Full wwPDB X-ray Structure Validation Report (i)

Aug 25, 2020 – 05:50 PM BST

PDB ID	:	3P9P
Title	:	Structure of I274V variant of E. coli KatE
Authors	:	Loewen, P.C.; Jha, V.; Louis, S.; Chelikani, P.; Carpena, X.; Fita, I.
Deposited on	:	2010-10-18
Resolution	:	1.50 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 following versions of software and data (see references (i)) were used in the production of this report:

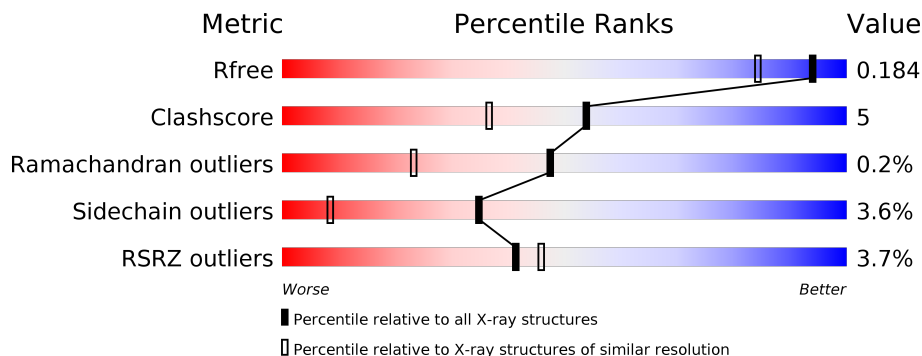|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

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 1.50 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	Percentile Ranks	Value
Rfree		0.184
Clashscore		5
Ramachandran outliers		0.2%
Sidechain outliers		3.6%
RSRZ outliers		3.7%

Worse *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 on 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	3% / 84% / 10%
1	B	753	5% / 82% / 12%
1	C	753	4% / 84% / 11%
1	D	753	2% / 84% / 12%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 27001 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	726	Total 5764	C 3658	N 1011	O 1083	S 12	0	5	0
1	B	726	Total 5749	C 3649	N 1007	O 1081	S 12	0	3	0
1	C	726	Total 5766	C 3661	N 1008	O 1085	S 12	0	5	0
1	D	726	Total 5757	C 3652	N 1008	O 1085	S 12	0	6	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	274	VAL	ILE	ENGINEERED MUTATION	UNP P21179
B	274	VAL	ILE	ENGINEERED MUTATION	UNP P21179
C	274	VAL	ILE	ENGINEERED MUTATION	UNP P21179
D	274	VAL	ILE	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	1
			43	34	1	4	4		
2	A	1	Total	C	Fe	N	O	0	1
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	1
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	1
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	1
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	1
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	1
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	1
			43	34	1	4	4		

- Molecule 3 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE 17R, 18S (three-letter code: HDE) (formula: $C_{34}H_{38}FeN_4O_5$).

HDE

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		
3	B	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		
3	C	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		
3	D	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		

- Molecule 4 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (three-letter code: HDD) (formula: $C_{34}H_{32}FeN_4O_5$).

HDD

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 44	C 34	Fe 1	N 4	O 5	0	1
4	B	1	Total 44	C 34	Fe 1	N 4	O 5	0	1
4	C	1	Total 44	C 34	Fe 1	N 4	O 5	0	1
4	D	1	Total 44	C 34	Fe 1	N 4	O 5	0	1

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	842	Total 842	O 842	0	0
5	B	754	Total 754	O 754	0	0
5	C	807	Total 807	O 807	0	0
5	D	866	Total 866	O 866	0	0

3 Residue-property plots ⓘ

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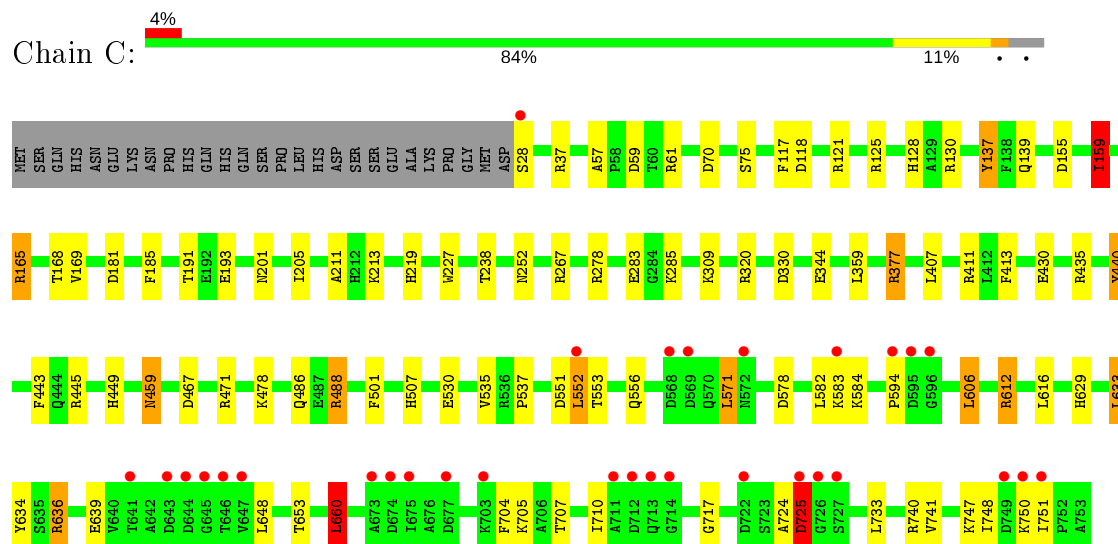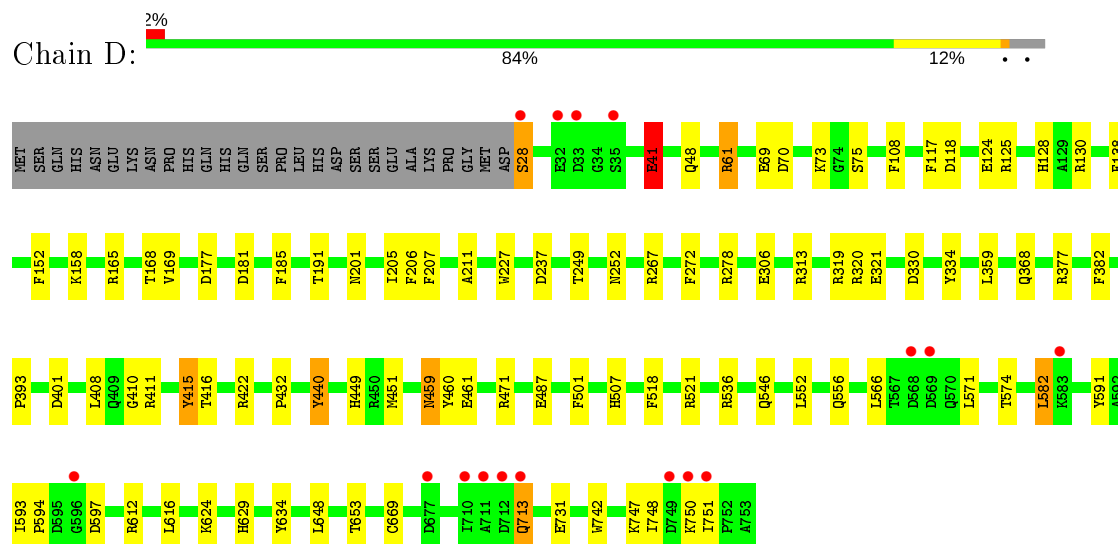
- Molecule 1: Catalase HPII
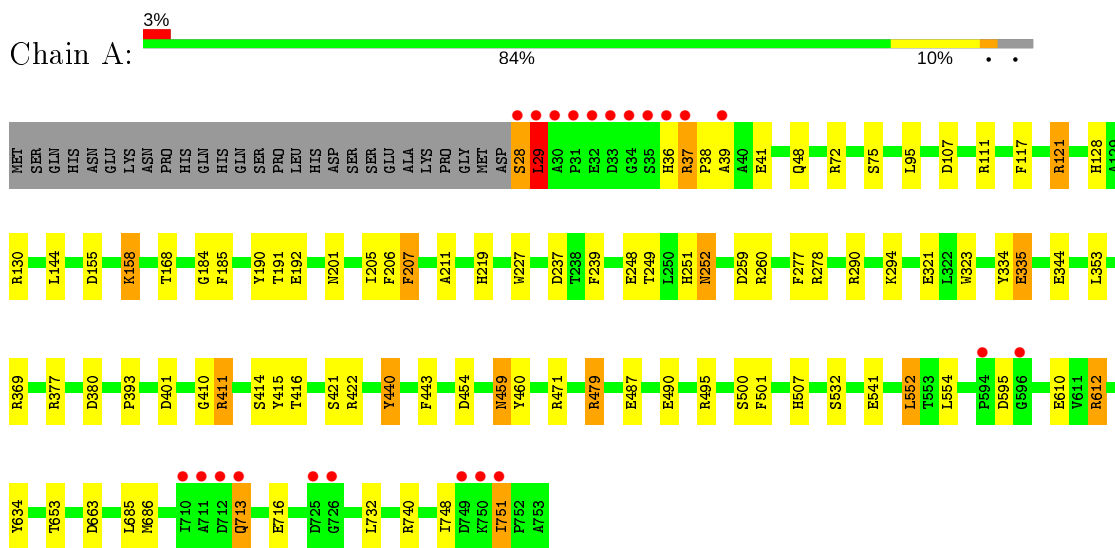
- Molecule 1: Catalase HPII

● Molecule 1: Catalase HPII

Chain C:

● Molecule 1: Catalase HPII

Chain D:
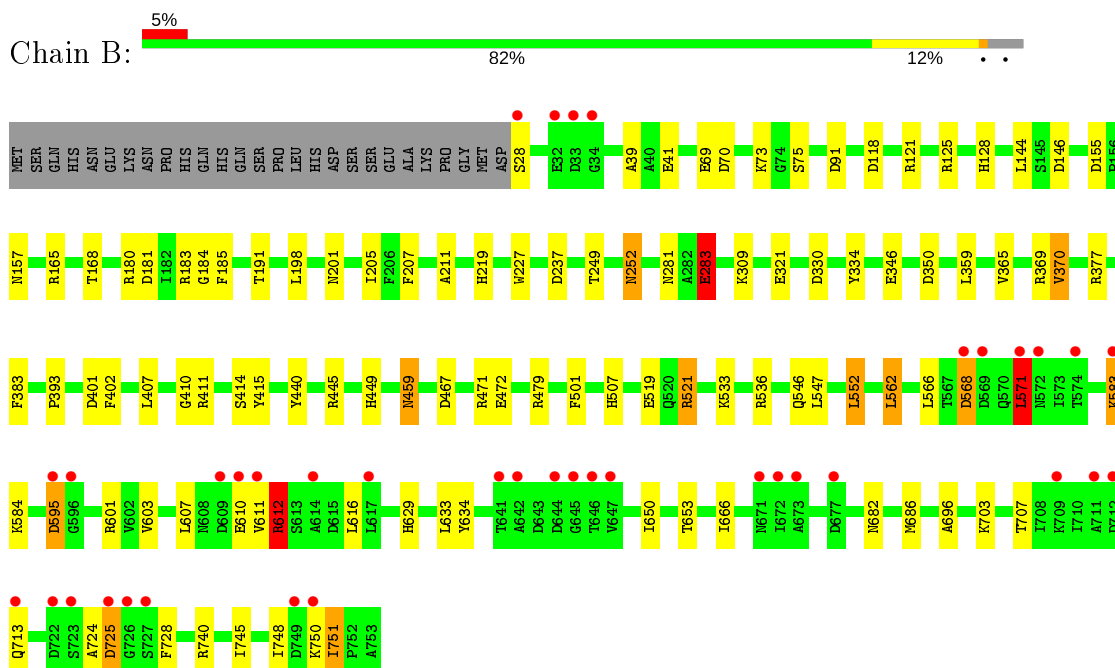
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.50Å 132.82Å 122.59Å 90.00° 109.47° 90.00°	Depositor
Resolution (Å)	29.16 – 1.50 29.16 – 1.50	Depositor EDS
% Data completeness (in resolution range)	94.8 (29.16-1.50) 94.8 (29.16-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.81 (at 1.50Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.149 , 0.185 0.148 , 0.184	Depositor DCC
R_{free} test set	21394 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	9.4	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 40.4	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	27001	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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, HDE, HDD

