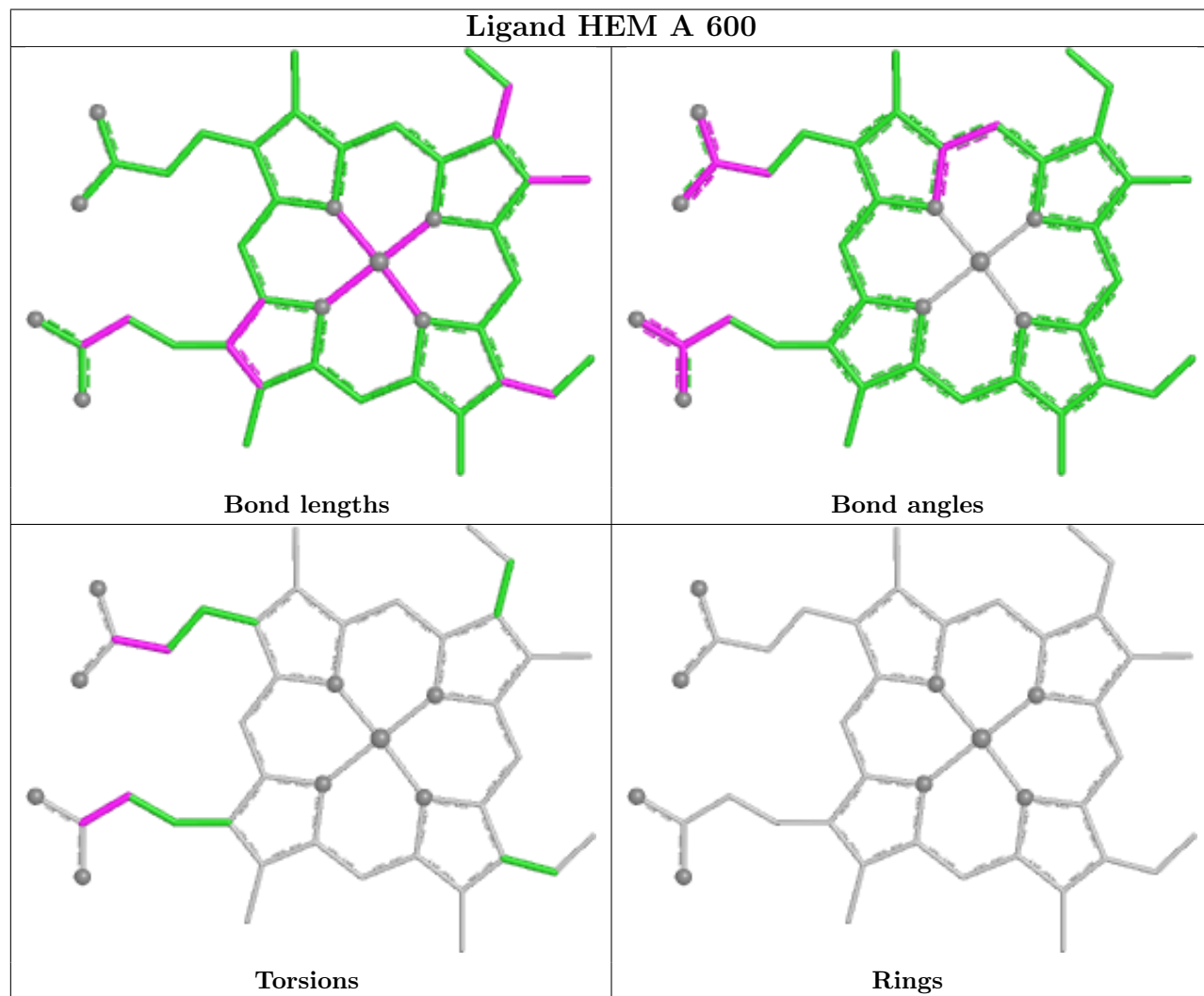
There are no ring outliers.