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	1.31	19/5937 (0.3%)	1.21	39/8071 (0.5%)
1	B	1.27	12/5918 (0.2%)	1.19	35/8046 (0.4%)
1	C	1.27	10/5940 (0.2%)	1.18	31/8076 (0.4%)
1	D	1.33	22/5938 (0.4%)	1.20	30/8073 (0.4%)
All	All	1.30	63/23733 (0.3%)	1.20	135/32266 (0.4%)

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	C	1	2
All	All	1	3

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	440	TYR	CE1-CZ	9.19	1.50	1.38
1	D	41	GLU	CG-CD	8.82	1.65	1.51
1	B	321	GLU	CB-CG	8.13	1.67	1.52
1	A	321	GLU	CD-OE1	6.96	1.33	1.25
1	A	440	TYR	CE1-CZ	6.91	1.47	1.38
1	B	283	GLU	CG-CD	6.79	1.62	1.51
1	A	334	TYR	CD1-CE1	6.56	1.49	1.39
1	A	377	ARG	CZ-NH1	6.49	1.41	1.33
1	B	521	ARG	CG-CD	6.43	1.68	1.51
1	C	530	GLU	CD-OE1	6.37	1.32	1.25
1	D	272	PHE	CG-CD1	6.33	1.48	1.38
1	C	137	TYR	CD2-CE2	6.31	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	321	GLU	CD-OE1	6.26	1.32	1.25
1	D	518	PHE	CD2-CE2	6.25	1.51	1.39
1	D	69	GLU	CG-CD	5.93	1.60	1.51
1	B	69	GLU	CB-CG	5.83	1.63	1.52
1	A	323	TRP	CE3-CZ3	5.76	1.48	1.38
1	C	344	GLU	CG-CD	5.70	1.60	1.51
1	A	460	TYR	CD2-CE2	5.66	1.47	1.39
1	C	344	GLU	CD-OE1	5.66	1.31	1.25
1	D	591	TYR	CE2-CZ	5.65	1.45	1.38
1	D	28	SER	CB-OG	5.60	1.49	1.42
1	C	159	ILE	CB-CG1	-5.57	1.38	1.54
1	A	184	GLY	N-CA	5.57	1.54	1.46
1	B	402	PHE	CD2-CE2	5.56	1.50	1.39
1	B	568	ASP	CB-CG	5.48	1.63	1.51
1	A	595	ASP	CB-CG	5.45	1.63	1.51
1	D	382	PHE	CE1-CZ	5.41	1.47	1.37
1	A	500	SER	CB-OG	5.39	1.49	1.42
1	A	443	PHE	CE2-CZ	5.37	1.47	1.37
1	D	306	GLU	CD-OE2	5.37	1.31	1.25
1	A	239	PHE	CE1-CZ	5.37	1.47	1.37
1	B	472	GLU	CD-OE2	5.34	1.31	1.25
1	D	440	TYR	CD2-CE2	5.33	1.47	1.39
1	D	165	ARG	CZ-NH2	5.31	1.40	1.33
1	A	190	TYR	CD1-CE1	5.30	1.47	1.39
1	C	193	GLU	CD-OE1	5.30	1.31	1.25
1	B	365	VAL	CB-CG1	5.29	1.64	1.52
1	C	278	ARG	CZ-NH2	5.28	1.40	1.33
1	A	344	GLU	CD-OE1	5.26	1.31	1.25
1	A	248	GLU	CD-OE2	5.26	1.31	1.25
1	C	430	GLU	CB-CG	5.24	1.62	1.52
1	B	519	GLU	CD-OE1	5.22	1.31	1.25
1	A	490	GLU	CG-CD	5.21	1.59	1.51
1	A	206	PHE	CE2-CZ	5.20	1.47	1.37
1	B	334	TYR	CD2-CE2	5.19	1.47	1.39
1	B	181	ASP	CB-CG	5.16	1.62	1.51
1	B	346	GLU	CD-OE1	5.15	1.31	1.25
1	D	206	PHE	CD1-CE1	5.15	1.49	1.39
1	D	181	ASP	CB-CG	5.15	1.62	1.51
1	D	742	TRP	CB-CG	-5.14	1.41	1.50
1	D	377	ARG	CZ-NH1	5.12	1.39	1.33
1	D	669	CYS	CB-SG	5.12	1.91	1.82
1	D	108	PHE	CE2-CZ	5.10	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	70	ASP	CB-CG	5.07	1.62	1.51
1	A	29	LEU	N-CA	-5.07	1.36	1.46
1	C	181	ASP	CB-CG	5.07	1.62	1.51
1	D	272	PHE	CE2-CZ	5.06	1.47	1.37
1	D	124	GLU	CG-CD	5.05	1.59	1.51
1	D	334	TYR	CD1-CE1	5.03	1.46	1.39
1	A	335	GLU	CB-CG	5.02	1.61	1.52
1	C	57	ALA	CA-CB	5.01	1.62	1.52
1	A	421	SER	CB-OG	5.00	1.48	1.42

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	130	ARG	NE-CZ-NH2	-9.82	115.39	120.30
1	C	37	ARG	NE-CZ-NH2	-9.15	115.72	120.30
1	D	377	ARG	NE-CZ-NH1	-8.71	115.94	120.30
1	A	495	ARG	NE-CZ-NH1	8.69	124.65	120.30
1	C	501	PHE	CB-CG-CD2	-8.64	114.75	120.80
1	D	130	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	B	125	ARG	NE-CZ-NH2	-8.38	116.11	120.30
1	C	471	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	B	445	ARG	NE-CZ-NH1	8.27	124.44	120.30
1	B	377	ARG	NE-CZ-NH1	-8.07	116.26	120.30
1	B	383	PHE	CB-CG-CD2	-8.04	115.17	120.80
1	B	536	ARG	NE-CZ-NH2	-8.03	116.28	120.30
1	B	521	ARG	NE-CZ-NH1	8.01	124.31	120.30
1	A	377	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	B	445	ARG	NE-CZ-NH2	-7.97	116.31	120.30
1	A	411	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	D	411	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	C	159	ILE	CB-CG1-CD1	-7.66	92.46	113.90
1	A	612	ARG	NE-CZ-NH2	7.60	124.10	120.30
1	C	278	ARG	NE-CZ-NH1	-7.54	116.53	120.30
1	A	121	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	A	686	MET	CG-SD-CE	7.39	112.03	100.20
1	D	401	ASP	CB-CG-OD2	7.39	124.95	118.30
1	C	320	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	C	740	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	A	130	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	C	445	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	C	636	ARG	NE-CZ-NH1	7.19	123.89	120.30
1	D	177	ASP	CB-CG-OD1	-7.06	111.95	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	260	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	D	125	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	D	582	LEU	CB-CG-CD1	6.90	122.74	111.00
1	C	660	LEU	CB-CG-CD1	6.86	122.67	111.00
1	A	111	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	C	59	ASP	CB-CG-OD2	-6.84	112.15	118.30
1	B	467	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	A	663	ASP	CB-CG-OD1	6.71	124.34	118.30
1	C	159	ILE	CG1-CB-CG2	6.71	126.15	111.40
1	A	501	PHE	CB-CG-CD2	-6.66	116.14	120.80
1	A	37	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	B	471	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	B	595	ASP	CB-CG-OD2	-6.52	112.44	118.30
1	A	380	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	D	377	ARG	CG-CD-NE	-6.49	98.17	111.80
1	A	552	LEU	CB-CG-CD2	6.49	122.03	111.00
1	D	408	LEU	CB-CG-CD2	-6.46	100.01	111.00
1	B	562	LEU	CB-CG-CD1	6.46	121.99	111.00
1	D	377	ARG	NH1-CZ-NH2	6.38	126.42	119.40
1	D	152	PHE	CB-CG-CD2	-6.36	116.34	120.80
1	D	521	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	A	290	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	C	125	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	B	369	ARG	NE-CZ-NH1	-6.27	117.17	120.30
1	A	401	ASP	CB-CG-OD2	6.25	123.92	118.30
1	A	294	LYS	CD-CE-NZ	-6.19	97.47	111.70
1	A	259	ASP	CB-CG-OD2	6.18	123.86	118.30
1	A	740	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	A	353	LEU	CB-CG-CD1	-6.14	100.56	111.00
1	C	377	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	D	313	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	B	370	VAL	CA-CB-CG2	-6.11	101.74	110.90
1	D	165	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	C	443	PHE	CB-CG-CD1	-6.10	116.53	120.80
1	A	144	LEU	CB-CG-CD1	-6.08	100.66	111.00
1	A	277	PHE	CB-CG-CD1	-6.07	116.55	120.80
1	D	401	ASP	CB-CG-OD1	-6.06	112.84	118.30
1	A	72	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	B	118	ASP	CB-CG-OD1	-6.03	112.88	118.30
1	A	207	PHE	CB-CG-CD1	-6.02	116.59	120.80
1	B	401	ASP	CB-CG-OD2	6.02	123.72	118.30
1	B	118	ASP	CB-CG-OD2	5.99	123.69	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	571	LEU	CA-CB-CG	5.98	129.06	115.30
1	A	471	ARG	NE-CZ-NH1	-5.95	117.32	120.30
1	B	146	ASP	CB-CG-OD2	5.94	123.65	118.30
1	C	725	ASP	N-CA-C	5.94	127.04	111.00
1	C	606	LEU	CB-CG-CD2	5.92	121.07	111.00
1	C	633	LEU	CB-CG-CD1	5.91	121.04	111.00
1	A	495	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	A	554	LEU	CB-CG-CD2	-5.87	101.02	111.00
1	A	29	LEU	CB-CA-C	5.87	121.35	110.20
1	D	501	PHE	CB-CG-CD1	5.86	124.90	120.80
1	A	479	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	A	685	LEU	CB-CG-CD1	-5.82	101.11	111.00
1	A	501	PHE	CB-CG-CD1	5.79	124.85	120.80
1	B	309	LYS	CD-CE-NZ	-5.77	98.42	111.70
1	C	165	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	D	181	ASP	CB-CG-OD2	5.76	123.48	118.30
1	D	320	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	B	479	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	D	501	PHE	CB-CG-CD2	-5.73	116.79	120.80
1	C	467	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	C	501	PHE	CB-CG-CD1	5.71	124.80	120.80
1	D	377	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	D	138	PHE	CB-CG-CD2	-5.68	116.82	120.80
1	A	454	ASP	CB-CG-OD1	-5.67	113.20	118.30
1	D	422	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	C	121	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	260	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	B	165	ARG	NE-CZ-NH1	-5.57	117.52	120.30
1	B	198	LEU	CB-CG-CD2	-5.53	101.61	111.00
1	B	612	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	595	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	595	ASP	CB-CG-OD1	5.49	123.24	118.30
1	C	435	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	D	471	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	D	536	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	B	595	ASP	CB-CA-C	5.42	121.24	110.40
1	C	117	PHE	CB-CG-CD2	-5.41	117.01	120.80
1	B	183	ARG	NE-CZ-NH2	5.40	123.00	120.30
1	A	117	PHE	CB-CG-CD1	-5.40	117.02	120.80
1	B	501	PHE	CB-CG-CD2	-5.38	117.03	120.80
1	D	415	TYR	CG-CD1-CE1	-5.36	117.01	121.30
1	D	319	ARG	NE-CZ-NH1	5.36	122.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	454	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	70	ASP	CB-CG-OD1	5.34	123.11	118.30
1	C	139	GLN	N-CA-CB	-5.34	100.99	110.60
1	D	118	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	601	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	D	117	PHE	CB-CG-CD1	-5.25	117.12	120.80
1	A	411	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	C	660	LEU	CB-CG-CD2	5.21	119.85	111.00
1	C	155	ASP	CB-CG-OD2	5.20	122.98	118.30
1	D	61	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	121	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	547	LEU	CB-CG-CD1	-5.17	102.22	111.00
1	C	125	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	37	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	B	740	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	C	118	ASP	CB-CG-OD1	-5.14	113.67	118.30
1	B	369	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	C	413	PHE	CB-CG-CD2	-5.07	117.25	120.80
1	B	350	ASP	CB-CG-OD1	-5.06	113.75	118.30
1	A	121	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	B	180	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	D	368	GLN	CA-CB-CG	-5.00	102.39	113.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	159	ILE	CB

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	ARG	Sidechain
1	C	724	ALA	Peptide
1	C	725	ASP	Peptide

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	5764	0	5599	43	0
1	B	5749	0	5577	62	0
1	C	5766	0	5595	52	0
1	D	5757	0	5585	50	0
2	A	86	0	60	8	0
2	B	86	0	60	10	0
2	C	86	0	60	8	0
2	D	86	0	60	4	0
3	A	44	0	37	7	0
3	B	44	0	37	4	0
3	C	44	0	37	7	0
3	D	44	0	37	4	0
4	A	44	0	31	5	0
4	B	44	0	31	6	0
4	C	44	0	31	6	0
4	D	44	0	31	4	0
5	A	842	0	0	12	0
5	B	754	0	0	15	0
5	C	807	0	0	19	0
5	D	866	0	0	17	1
All	All	27001	0	22868	247	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 5.

All (247) 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:C:449[B]:HIS:CE1	5:C:3363:HOH:O	1.74	1.36
5:A:2649:HOH:O	1:C:28:SER:HA	1.44	1.16
1:D:451:MET:SD	5:D:3617:HOH:O	1.99	1.15
1:A:369[B]:ARG:HG3	1:A:369[B]:ARG:HH21	1.12	1.15
1:B:157:ASN:HB2	5:B:3138:HOH:O	1.48	1.11
5:B:2705:HOH:O	1:D:73:LYS:HD3	1.49	1.10
1:D:41:GLU:HG2	5:D:3312:HOH:O	1.52	1.06
1:D:267:ARG:HG3	5:D:1920:HOH:O	1.57	1.04
1:B:546:GLN:HG3	5:B:3324:HOH:O	1.58	1.03
1:A:369[B]:ARG:CG	1:A:369[B]:ARG:HH21	1.73	1.00
1:C:267:ARG:HG3	5:C:2916:HOH:O	1.62	0.99
3:C:761[B]:HDE:HBBB	3:C:761[B]:HDE:HMB	1.47	0.97
1:A:713:GLN:HG2	5:A:3248:HOH:O	1.65	0.94
1:A:28:SER:OG	1:A:28:SER:O	1.84	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:748:ILE:O	1:A:751:ILE:HG22	1.69	0.93
1:B:521:ARG:HH21	1:B:745:ILE:HG21	1.33	0.91
3:A:761[B]:HDE:HBBB	3:A:761[B]:HDE:HMB	1.55	0.88
1:D:28:SER:HB3	5:D:2467:HOH:O	1.76	0.85
1:A:541:GLU:OE2	5:A:2550:HOH:O	1.94	0.85
3:D:761[B]:HDE:HMB	3:D:761[B]:HDE:CBB	2.07	0.84
2:B:754[A]:HEM:CMB	2:B:754[A]:HEM:HBB2	2.05	0.83
1:B:521:ARG:NH2	1:B:745:ILE:HG21	1.94	0.82
1:A:416[B]:THR:HG22	5:A:901:HOH:O	1.79	0.81
1:C:751:ILE:HB	5:C:2367:HOH:O	1.81	0.80
2:B:755[C]:HEM:HMC2	2:B:755[C]:HEM:HBC2	1.63	0.79
1:B:155:ASP:OD1	5:B:3138:HOH:O	1.98	0.79
1:D:416[B]:THR:CG2	5:D:1415:HOH:O	2.30	0.78
1:D:416[B]:THR:HG22	5:D:1415:HOH:O	1.83	0.77
3:C:761[B]:HDE:HBCB	3:C:761[B]:HDE:HMC	1.68	0.76
1:D:552:LEU:CD1	1:D:556:GLN:NE2	2.49	0.75
3:D:761[B]:HDE:HBBB	3:D:761[B]:HDE:HMB	1.67	0.75
1:C:636:ARG:HD3	5:C:2717:HOH:O	1.87	0.75
2:B:754[A]:HEM:HMB1	2:B:754[A]:HEM:HBB2	1.70	0.74
1:C:748:ILE:O	1:C:751:ILE:HG22	1.86	0.74
1:B:546:GLN:CG	5:B:3324:HOH:O	2.27	0.74
3:B:761[B]:HDE:HBBB	3:B:761[B]:HDE:HMB	1.69	0.74
1:B:533:LYS:HE2	5:B:3100:HOH:O	1.88	0.73
1:D:552:LEU:HD13	1:D:556:GLN:NE2	2.04	0.72
1:B:201:ASN:CG	4:B:760[D]:HDD:HMB2	2.09	0.72
2:A:755[C]:HEM:HBC2	2:A:755[C]:HEM:HMC1	1.71	0.71
1:B:144:LEU:HD11	1:B:370:VAL:HG13	1.71	0.71
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.73	0.71
1:D:201:ASN:CG	4:D:760[D]:HDD:HMB2	2.11	0.71
1:D:449[A]:HIS:HD2	5:D:3615:HOH:O	1.72	0.70
2:A:755[C]:HEM:HBB2	2:A:755[C]:HEM:CMB	2.22	0.69
1:A:201:ASN:CG	4:A:760[D]:HDD:HMB2	2.13	0.69
3:C:761[B]:HDE:HMB	3:C:761[B]:HDE:CBB	2.21	0.69
1:C:70:ASP:OD1	5:C:2554:HOH:O	2.09	0.69
2:A:755[C]:HEM:HMB2	2:A:755[C]:HEM:HBB2	1.75	0.68
1:C:578[A]:ASP:OD1	5:C:3157:HOH:O	2.11	0.68
1:D:748:ILE:O	1:D:751:ILE:HG22	1.93	0.68
1:B:607:LEU:HD12	1:B:650[B]:ILE:CD1	2.23	0.68
1:A:612:ARG:NH1	5:A:3360:HOH:O	2.26	0.67
1:A:369[B]:ARG:HG3	1:A:369[B]:ARG:NH2	1.96	0.66
3:A:761[B]:HDE:HBCB	3:A:761[B]:HDE:HMC	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:ASN:CG	4:C:760[D]:HDD:HMB2	2.16	0.66
1:D:597:ASP:OD1	5:D:3292:HOH:O	2.14	0.66
3:D:761[B]:HDE:HBBA	3:D:761[B]:HDE:HMB	1.78	0.65
1:B:449[B]:HIS:HD2	5:B:3613:HOH:O	1.79	0.65
1:C:486:GLN:OE1	5:C:2892:HOH:O	2.13	0.65
1:C:583:LYS:O	1:C:584:LYS:HB3	1.97	0.65
1:C:449[A]:HIS:HD2	5:C:3611:HOH:O	1.79	0.65
1:C:612:ARG:HB2	1:C:612:ARG:CZ	2.27	0.65
5:B:2705:HOH:O	1:D:73:LYS:CD	2.23	0.64
2:B:754[A]:HEM:CBB	2:B:754[A]:HEM:HMB1	2.26	0.64
1:A:411:ARG:HG3	3:A:761[B]:HDE:HBBA	1.78	0.64
1:B:407:LEU:HD12	2:B:755[C]:HEM:HBB1	1.79	0.63
4:C:760[D]:HDD:HBC1	4:C:760[D]:HDD:HMC1	1.79	0.63
1:C:556:GLN:NE2	5:C:2533:HOH:O	2.31	0.63
2:C:755[C]:HEM:HBB2	2:C:755[C]:HEM:HMB2	1.80	0.63
1:B:546:GLN:CD	5:B:3324:HOH:O	2.36	0.63
1:A:416[B]:THR:CG2	5:A:901:HOH:O	2.43	0.62
1:C:634:TYR:O	1:C:653:THR:HA	1.99	0.62
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.83	0.62
1:D:629:HIS:HD2	5:D:1554:HOH:O	1.83	0.62
3:B:761[B]:HDE:HMB	3:B:761[B]:HDE:CBB	2.29	0.62
1:B:583:LYS:NZ	1:B:583:LYS:H	1.98	0.61
1:D:552:LEU:HD11	1:D:556:GLN:NE2	2.14	0.61
1:C:211:ALA:CB	2:C:755[C]:HEM:HBB1	2.30	0.61
1:A:29:LEU:HB2	5:C:2405:HOH:O	2.01	0.60
1:A:532[A]:SER:OG	5:A:3443:HOH:O	2.12	0.60
1:D:556:GLN:NE2	5:D:2773:HOH:O	2.33	0.60
2:B:755[C]:HEM:HBC2	2:B:755[C]:HEM:CMC	2.30	0.60
1:B:748:ILE:O	1:B:751:ILE:HG22	2.02	0.60
4:C:760[D]:HDD:HMC1	4:C:760[D]:HDD:CBC	2.30	0.60
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.84	0.59
1:A:369[B]:ARG:CG	1:A:369[B]:ARG:NH2	2.44	0.59
4:B:760[D]:HDD:HMC1	4:B:760[D]:HDD:HBC1	1.83	0.59
1:D:552:LEU:HD13	1:D:556:GLN:HE21	1.68	0.58
1:A:479:ARG:NH2	5:A:2607:HOH:O	2.18	0.57
1:C:449[B]:HIS:NE2	5:C:3363:HOH:O	2.04	0.57
1:B:201:ASN:ND2	4:B:760[D]:HDD:HMB2	2.18	0.57
1:B:411:ARG:HG3	3:B:761[B]:HDE:HBBA	1.85	0.57
1:A:201:ASN:ND2	4:A:760[D]:HDD:HMB2	2.19	0.57
1:C:578[A]:ASP:HB2	1:C:582:LEU:O	2.04	0.57
1:A:713:GLN:HA	1:A:713:GLN:HE21	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:ARG:HG3	3:C:761[B]:HDE:HBBA	1.86	0.57
1:D:211:ALA:HB2	2:D:755[C]:HEM:HBB1	1.86	0.56
1:C:359:LEU:H	1:C:507:HIS:HD2	1.52	0.56
1:B:634:TYR:O	1:B:653:THR:HA	2.05	0.56
1:B:521:ARG:NH2	1:B:745:ILE:HD13	2.21	0.56
1:C:201:ASN:ND2	4:C:760[D]:HDD:HMB2	2.21	0.55
1:B:359:LEU:H	1:B:507:HIS:HD2	1.53	0.55
1:C:636:ARG:NH2	1:C:639:GLU:O	2.39	0.55
2:C:754[A]:HEM:CMB	2:C:754[A]:HEM:HBB2	2.37	0.55
4:A:760[D]:HDD:HMC1	4:A:760[D]:HDD:HBC1	1.88	0.54
1:B:629:HIS:HD2	5:B:1052:HOH:O	1.92	0.53
1:B:724:ALA:O	1:B:725:ASP:O	2.27	0.53
1:D:158:LYS:HB3	5:D:3367:HOH:O	2.08	0.53
4:A:760[D]:HDD:HBC1	4:A:760[D]:HDD:CMC	2.39	0.52
1:D:211:ALA:CB	2:D:755[C]:HEM:HBB1	2.40	0.52
1:C:440[B]:TYR:CZ	5:C:1792:HOH:O	2.54	0.52
3:C:761[B]:HDE:HBAA	5:C:964:HOH:O	2.09	0.52
4:B:760[D]:HDD:HMC1	4:B:760[D]:HDD:CBC	2.40	0.51
3:A:761[B]:HDE:CBB	3:A:761[B]:HDE:HMB	2.36	0.51