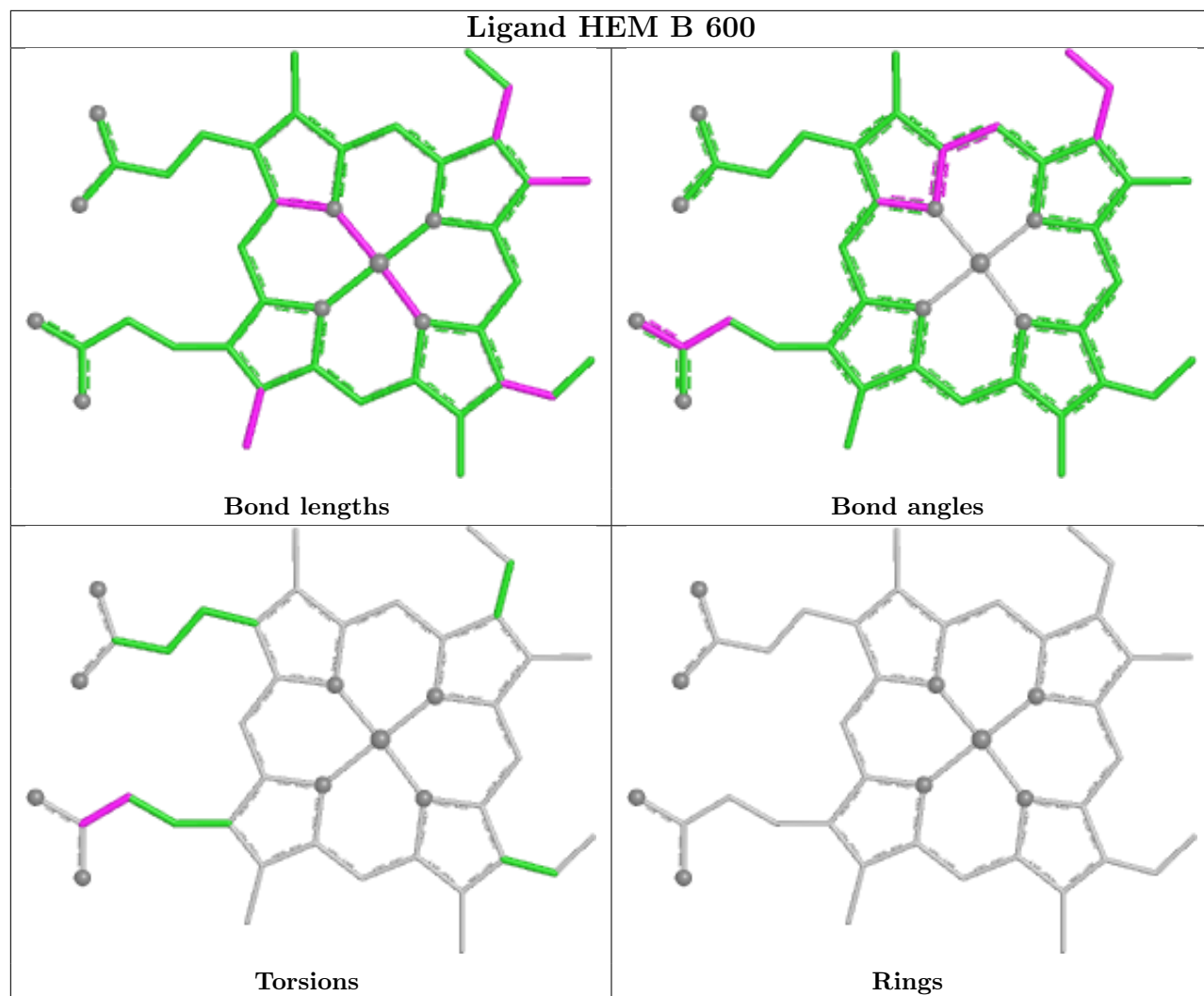
1 monomer is involved in 2 short contacts:

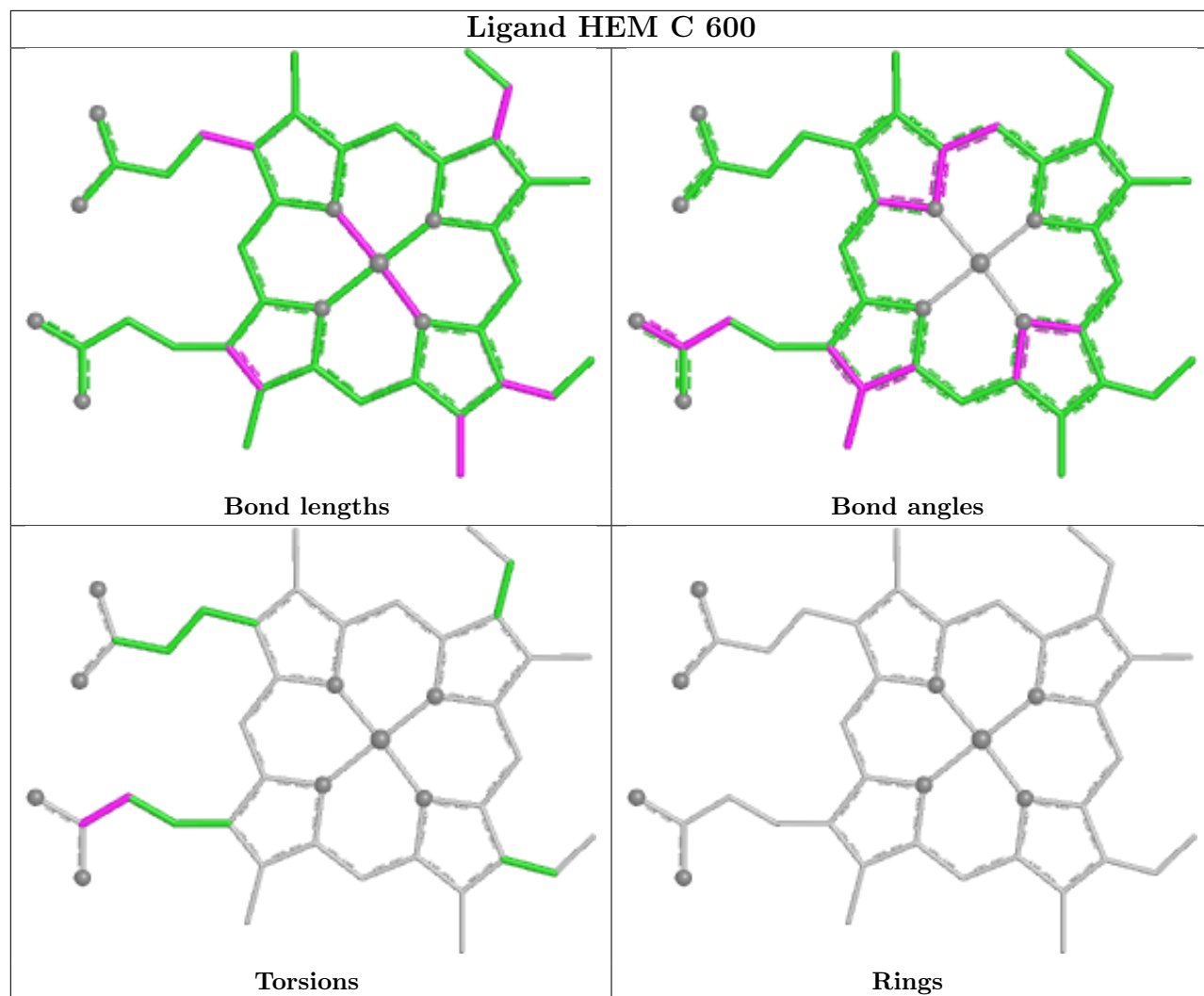
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	HEM	2	0