1:B:533:LYS:HE3	5:C:2623:HOH:O	2.12	0.50
1:B:552:LEU:HD21	1:B:571:LEU:HD12	1.93	0.50
1:C:535:VAL:O	1:C:537:PRO:HD3	2.11	0.50
1:A:36:HIS:H	1:A:36:HIS:CD2	2.30	0.49
1:A:192:GLU:OE1	1:A:479:ARG:NH2	2.45	0.49
1:B:603:VAL:HG11	1:B:666:ILE:HD12	1.95	0.49
4:C:760[D]:HDD:HBD2	5:C:964:HOH:O	2.12	0.49
4:C:760[D]:HDD:HBC1	4:C:760[D]:HDD:CMC	2.43	0.49
2:A:755[C]:HEM:HBC2	2:A:755[C]:HEM:CMC	2.41	0.49
1:D:201:ASN:ND2	4:D:760[D]:HDD:HMB2	2.26	0.49
1:B:583:LYS:O	1:B:584:LYS:HB3	2.13	0.49
1:D:61:ARG:NH2	5:D:3239:HOH:O	2.36	0.49
1:B:449[B]:HIS:HE1	5:B:1789:HOH:O	1.96	0.48
1:D:359:LEU:H	1:D:507:HIS:HD2	1.61	0.48
1:A:414:SER:OG	2:A:754[A]:HEM:HHD	2.13	0.48
1:D:713:GLN:O	1:D:713:GLN:HG2	2.14	0.48
1:B:612:ARG:CZ	1:B:612:ARG:HB2	2.43	0.48
1:A:278:ARG:HH12	1:A:487:GLU:CD	2.17	0.48
1:B:546:GLN:NE2	5:B:3324:HOH:O	2.47	0.47
1:C:128:HIS:HA	1:C:168:THR:O	2.13	0.47
1:C:748:ILE:O	1:C:751:ILE:CG2	2.58	0.47
1:B:281:ASN:OD1	1:B:283:GLU:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:ASN:HD22	1:A:459:ASN:H	1.63	0.47
4:B:760[D]:HDD:CMC	4:B:760[D]:HDD:HBC1	2.44	0.47
1:C:488:ARG:HB2	1:C:488:ARG:HE	1.39	0.47
1:B:73:LYS:NZ	5:B:1110:HOH:O	2.47	0.47
1:B:407:LEU:CD1	2:B:755[C]:HEM:HBB1	2.45	0.47
1:B:359:LEU:H	1:B:507:HIS:CD2	2.31	0.47
3:C:761[B]:HDE:CBC	3:C:761[B]:HDE:HMC	2.41	0.47
1:D:207:PHE:O	1:D:249:THR:HA	2.14	0.47
4:D:760[D]:HDD:HMC1	4:D:760[D]:HDD:CBC	2.44	0.47
1:A:612:ARG:CZ	5:A:3400:HOH:O	2.62	0.47
1:C:583:LYS:O	1:C:584:LYS:CB	2.63	0.47
1:C:629:HIS:HD2	5:C:1129:HOH:O	1.98	0.47
1:D:731:GLU:OE2	5:D:3028:HOH:O	2.20	0.47
2:D:755[C]:HEM:HBC2	2:D:755[C]:HEM:CMC	2.46	0.47
1:B:583:LYS:HZ2	1:B:583:LYS:H	1.62	0.46
1:A:155:ASP:HB3	1:A:158:LYS:HB2	1.97	0.46
1:B:634:TYR:HB2	1:B:650[B]:ILE:HD12	1.96	0.46
1:B:603:VAL:HG11	1:B:666:ILE:CD1	2.46	0.46
1:D:128:HIS:HA	1:D:168:THR:O	2.15	0.46
1:C:411:ARG:HG2	2:C:755[C]:HEM:C3B	2.50	0.46
4:A:760[D]:HDD:HMC1	4:A:760[D]:HDD:CBC	2.45	0.46
1:B:521:ARG:NH2	1:B:745:ILE:CG2	2.74	0.45
1:C:612:ARG:HG3	5:C:3087:HOH:O	2.15	0.45
1:B:184:GLY:HA3	4:B:760[D]:HDD:HMA2	1.98	0.45
1:A:211:ALA:CB	1:A:410:GLY:HA3	2.46	0.45
1:D:552:LEU:HD21	1:D:571:LEU:HD23	1.97	0.45
1:B:696:ALA:HB1	1:B:728:PHE:CZ	2.51	0.45
2:A:754[A]:HEM:CMB	2:A:754[A]:HEM:HBB2	2.47	0.45
1:C:137:TYR:HB2	1:C:159:ILE:HD11	1.97	0.45
1:D:359:LEU:HD21	5:D:2971:HOH:O	2.17	0.45
1:B:211:ALA:HA	2:B:755[C]:HEM:HBB1	1.98	0.45
1:B:414:SER:OG	2:B:754[A]:HEM:HHD	2.16	0.45
1:B:533:LYS:CE	5:C:2623:HOH:O	2.65	0.45
1:B:39:ALA:HB1	1:B:41:GLU:HG2	1.98	0.45
5:A:1788:HOH:O	1:C:449[A]:HIS:HE1	1.99	0.45
1:C:704:PHE:O	1:C:707:THR:HG22	2.17	0.45
1:C:165:ARG:HD3	2:C:755[C]:HEM:O1D	2.16	0.45
2:C:755[C]:HEM:HBB2	2:C:755[C]:HEM:CMB	2.46	0.45
1:A:128:HIS:HA	1:A:168:THR:O	2.17	0.45
1:A:634:TYR:O	1:A:653:THR:HA	2.16	0.45
1:A:411:ARG:CG	3:A:761[B]:HDE:HBBA	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:393:PRO:HD2	1:D:415:TYR:CG	2.52	0.45
1:B:459:ASN:H	1:B:459:ASN:HD22	1.65	0.44
1:B:211:ALA:CB	1:B:410:GLY:HA3	2.47	0.44
1:B:686:MET:HB3	1:B:751:ILE:HD11	1.98	0.44
1:C:488:ARG:NH1	5:C:2379:HOH:O	2.25	0.44
1:C:717:GLY:HA3	1:C:741:VAL:HG11	1.99	0.44
1:B:157:ASN:CB	5:B:3138:HOH:O	2.28	0.44
1:D:556:GLN:HG2	1:D:566:LEU:HD12	1.98	0.44
1:C:552:LEU:HD22	1:C:556:GLN:HG3	2.00	0.44
1:C:705:LYS:HG2	1:C:710:ILE:HB	2.00	0.44
1:B:128:HIS:HA	1:B:168:THR:O	2.18	0.44
2:B:754[A]:HEM:HMB3	2:B:754[A]:HEM:HBB2	1.93	0.44
1:C:28:SER:OG	1:C:28:SER:O	2.35	0.44
1:C:309:LYS:HB3	1:C:660:LEU:HD21	1.98	0.44
1:C:128:HIS:CE1	1:C:169:VAL:HG22	2.53	0.44
1:C:551:ASP:OD1	1:C:553:THR:HB	2.18	0.44
1:D:278:ARG:HH12	1:D:487:GLU:CD	2.21	0.44
1:A:393:PRO:HD2	1:A:415:TYR:CG	2.53	0.43
1:C:359:LEU:H	1:C:507:HIS:CD2	2.32	0.43
1:B:393:PRO:HD2	1:B:415:TYR:CG	2.54	0.43
2:A:755[C]:HEM:HMB2	2:A:755[C]:HEM:CBB	2.46	0.43
1:B:521:ARG:NH2	1:B:745:ILE:CD1	2.81	0.43
2:D:755[C]:HEM:HBC2	2:D:755[C]:HEM:HMC2	2.00	0.43
1:A:252:ASN:HA	1:A:252:ASN:HD22	1.69	0.43
4:D:760[D]:HDD:HMC1	4:D:760[D]:HDD:HBC1	2.00	0.43
1:D:128:HIS:CE1	1:D:169:VAL:HG22	2.54	0.43
5:B:1789:HOH:O	1:D:449[A]:HIS:HE1	2.02	0.43
1:B:583:LYS:HZ3	1:B:583:LYS:H	1.65	0.43
2:C:754[A]:HEM:HMB1	2:C:754[A]:HEM:HBB2	2.00	0.43
1:C:552:LEU:HD21	1:C:571:LEU:HD12	2.00	0.42
1:D:393:PRO:HD2	1:D:415:TYR:CD2	2.54	0.42
1:D:48:GLN:HB3	1:D:48:GLN:HE21	1.69	0.42
1:A:335:GLU:OE1	1:A:369[B]:ARG:HD3	2.20	0.42
1:B:252:ASN:HA	1:B:252:ASN:HD22	1.75	0.42
1:D:416[B]:THR:HG21	5:D:1415:HOH:O	2.07	0.42
3:A:761[B]:HDE:HABA	3:A:761[B]:HDE:HHCA	1.86	0.42
1:D:597:ASP:OD2	5:D:2709:HOH:O	2.21	0.42
1:A:414:SER:OG	3:A:761[B]:HDE:HHB	2.20	0.42
1:A:610:GLU:HG2	5:A:2551:HOH:O	2.19	0.42
1:C:211:ALA:HB2	2:C:755[C]:HEM:HBB1	2.02	0.42
1:A:422:ARG:NE	2:A:754[A]:HEM:O1D	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:682:ASN:HB3	1:B:707:THR:HG21	2.02	0.41
1:A:38:PRO:HA	1:A:48:GLN:OE1	2.19	0.41
1:D:593:ILE:HA	1:D:594:PRO:HD3	1.94	0.41
1:C:459:ASN:H	1:C:459:ASN:HD22	1.68	0.41
1:D:211:ALA:CB	1:D:410:GLY:HA3	2.51	0.41
1:D:459:ASN:HD22	1:D:459:ASN:H	1.68	0.41
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.36	0.41
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.36	0.41
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.36	0.41
1:A:716:GLU:HG2	5:A:1656:HOH:O	2.21	0.41
1:B:207:PHE:O	1:B:249:THR:HA	2.21	0.41
1:B:91:ASP:OD1	1:D:461:GLU:OE1	2.39	0.41
1:C:583:LYS:HB2	1:C:583:LYS:HE3	1.90	0.41
1:D:556:GLN:CG	1:D:566:LEU:HD12	2.51	0.41
1:D:634:TYR:O	1:D:653:THR:HA	2.20	0.41
1:B:521:ARG:HH22	1:B:745:ILE:CD1	2.34	0.40
1:B:607:LEU:HD22	1:B:611:VAL:HG21	2.02	0.40
1:A:207:PHE:O	1:A:249:THR:HA	2.21	0.40
1:A:39:ALA:HB1	1:A:41:GLU:HG2	2.04	0.40
1:C:238:THR:HB	1:D:460:TYR:CE2	2.56	0.40
1:D:61:ARG:NH1	5:D:3245:HOH:O	2.53	0.40
1:A:95:LEU:HB3	1:A:107:ASP:HB2	2.03	0.40
1:A:251:HIS:CE1	1:A:507:HIS:HB3	2.56	0.40
1:B:411:ARG:HG2	3:B:761[B]:HDE:C3B	2.51	0.40
1:C:407:LEU:HD12	3:C:761[B]:HDE:HBB	2.04	0.40
1:B:144:LEU:HD11	1:B:370:VAL:CG1	2.48	0.40
3:D:761[B]:HDE:HBBB	3:D:761[B]:HDE:CMB	2.44	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)
5:D:2178:HOH:O	5:D:2976:HOH:O[1_655]	2.13	0.07

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	729/753 (97%)	713 (98%)	15 (2%)	1 (0%)	51	25
1	B	727/753 (96%)	706 (97%)	19 (3%)	2 (0%)	41	18
1	C	729/753 (97%)	717 (98%)	11 (2%)	1 (0%)	51	25
1	D	730/753 (97%)	716 (98%)	13 (2%)	1 (0%)	51	25
All	All	2915/3012 (97%)	2852 (98%)	58 (2%)	5 (0%)	47	23

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	725	ASP
1	A	75	SER
1	B	75	SER
1	C	75	SER
1	D	75	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	616/636 (97%)	600 (97%)	16 (3%)	46	16
1	B	614/636 (96%)	589 (96%)	25 (4%)	30	6
1	C	616/636 (97%)	587 (95%)	29 (5%)	26	4
1	D	617/636 (97%)	598 (97%)	19 (3%)	40	11
All	All	2463/2544 (97%)	2374 (96%)	89 (4%)	35	8

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	SER

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Mol	Chain	Res	Type
1	A	29	LEU
1	A	37	ARG
1	A	158	LYS
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	440	TYR
1	A	459	ASN
1	A	552	LEU
1	A	713	GLN
1	A	732	LEU
1	A	751	ILE
1	B	28	SER
1	B	185	PHE
1	B	191	THR
1	B	205	ILE
1	B	227	TRP
1	B	237	ASP
1	B	252	ASN
1	B	283	GLU
1	B	440	TYR
1	B	459	ASN
1	B	552	LEU
1	B	562	LEU
1	B	566	LEU
1	B	568	ASP
1	B	571	LEU
1	B	583	LYS
1	B	595	ASP
1	B	610	GLU
1	B	612	ARG
1	B	616	LEU
1	B	633	LEU
1	B	703	LYS
1	B	713	GLN
1	B	750	LYS
1	B	751	ILE
1	C	61	ARG
1	C	159	ILE

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Mol	Chain	Res	Type
1	C	185	PHE
1	C	191	THR
1	C	205	ILE
1	C	213	LYS
1	C	227	TRP
1	C	252	ASN
1	C	283	GLU
1	C	285	LYS
1	C	377	ARG
1	C	440[A]	TYR
1	C	440[B]	TYR
1	C	459	ASN
1	C	478	LYS
1	C	488	ARG
1	C	552	LEU
1	C	571	LEU
1	C	594	PRO
1	C	606	LEU
1	C	612	ARG
1	C	616	LEU
1	C	633	LEU
1	C	648	LEU
1	C	660	LEU
1	C	725	ASP
1	C	733	LEU
1	C	747	LYS
1	C	750	LYS
1	D	41	GLU
1	D	185	PHE
1	D	191	THR
1	D	205	ILE
1	D	227	TRP
1	D	237	ASP
1	D	252	ASN
1	D	432	PRO
1	D	440	TYR
1	D	459	ASN
1	D	574	THR
1	D	582	LEU
1	D	612	ARG
1	D	616	LEU
1	D	624	LYS

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Mol	Chain	Res	Type
1	D	648	LEU
1	D	713	GLN
1	D	747	LYS
1	D	750	LYS

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

Mol	Chain	Res	Type
1	A	36	HIS
1	A	252	ASN
1	A	459	ASN
1	A	515	GLN
1	A	713	GLN
1	B	252	ASN
1	B	459	ASN
1	B	507	HIS
1	B	546	GLN
1	B	629	HIS
1	C	252	ASN
1	C	459	ASN
1	C	486	GLN
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	459	ASN
1	D	507	HIS
1	D	556	GLN
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)

16 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	$\#|Z| > 2$
3	HDE	C	761[B]	1,5	41,52,52	2.66	15 (36%)	38,89,89	2.43	16 (42%)
3	HDE	B	761[B]	1,5	41,52,52	2.64	14 (34%)	38,89,89	3.00	20 (52%)
3	HDE	D	761[B]	1	41,52,52	2.76	15 (36%)	38,89,89	2.99	19 (50%)
2	HEM	C	754[A]	1,5	27,50,50	2.10	7 (25%)	17,82,82	2.82	10 (58%)
2	HEM	A	754[A]	1,5	27,50,50	2.18	9 (33%)	17,82,82	2.44	6 (35%)
2	HEM	D	754[A]	1	27,50,50	2.06	7 (25%)	17,82,82	2.23	6 (35%)
4	HDD	A	760[D]	1,5	38,52,52	2.46	11 (28%)	28,89,89	2.42	7 (25%)
4	HDD	C	760[D]	1,5	38,52,52	2.33	11 (28%)	28,89,89	2.16	10 (35%)
2	HEM	D	755[C]	1	27,50,50	2.17	5 (18%)	17,82,82	2.47	5 (29%)
4	HDD	D	760[D]	1	38,52,52	2.41	10 (26%)	28,89,89	1.66	8 (28%)
2	HEM	C	755[C]	1,5	27,50,50	1.97	7 (25%)	17,82,82	2.11	5 (29%)
2	HEM	B	754[A]	1,5	27,50,50	2.17	9 (33%)	17,82,82	2.66	7 (41%)
2	HEM	B	755[C]	1,5	27,50,50	2.04	6 (22%)	17,82,82	2.43	5 (29%)
4	HDD	B	760[D]	1,5	38,52,52	2.28	13 (34%)	28,89,89	2.23	10 (35%)
2	HEM	A	755[C]	1,5	27,50,50	2.08	8 (29%)	17,82,82	1.85	4 (23%)
3	HDE	A	761[B]	1,5	41,52,52	2.52	17 (41%)	38,89,89	3.02	19 (50%)

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
3	HDE	C	761[B]	1,5	-	4/7/89/89	0/1/9/9
3	HDE	B	761[B]	1,5	-	4/7/89/89	0/1/9/9
3	HDE	D	761[B]	1	-	4/7/89/89	0/1/9/9
2	HEM	C	754[A]	1,5	-	0/6/54/54	-
2	HEM	A	754[A]	1,5	-	0/6/54/54	-
2	HEM	D	754[A]	1	-	0/6/54/54	-
4	HDD	A	760[D]	1,5	-	0/3/89/89	0/1/9/9
4	HDD	C	760[D]	1,5	-	0/3/89/89	0/1/9/9
2	HEM	D	755[C]	1	-	0/6/54/54	-
4	HDD	D	760[D]	1	-	0/3/89/89	0/1/9/9
2	HEM	C	755[C]	1,5	-	0/6/54/54	-
2	HEM	B	754[A]	1,5	-	0/6/54/54	-
2	HEM	B	755[C]	1,5	-	0/6/54/54	-
4	HDD	B	760[D]	1,5	-	0/3/89/89	0/1/9/9
2	HEM	A	755[C]	1,5	-	0/6/54/54	-
3	HDE	A	761[B]	1,5	-	4/7/89/89	0/1/9/9