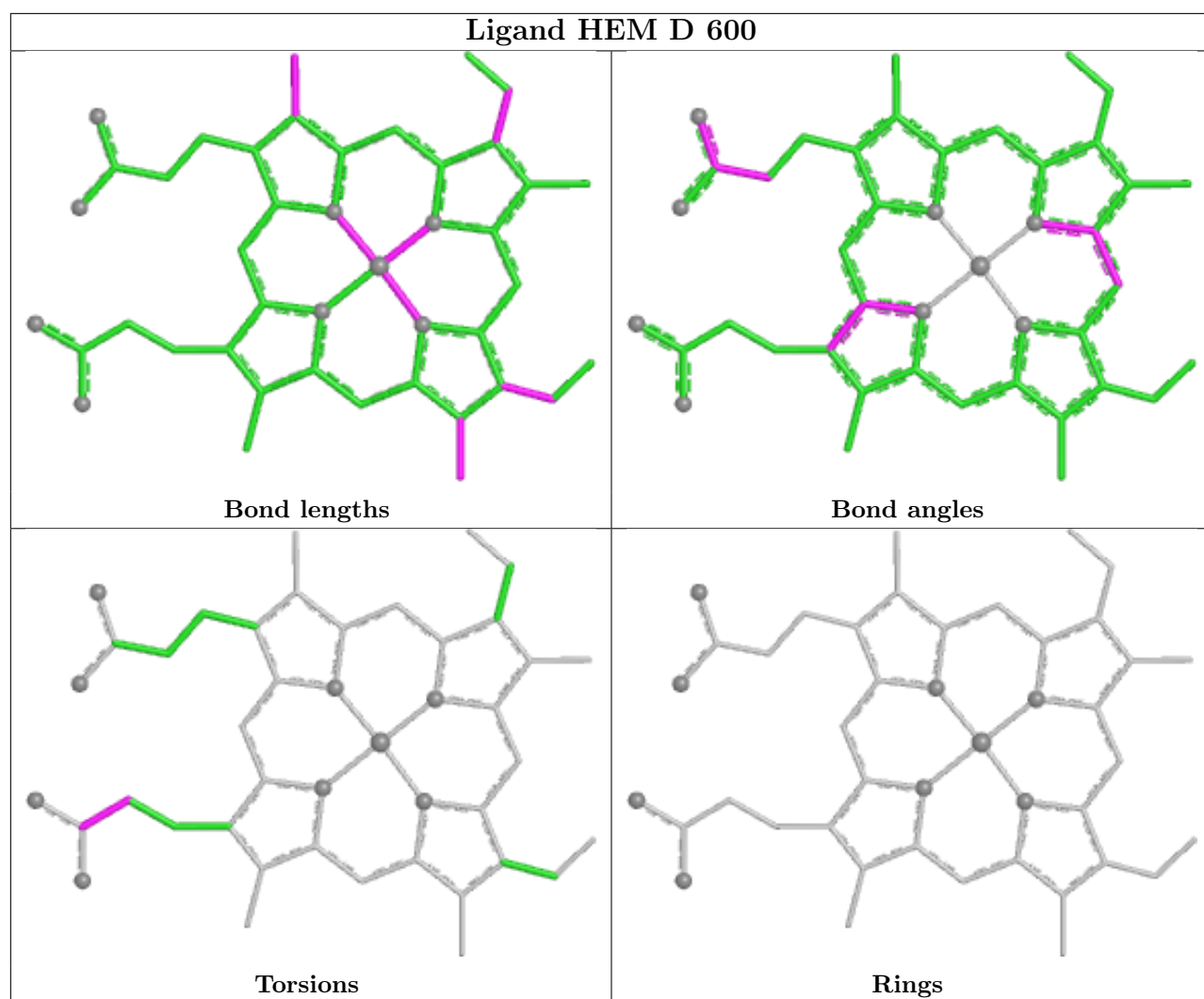
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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	484/484 (100%)	-0.43	5 (1%) 79 80	5, 12, 24, 39	3 (0%)
1	B	483/484 (99%)	0.19	8 (1%) 69 69	5, 20, 34, 51	3 (0%)
1	C	483/484 (99%)	0.12	5 (1%) 79 80	8, 20, 33, 47	3 (0%)
1	D	484/484 (100%)	-0.48	6 (1%) 76 77	4, 11, 23, 43	3 (0%)
All	All	1934/1936 (99%)	-0.15	24 (1%) 76 77	4, 15, 31, 51	12 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	510	ASP	3.8
1	D	27	THR	3.0
1	A	87	GLU	3.0
1	A	510	ASP	2.9
1	A	27	THR	2.8
1	A	466	ASP	2.7
1	C	466	ASP	2.6
1	D	307	ASP	2.6
1	C	122[A]	ASN	2.6
1	B	96	ASP	2.5
1	B	510	ASP	2.4
1	B	466	ASP	2.4
1	C	497	ASP	2.4
1	B	508	LEU	2.3
1	B	121[A]	GLY	2.3
1	B	480	TYR	2.3
1	D	510	ASP	2.3
1	C	254	GLN	2.3
1	D	96	ASP	2.2
1	D	122[A]	ASN	2.2
1	D	254	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	494	ALA	2.1
1	A	96	ASP	2.0
1	B	294	PHE	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](#)