All (164) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	761[B]	HDE	C4C-C3C	8.26	1.49	1.38
3	C	761[B]	HDE	C4C-C3C	7.76	1.48	1.38
4	D	760[D]	HDD	FE-ND	6.99	2.22	1.95
3	D	761[B]	HDE	C4C-C3C	6.91	1.47	1.38
4	C	760[D]	HDD	FE-ND	6.81	2.22	1.95
4	A	760[D]	HDD	FE-ND	6.81	2.22	1.95
4	A	760[D]	HDD	O1D-C3D	-6.79	1.35	1.46
3	C	761[B]	HDE	CHC-C1C	-6.41	1.44	1.51
3	A	761[B]	HDE	CHD-C1D	-6.27	1.44	1.51
3	D	761[B]	HDE	CHC-C4B	-6.23	1.44	1.51
2	D	755[C]	HEM	C3B-C2B	-6.03	1.32	1.40
3	D	761[B]	HDE	CHC-C1C	-6.03	1.45	1.51
3	B	761[B]	HDE	CHC-C4B	-5.98	1.45	1.51
4	B	760[D]	HDD	FE-ND	5.93	2.18	1.95
3	A	761[B]	HDE	C4C-C3C	5.83	1.46	1.38
3	D	761[B]	HDE	CHD-C4C	-5.75	1.45	1.51
4	B	760[D]	HDD	C3B-C2B	-5.70	1.32	1.40
4	D	760[D]	HDD	C3C-C2C	-5.54	1.32	1.40
3	D	761[B]	HDE	CHD-C1D	-5.46	1.45	1.51
4	A	760[D]	HDD	C3C-C2C	-5.43	1.32	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	760[D]	HDD	O1D-C3D	-5.42	1.38	1.46
3	A	761[B]	HDE	CHC-C4B	-5.34	1.45	1.51
2	B	754[A]	HEM	C3B-C2B	-5.31	1.33	1.40
2	A	754[A]	HEM	C3C-C2C	-5.22	1.33	1.40
2	D	754[A]	HEM	C3D-C2D	5.17	1.53	1.37
4	C	760[D]	HDD	C3B-C2B	-5.15	1.33	1.40
2	A	755[C]	HEM	C3B-C2B	-5.14	1.33	1.40
3	C	761[B]	HDE	CHD-C1D	-5.10	1.45	1.51
2	A	754[A]	HEM	C3D-C2D	5.00	1.52	1.37
2	C	754[A]	HEM	C3D-C2D	4.88	1.52	1.37
2	D	755[C]	HEM	C3D-C2D	4.86	1.52	1.37
4	B	760[D]	HDD	O1D-C3D	-4.85	1.38	1.46
4	D	760[D]	HDD	C3B-C2B	-4.81	1.33	1.40
2	B	754[A]	HEM	C3D-C2D	4.80	1.51	1.37
2	C	754[A]	HEM	C3C-C2C	-4.79	1.33	1.40
4	A	760[D]	HDD	C3B-C2B	-4.78	1.33	1.40
3	C	761[B]	HDE	CHD-C4C	-4.78	1.46	1.51
2	C	755[C]	HEM	C3D-C2D	4.74	1.51	1.37
3	B	761[B]	HDE	C4A-NA	4.70	1.45	1.37
2	A	755[C]	HEM	C3D-C2D	4.68	1.51	1.37
2	B	755[C]	HEM	C3D-C2D	4.65	1.51	1.37
2	C	755[C]	HEM	C3C-C2C	-4.64	1.33	1.40
2	C	754[A]	HEM	C3B-C2B	-4.62	1.34	1.40
4	D	760[D]	HDD	O1D-C3D	-4.60	1.39	1.46
3	C	761[B]	HDE	O1A-CGA	4.55	1.43	1.35
4	C	760[D]	HDD	C3C-C2C	-4.53	1.34	1.40
3	B	761[B]	HDE	CHD-C4C	-4.50	1.46	1.51
3	B	761[B]	HDE	O1A-CGA	4.47	1.43	1.35
3	A	761[B]	HDE	CHD-C4C	-4.47	1.46	1.51
2	D	755[C]	HEM	C3C-C2C	-4.47	1.34	1.40
3	B	761[B]	HDE	C1A-NA	4.38	1.45	1.37
2	B	755[C]	HEM	C3C-C2C	-4.33	1.34	1.40
2	D	754[A]	HEM	C3B-C2B	-4.26	1.34	1.40
3	D	761[B]	HDE	C4A-NA	4.25	1.45	1.37
2	D	754[A]	HEM	C3C-C2C	-4.21	1.34	1.40
2	B	755[C]	HEM	C3B-CAB	4.20	1.56	1.47
3	B	761[B]	HDE	CHD-C1D	-4.20	1.46	1.51
2	B	754[A]	HEM	C3C-C2C	-4.09	1.34	1.40
3	A	761[B]	HDE	O1A-CGA	4.08	1.42	1.35
4	B	760[D]	HDD	C3C-C2C	-4.07	1.34	1.40
2	C	755[C]	HEM	C3B-C2B	-3.95	1.34	1.40
2	A	754[A]	HEM	C3B-C2B	-3.95	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	761[B]	HDE	C1A-NA	3.93	1.44	1.37
3	A	761[B]	HDE	CHC-C1C	-3.93	1.47	1.51
3	C	761[B]	HDE	CHC-C4B	-3.84	1.47	1.51
3	D	761[B]	HDE	O1A-CGA	3.82	1.42	1.35
3	B	761[B]	HDE	C3C-C2C	3.78	1.48	1.37
3	C	761[B]	HDE	C3B-C2B	3.73	1.48	1.37
3	D	761[B]	HDE	C3C-C2C	3.68	1.48	1.37
3	C	761[B]	HDE	C1A-NA	3.67	1.44	1.37
3	D	761[B]	HDE	C1A-NA	3.62	1.43	1.37
3	B	761[B]	HDE	C3B-C2B	3.59	1.48	1.37
3	C	761[B]	HDE	C4A-NA	3.57	1.43	1.37
3	C	761[B]	HDE	C3D-C2D	3.50	1.48	1.37
3	B	761[B]	HDE	CHC-C1C	-3.49	1.47	1.51
2	B	755[C]	HEM	C3B-C2B	-3.48	1.35	1.40
4	D	760[D]	HDD	CHD-C1D	3.48	1.41	1.36
3	A	761[B]	HDE	C4A-NA	3.47	1.43	1.37
3	D	761[B]	HDE	C3B-C2B	3.44	1.47	1.37
2	A	754[A]	HEM	C3C-CAC	3.44	1.54	1.47
4	D	760[D]	HDD	C3C-CAC	3.44	1.54	1.47
3	A	761[B]	HDE	C3D-C2D	3.41	1.47	1.37
4	C	760[D]	HDD	CHA-C4D	3.40	1.41	1.36
4	D	760[D]	HDD	C3B-CAB	3.38	1.54	1.47
2	A	755[C]	HEM	C3C-C2C	-3.35	1.35	1.40
3	C	761[B]	HDE	C3C-C2C	3.35	1.47	1.37
4	B	760[D]	HDD	C3B-CAB	3.33	1.54	1.47
3	A	761[B]	HDE	C3B-C2B	3.28	1.47	1.37
4	C	760[D]	HDD	CHD-C1D	3.21	1.41	1.36
3	A	761[B]	HDE	C3C-C2C	3.20	1.47	1.37
4	A	760[D]	HDD	CHA-C4D	3.18	1.41	1.36
2	A	755[C]	HEM	C3C-CAC	3.18	1.54	1.47
4	D	760[D]	HDD	CMD-C2D	3.17	1.57	1.53
2	D	754[A]	HEM	C3C-CAC	3.15	1.54	1.47
2	D	755[C]	HEM	C3B-CAB	3.06	1.54	1.47
2	C	754[A]	HEM	C3C-CAC	3.02	1.54	1.47
3	D	761[B]	HDE	C1B-NB	3.02	1.42	1.36
2	A	755[C]	HEM	C3B-CAB	3.01	1.54	1.47
3	C	761[B]	HDE	C1B-NB	2.99	1.42	1.36
2	C	754[A]	HEM	C3B-CAB	2.99	1.54	1.47
2	A	754[A]	HEM	C3B-CAB	2.93	1.53	1.47
4	C	760[D]	HDD	C3C-CAC	2.92	1.53	1.47
3	D	761[B]	HDE	C4D-CHA	2.91	1.49	1.41
2	B	755[C]	HEM	C3C-CAC	2.91	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	760[D]	HDD	C3B-CAB	2.91	1.53	1.47
4	A	760[D]	HDD	C3C-CAC	2.84	1.53	1.47
4	B	760[D]	HDD	CHA-C4D	2.77	1.40	1.36
3	A	761[B]	HDE	C1B-NB	2.73	1.41	1.36
4	B	760[D]	HDD	C1A-NA	2.73	1.41	1.36
2	C	755[C]	HEM	C3B-CAB	2.71	1.53	1.47
4	B	760[D]	HDD	CMD-C2D	2.70	1.57	1.53
2	B	754[A]	HEM	C3B-CAB	2.70	1.53	1.47
4	A	760[D]	HDD	CAA-C2A	2.69	1.56	1.52
4	A	760[D]	HDD	CHD-C1D	2.67	1.40	1.36
2	D	755[C]	HEM	C3C-CAC	2.67	1.53	1.47
3	A	761[B]	HDE	C1C-C2C	2.62	1.41	1.38
2	D	754[A]	HEM	C3B-CAB	2.61	1.53	1.47
4	D	760[D]	HDD	CHA-C4D	2.61	1.40	1.36
3	D	761[B]	HDE	C3D-C2D	2.60	1.45	1.37
4	B	760[D]	HDD	CHD-C1D	2.57	1.40	1.36
4	B	760[D]	HDD	C3C-CAC	2.57	1.53	1.47
2	A	755[C]	HEM	C1D-ND	2.54	1.41	1.36
3	A	761[B]	HDE	C4D-CHA	2.54	1.48	1.41
2	C	755[C]	HEM	C3C-CAC	2.54	1.53	1.47
4	C	760[D]	HDD	CAA-C2A	2.54	1.55	1.52
4	A	760[D]	HDD	C3B-CAB	2.53	1.53	1.47
4	D	760[D]	HDD	OND-C2D	2.51	1.47	1.42
2	C	754[A]	HEM	CAA-C2A	2.50	1.55	1.52
3	B	761[B]	HDE	C1B-NB	2.50	1.41	1.36
3	D	761[B]	HDE	CAD-C3D	-2.48	1.48	1.52
2	B	754[A]	HEM	C3C-CAC	2.48	1.52	1.47
3	B	761[B]	HDE	C4D-CHA	2.47	1.47	1.41
3	A	761[B]	HDE	C1B-CHB	2.46	1.47	1.41
2	A	754[A]	HEM	C1D-ND	2.45	1.41	1.36
3	C	761[B]	HDE	C1B-CHB	2.44	1.47	1.41
2	B	754[A]	HEM	C1D-ND	2.44	1.41	1.36
4	A	760[D]	HDD	C1C-NC	2.41	1.41	1.36
2	A	754[A]	HEM	CAA-C2A	2.38	1.55	1.52
2	C	755[C]	HEM	C1D-ND	2.35	1.41	1.36
2	B	754[A]	HEM	CAA-C2A	2.34	1.55	1.52
4	B	760[D]	HDD	CAA-C2A	2.32	1.55	1.52
2	A	754[A]	HEM	C4A-NA	2.30	1.40	1.36
4	C	760[D]	HDD	CMD-C2D	2.30	1.56	1.53
3	B	761[B]	HDE	C1B-CHB	2.28	1.47	1.41
2	D	754[A]	HEM	C4A-NA	2.27	1.40	1.36
3	B	761[B]	HDE	C3D-C2D	2.26	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	761[B]	HDE	C1C-C2C	2.26	1.41	1.38
4	A	760[D]	HDD	C1A-NA	2.25	1.40	1.36
4	B	760[D]	HDD	C4D-ND	2.24	1.41	1.37
3	C	761[B]	HDE	C4D-CHA	2.20	1.47	1.41
2	A	754[A]	HEM	C4B-NB	2.20	1.40	1.36
2	C	755[C]	HEM	C2A-C3A	-2.19	1.31	1.37
3	A	761[B]	HDE	CAD-C3D	-2.17	1.48	1.52
2	A	755[C]	HEM	C4B-NB	2.16	1.40	1.36
2	B	754[A]	HEM	CMA-C3A	2.12	1.56	1.51
4	B	760[D]	HDD	C2A-C3A	-2.10	1.31	1.37
3	A	761[B]	HDE	O1A-C2A	-2.10	1.43	1.46
4	C	760[D]	HDD	C4A-NA	2.09	1.40	1.36
2	D	754[A]	HEM	CMC-C2C	2.06	1.56	1.51
3	D	761[B]	HDE	C1B-CHB	2.06	1.46	1.41
2	A	755[C]	HEM	C1C-C2C	2.05	1.47	1.42
2	C	754[A]	HEM	C4A-NA	2.04	1.40	1.36
2	B	754[A]	HEM	C4B-NB	2.04	1.40	1.36
2	B	755[C]	HEM	C2A-C3A	-2.02	1.31	1.37