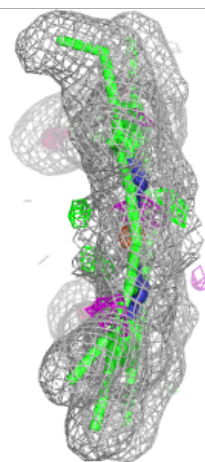
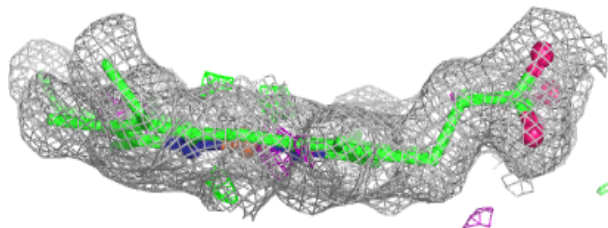
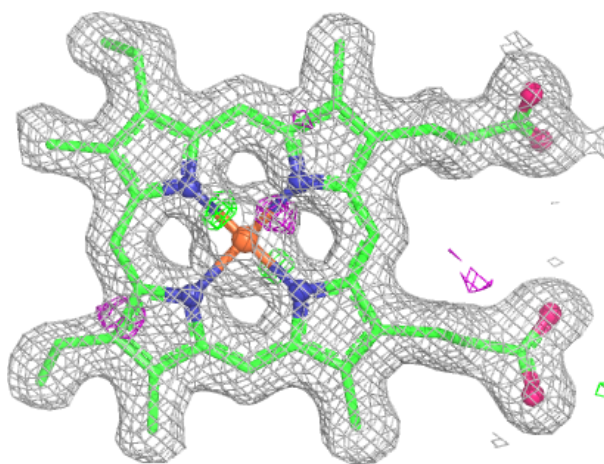
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	HEM	B	600	43/43	0.97	0.06	9,14,17,19	0
2	HEM	A	600	43/43	0.98	0.05	4,7,12,14	0
2	HEM	C	600	43/43	0.98	0.06	8,14,18,20	0
2	HEM	D	600	43/43	0.98	0.05	3,7,12,15	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.

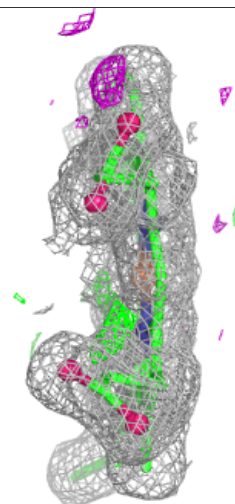
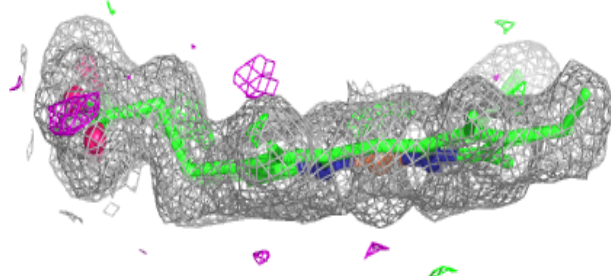
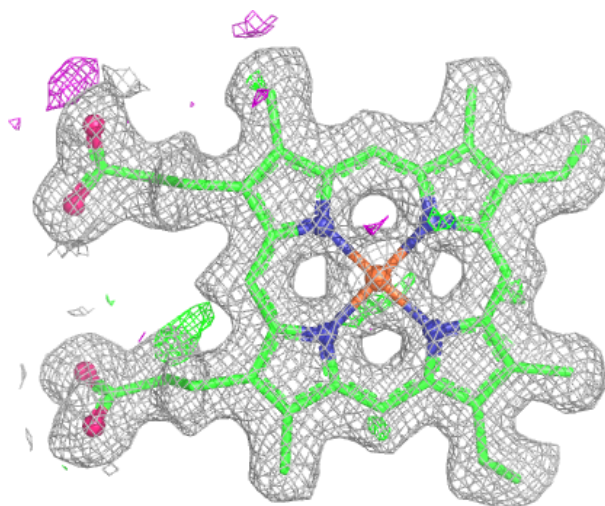
Electron density around HEM B 600:

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



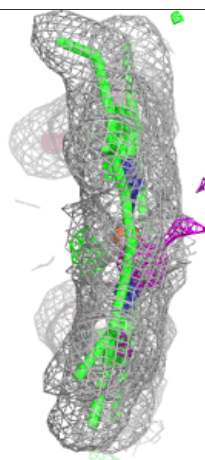
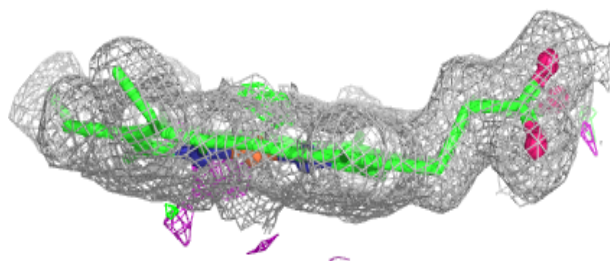
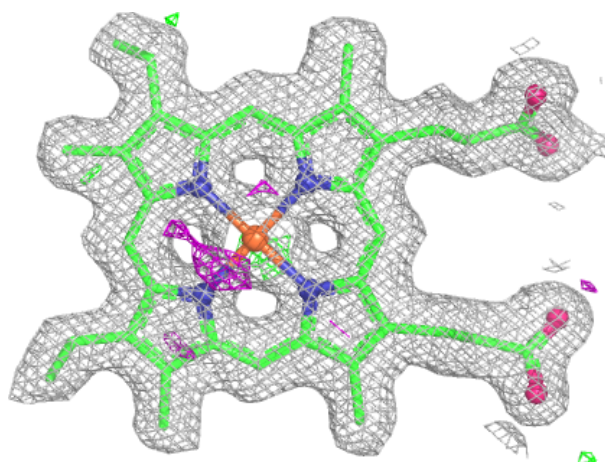
Electron density around HEM A 600:

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



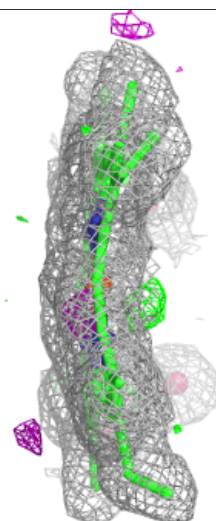
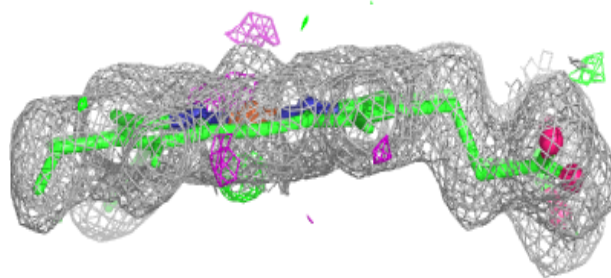
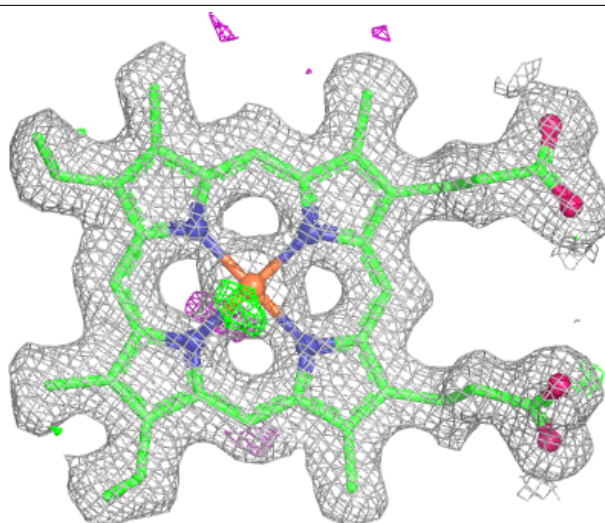
Electron density around HEM C 600:

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



Electron density around HEM D 600:

$2mF_o-DF_c$ (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.