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	761[B]	HDE	CHC-C4B-C3B	-7.48	120.65	129.68
3	A	761[B]	HDE	CHC-C4B-C3B	-7.47	120.66	129.68
3	B	761[B]	HDE	CAC-C3C-C4C	-7.42	118.27	127.19
2	C	754[A]	HEM	CBD-CAD-C3D	-6.92	99.73	112.48
3	B	761[B]	HDE	CHC-C4B-C3B	-6.74	121.54	129.68
2	D	754[A]	HEM	CBD-CAD-C3D	-6.69	100.15	112.48
3	A	761[B]	HDE	CHD-C4C-C3C	-6.55	121.78	129.68
2	B	754[A]	HEM	CBD-CAD-C3D	-6.51	100.49	112.48
2	B	755[C]	HEM	CAD-CBD-CGD	-6.48	101.80	112.67
3	D	761[B]	HDE	CAC-C3C-C4C	-6.39	119.51	127.19
2	A	754[A]	HEM	CBD-CAD-C3D	-6.27	100.92	112.48
3	D	761[B]	HDE	CHD-C1D-C2D	-6.25	119.07	129.53
3	A	761[B]	HDE	CAD-CBD-CGD	-6.14	102.36	112.67
2	D	755[C]	HEM	CAD-CBD-CGD	-5.74	103.05	112.67
3	D	761[B]	HDE	CAD-CBD-CGD	-5.72	103.08	112.67
3	A	761[B]	HDE	CHD-C1D-C2D	-5.56	120.23	129.53
3	B	761[B]	HDE	CHD-C1D-C2D	-5.41	120.48	129.53
4	A	760[D]	HDD	CAD-CBD-CGD	-5.33	96.32	104.56
4	A	760[D]	HDD	CMC-C2C-C1C	-5.30	120.32	128.46
3	A	761[B]	HDE	CAC-C3C-C4C	-5.29	120.83	127.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	761[B]	HDE	CAD-CBD-CGD	-5.22	103.92	112.67
4	B	760[D]	HDD	CAA-CBA-CGA	-5.06	104.18	112.67
3	C	761[B]	HDE	CHD-C1D-C2D	-5.05	121.09	129.53
3	B	761[B]	HDE	CHD-C4C-C3C	-5.04	123.59	129.68
3	D	761[B]	HDE	CHD-C4C-C3C	-5.04	123.59	129.68
3	C	761[B]	HDE	CAD-CBD-CGD	-4.92	104.42	112.67
2	A	755[C]	HEM	CAD-CBD-CGD	-4.80	104.62	112.67
2	B	754[A]	HEM	CAA-CBA-CGA	-4.65	104.87	112.67
3	C	761[B]	HDE	CHD-C4C-C3C	-4.59	124.14	129.68
4	C	760[D]	HDD	C4B-C3B-C2B	4.54	110.07	106.90
3	C	761[B]	HDE	CHC-C4B-C3B	-4.51	124.24	129.68
2	D	755[C]	HEM	C1D-C2D-C3D	-4.44	103.91	107.00
4	A	760[D]	HDD	CMA-C3A-C4A	-4.42	121.68	128.46
4	C	760[D]	HDD	O1D-CGD-O2D	4.39	124.72	120.80
2	C	755[C]	HEM	CBA-CAA-C2A	-4.37	104.42	112.49
3	D	761[B]	HDE	C4C-CHD-C1D	4.36	123.52	112.87
2	D	755[C]	HEM	CBA-CAA-C2A	-4.36	104.44	112.49
4	A	760[D]	HDD	O1D-CGD-CBD	-4.32	105.83	110.19
3	D	761[B]	HDE	C1B-C2B-C3B	-4.27	104.02	107.00
4	B	760[D]	HDD	C4A-C3A-C2A	4.24	109.95	107.00
3	C	761[B]	HDE	C4C-CHD-C1D	4.15	122.99	112.87
4	B	760[D]	HDD	O1D-CGD-O2D	4.13	124.48	120.80
3	B	761[B]	HDE	C4C-CHD-C1D	4.06	122.77	112.87
4	A	760[D]	HDD	C4A-C3A-C2A	4.04	109.81	107.00
4	A	760[D]	HDD	CAA-CBA-CGA	-4.03	105.91	112.67
3	B	761[B]	HDE	CHC-C1C-C2C	-4.03	122.79	129.53
3	A	761[B]	HDE	C1C-C2C-C3C	-4.00	101.55	105.81
2	C	755[C]	HEM	CAD-CBD-CGD	-3.99	105.97	112.67
3	C	761[B]	HDE	C4B-CHC-C1C	3.96	122.54	112.87
3	A	761[B]	HDE	C1B-CHB-C4A	-3.96	122.27	130.12
3	A	761[B]	HDE	CMD-C2D-C3D	3.93	132.35	124.94
3	D	761[B]	HDE	CHC-C1C-C2C	-3.86	123.08	129.53
2	C	754[A]	HEM	C4A-C3A-C2A	3.79	109.63	107.00
2	C	754[A]	HEM	CBA-CAA-C2A	-3.78	105.52	112.49
3	A	761[B]	HDE	CAB-C3B-C4B	-3.74	122.69	127.19
4	C	760[D]	HDD	CAA-CBA-CGA	-3.73	106.42	112.67
2	C	755[C]	HEM	CMB-C2B-C3B	3.61	131.44	124.68
2	A	754[A]	HEM	CMA-C3A-C4A	-3.61	122.92	128.46
3	C	761[B]	HDE	CMD-C2D-C3D	3.59	131.70	124.94
2	B	755[C]	HEM	CMB-C2B-C3B	3.58	131.37	124.68
4	B	760[D]	HDD	O1D-CGD-CBD	-3.52	106.64	110.19
2	C	754[A]	HEM	C4C-C3C-C2C	3.51	109.35	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	761[B]	HDE	C4C-CHD-C1D	3.51	121.42	112.87
3	B	761[B]	HDE	CMC-C2C-C3C	3.50	131.53	124.94
3	D	761[B]	HDE	CMC-C2C-C3C	3.49	131.52	124.94
4	D	760[D]	HDD	CAA-CBA-CGA	-3.45	106.89	112.67
4	D	760[D]	HDD	O1D-CGD-O2D	3.44	123.87	120.80
2	B	754[A]	HEM	CBA-CAA-C2A	-3.42	106.18	112.49
4	C	760[D]	HDD	C4A-C3A-C2A	3.33	109.31	107.00
4	B	760[D]	HDD	CMC-C2C-C1C	-3.27	123.44	128.46
2	B	755[C]	HEM	CBA-CAA-C2A	-3.26	106.47	112.49
3	A	761[B]	HDE	C4D-CHA-C1A	-3.25	123.67	130.12
3	B	761[B]	HDE	C4D-CHA-C1A	-3.23	123.72	130.12
3	D	761[B]	HDE	C4B-CHC-C1C	3.18	120.62	112.87
3	C	761[B]	HDE	C1B-CHB-C4A	-3.13	123.92	130.12
4	B	760[D]	HDD	CBA-CAA-C2A	-3.13	106.71	112.49
2	B	754[A]	HEM	CMA-C3A-C4A	-3.13	123.66	128.46
3	B	761[B]	HDE	C1B-CHB-C4A	-3.13	123.93	130.12
3	A	761[B]	HDE	CHC-C1C-C2C	-3.12	124.32	129.53
3	B	761[B]	HDE	ONA-C3A-C4A	3.10	118.20	111.92
2	D	754[A]	HEM	C3B-C4B-NB	-3.09	105.21	109.21
2	A	755[C]	HEM	CMB-C2B-C3B	3.09	130.46	124.68
3	B	761[B]	HDE	C1C-C2C-C3C	-3.04	102.57	105.81
3	D	761[B]	HDE	CAB-C3B-C4B	-3.04	123.53	127.19
2	C	754[A]	HEM	CMA-C3A-C4A	-3.03	123.81	128.46
2	B	754[A]	HEM	C4A-C3A-C2A	2.99	109.08	107.00
4	C	760[D]	HDD	CMA-C3A-C4A	-2.99	123.88	128.46
4	B	760[D]	HDD	C3C-C4C-NC	-2.98	105.36	109.21
2	A	755[C]	HEM	CBA-CAA-C2A	-2.98	107.00	112.49
3	C	761[B]	HDE	C1D-C2D-C3D	-2.98	102.64	105.81
3	B	761[B]	HDE	O1A-CGA-O2A	2.96	123.44	120.80
2	D	755[C]	HEM	CMB-C2B-C3B	2.94	130.18	124.68
2	C	755[C]	HEM	C4C-C3C-C2C	2.93	108.95	106.90
2	C	754[A]	HEM	C1D-C2D-C3D	-2.90	104.98	107.00
4	B	760[D]	HDD	CMA-C3A-C4A	-2.90	124.01	128.46
2	A	754[A]	HEM	CAA-CBA-CGA	-2.89	107.82	112.67
3	B	761[B]	HDE	CHB-C4A-NA	-2.87	119.99	124.20
4	C	760[D]	HDD	C3B-C4B-NB	-2.87	105.53	110.94
3	C	761[B]	HDE	C1C-C2C-C3C	-2.86	102.77	105.81
2	A	755[C]	HEM	CAA-CBA-CGA	-2.84	107.91	112.67
2	B	755[C]	HEM	CAA-CBA-CGA	-2.82	107.93	112.67
3	D	761[B]	HDE	C1B-CHB-C4A	-2.82	124.53	130.12
3	B	761[B]	HDE	C4B-CHC-C1C	2.81	119.71	112.87
2	A	754[A]	HEM	C3B-C4B-NB	-2.79	105.61	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	754[A]	HEM	CMC-C2C-C3C	2.77	129.87	124.68
3	C	761[B]	HDE	CMC-C2C-C3C	2.77	130.17	124.94
3	D	761[B]	HDE	CMA-C3A-C4A	-2.70	107.83	112.63
4	C	760[D]	HDD	C3C-C4C-NC	-2.66	105.77	109.21
3	A	761[B]	HDE	C1D-C2D-C3D	-2.66	102.98	105.81
2	C	754[A]	HEM	CAA-CBA-CGA	-2.66	108.21	112.67
3	C	761[B]	HDE	CAA-CBA-CGA	-2.65	100.46	104.56
2	A	754[A]	HEM	C4A-C3A-C2A	2.65	108.84	107.00
2	C	754[A]	HEM	CMB-C2B-C3B	2.60	129.55	124.68
2	A	754[A]	HEM	C4C-C3C-C2C	2.56	108.69	106.90
3	A	761[B]	HDE	C4C-C3C-C2C	2.55	109.73	105.93
3	A	761[B]	HDE	C4B-CHC-C1C	2.53	119.04	112.87
2	C	754[A]	HEM	C3B-C4B-NB	-2.53	105.94	109.21
3	D	761[B]	HDE	C1C-C2C-C3C	-2.52	103.12	105.81
4	D	760[D]	HDD	O1D-CGD-CBD	-2.50	107.66	110.19
3	B	761[B]	HDE	CMA-C3A-C4A	-2.49	108.21	112.63
4	D	760[D]	HDD	CMC-C2C-C1C	-2.47	124.67	128.46
4	D	760[D]	HDD	CMB-C2B-C3B	2.45	129.27	124.68
3	C	761[B]	HDE	CHC-C1C-C2C	-2.44	125.44	129.53
3	C	761[B]	HDE	CAC-C3C-C4C	-2.44	124.26	127.19
2	B	754[A]	HEM	C3B-C4B-NB	-2.43	106.07	109.21
3	D	761[B]	HDE	C4D-CHA-C1A	-2.41	125.34	130.12
3	A	761[B]	HDE	ONA-C3A-C4A	-2.41	107.03	111.92
3	B	761[B]	HDE	CBD-CAD-C3D	-2.39	108.07	112.49
2	C	754[A]	HEM	C3C-C4C-NC	-2.38	106.45	110.94
3	C	761[B]	HDE	CHB-C4A-NA	-2.37	120.72	124.20
3	C	761[B]	HDE	C4D-CHA-C1A	-2.36	125.44	130.12
3	A	761[B]	HDE	CBC-CAC-C3C	2.36	118.27	112.27
4	A	760[D]	HDD	C3B-C4B-NB	-2.33	106.54	110.94
2	D	754[A]	HEM	CAA-CBA-CGA	-2.33	108.76	112.67
3	B	761[B]	HDE	O1A-C2A-C1A	2.32	112.97	108.25
3	D	761[B]	HDE	CBC-CAC-C3C	2.31	118.15	112.27
2	D	754[A]	HEM	C1D-C2D-C3D	-2.27	105.42	107.00
3	D	761[B]	HDE	CMD-C2D-C3D	2.26	129.20	124.94
2	C	755[C]	HEM	CMC-C2C-C3C	2.24	128.88	124.68
4	C	760[D]	HDD	CHA-C4D-ND	-2.23	120.93	124.20
4	C	760[D]	HDD	O1D-CGD-CBD	-2.23	107.94	110.19
4	B	760[D]	HDD	C1A-CHA-C4D	-2.19	125.79	130.12
3	B	761[B]	HDE	C1B-C2B-C3B	-2.18	105.48	107.00
2	B	754[A]	HEM	C1D-C2D-C3D	-2.16	105.49	107.00
2	D	754[A]	HEM	CMB-C2B-C3B	2.15	128.70	124.68
4	D	760[D]	HDD	C3B-C4B-NB	-2.13	106.92	110.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	761[B]	HDE	CAD-C3D-C2D	2.12	133.34	127.25
3	B	761[B]	HDE	CBC-CAC-C3C	2.08	117.57	112.27
4	D	760[D]	HDD	CMA-C3A-C4A	-2.07	125.28	128.46
3	D	761[B]	HDE	CBB-CAB-C3B	-2.06	107.02	112.27
2	D	755[C]	HEM	C4A-C3A-C2A	2.04	108.41	107.00
4	D	760[D]	HDD	CHA-C4D-ND	-2.04	121.22	124.20
3	A	761[B]	HDE	CMA-C3A-C4A	-2.02	109.04	112.63
2	B	755[C]	HEM	C1D-C2D-C3D	-2.02	105.59	107.00
4	B	760[D]	HDD	O1D-C3D-CAD	2.02	106.80	103.01
4	C	760[D]	HDD	OND-C2D-C1D	-2.01	107.85	111.92
3	D	761[B]	HDE	C3A-C4A-CHB	-2.00	120.97	124.28

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	761[B]	HDE	C2B-C3B-CAB-CBB
3	C	761[B]	HDE	C4B-C3B-CAB-CBB
3	C	761[B]	HDE	C2C-C3C-CAC-CBC
3	C	761[B]	HDE	C4C-C3C-CAC-CBC
3	B	761[B]	HDE	C2B-C3B-CAB-CBB
3	B	761[B]	HDE	C4B-C3B-CAB-CBB
3	B	761[B]	HDE	C2C-C3C-CAC-CBC
3	B	761[B]	HDE	C4C-C3C-CAC-CBC
3	D	761[B]	HDE	C2B-C3B-CAB-CBB
3	D	761[B]	HDE	C4B-C3B-CAB-CBB
3	D	761[B]	HDE	C2C-C3C-CAC-CBC
3	D	761[B]	HDE	C4C-C3C-CAC-CBC
3	A	761[B]	HDE	C2B-C3B-CAB-CBB
3	A	761[B]	HDE	C4B-C3B-CAB-CBB
3	A	761[B]	HDE	C2C-C3C-CAC-CBC
3	A	761[B]	HDE	C4C-C3C-CAC-CBC

There are no ring outliers.

15 monomers are involved in 73 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	761[B]	HDE	7	0
3	B	761[B]	HDE	4	0
3	D	761[B]	HDE	4	0
2	C	754[A]	HEM	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	754[A]	HEM	3	0
4	A	760[D]	HDD	5	0
4	C	760[D]	HDD	6	0
2	D	755[C]	HEM	4	0
4	D	760[D]	HDD	4	0
2	C	755[C]	HEM	6	0
2	B	754[A]	HEM	5	0
2	B	755[C]	HEM	5	0
4	B	760[D]	HDD	6	0
2	A	755[C]	HEM	5	0
3	A	761[B]	HDE	7	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 HDE C 761 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand HDE B 761 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand HDE D 761 (B)

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM C 754 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 754 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM D 754 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand HDD A 760 (D)

Bond lengths

Bond angles

Torsions

Rings

Ligand HDD C 760 (D)

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM D 755 (C)

Bond lengths

Bond angles

Torsions

Rings

Ligand HDD D 760 (D)

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM C 755 (C)

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM B 754 (A)

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM B 755 (C)

Bond lengths

Bond angles

Torsions

Rings

Ligand HDD B 760 (D)

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 755 (C)

Bond lengths

Bond angles

Torsions

Rings

Ligand HDE A 761 (B)

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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(Å²)	Q<0.9
1	A	726/753 (96%)	-0.34	22 (3%)	50	55	3, 10, 28, 48	1 (0%)
1	B	726/753 (96%)	-0.17	38 (5%)	27	30	3, 11, 34, 50	1 (0%)
1	C	726/753 (96%)	-0.26	31 (4%)	35	39	3, 11, 33, 50	1 (0%)
1	D	726/753 (96%)	-0.34	16 (2%)	62	67	3, 9, 28, 48	0
All	All	2904/3012 (96%)	-0.28	107 (3%)	41	46	3, 10, 31, 50	3 (0%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	726	GLY	7.2
1	D	28	SER	5.5
1	B	32	GLU	5.0
1	A	32	GLU	4.7
1	B	673	ALA	4.6
1	B	712	ASP	4.5
1	B	647	VAL	4.4
1	D	749	ASP	4.4
1	A	726	GLY	4.2
1	D	750	LYS	4.2
1	B	711	ALA	4.1
1	B	28	SER	4.1
1	B	677	ASP	4.0
1	B	645	GLY	3.8
1	B	611	VAL	3.8
1	B	713	GLN	3.7
1	C	711	ALA	3.7
1	B	646	THR	3.6
1	A	33	ASP	3.6
1	C	641	THR	3.6
1	C	712	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	726	GLY	3.5
1	B	596	GLY	3.5
1	A	749	ASP	3.5
1	D	712	ASP	3.4
1	A	29	LEU	3.4
1	D	33	ASP	3.4
1	B	725	ASP	3.4
1	C	645	GLY	3.3
1	C	594	PRO	3.3
1	D	751	ILE	3.3
1	B	609	ASP	3.3
1	B	641	THR	3.2
1	C	677	ASP	3.2
1	B	749	ASP	3.1
1	B	568	ASP	3.1
1	A	28	SER	3.1
1	C	750	LYS	3.1
1	B	727	SER	3.1
1	C	643	ASP	3.1
1	D	713	GLN	3.0
1	C	751	ILE	3.0
1	C	28	SER	3.0
1	A	34	GLY	3.0
1	B	33	ASP	3.0
1	A	713	GLN	2.9
1	A	710	ILE	2.9
1	C	673	ALA	2.9
1	B	750	LYS	2.9
1	A	39	ALA	2.9
1	A	37	ARG	2.9
1	C	644	ASP	2.9
1	B	610	GLU	2.8
1	D	32	GLU	2.8
1	C	568	ASP	2.8
1	C	725	ASP	2.8
1	D	711	ALA	2.8
1	A	712	ASP	2.7
1	D	596	GLY	2.7
1	C	595	ASP	2.7
1	B	572	ASN	2.7
1	A	31	PRO	2.7
1	B	583	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	596	GLY	2.7
1	A	750	LYS	2.7
1	C	675	ILE	2.6
1	B	642	ALA	2.6
1	B	644	ASP	2.6
1	C	552	LEU	2.6
1	A	35	SER	2.6
1	C	703	LYS	2.5
1	C	727	SER	2.5
1	B	617	LEU	2.5
1	C	646	THR	2.5
1	A	725	ASP	2.5
1	A	596	GLY	2.5
1	A	594	PRO	2.4
1	D	583	LYS	2.4
1	C	713	GLN	2.4
1	C	647	VAL	2.4
1	B	672	ILE	2.4
1	C	714	GLY	2.4
1	A	751	ILE	2.4
1	B	722	ASP	2.3
1	A	711	ALA	2.3
1	B	723	SER	2.3
1	B	614	ALA	2.3
1	B	709	LYS	2.2
1	C	583	LYS	2.2
1	B	574	THR	2.2
1	B	34	GLY	2.2
1	C	569	ASP	2.2
1	C	722	ASP	2.2
1	B	671	ASN	2.2
1	C	749	ASP	2.1
1	D	569	ASP	2.1
1	B	571	LEU	2.1
1	D	677	ASP	2.1
1	B	569	ASP	2.1
1	D	35	SER	2.1
1	A	30	ALA	2.1
1	C	674	ASP	2.1
1	D	568	ASP	2.1
1	D	710	ILE	2.0
1	C	572	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	36	HIS	2.0
1	B	595	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
3	HDE	C	761[B]	44/44	0.99	0.06	2,2,4,12	44
3	HDE	B	761[B]	44/44	0.99	0.07	2,3,6,11	44
3	HDE	D	761[B]	44/44	0.99	0.06	2,2,6,10	44
2	HEM	C	754[A]	43/43	0.99	0.06	2,4,6,8	43
2	HEM	A	754[A]	43/43	0.99	0.06	2,3,4,5	43
2	HEM	D	754[A]	43/43	0.99	0.06	2,2,6,8	43
4	HDD	A	760[D]	44/44	0.99	0.06	2,2,3,6	44
4	HDD	C	760[D]	44/44	0.99	0.06	2,3,7,9	44
2	HEM	D	755[C]	43/43	0.99	0.06	2,2,7,8	43
4	HDD	D	760[D]	44/44	0.99	0.06	2,2,4,7	44
2	HEM	C	755[C]	43/43	0.99	0.06	2,5,8,11	43
2	HEM	B	754[A]	43/43	0.99	0.07	2,4,7,9	43
2	HEM	B	755[C]	43/43	0.99	0.07	2,4,9,12	43
4	HDD	B	760[D]	44/44	0.99	0.07	2,3,5,7	44
2	HEM	A	755[C]	43/43	0.99	0.06	2,4,7,10	43
3	HDE	A	761[B]	44/44	0.99	0.06	2,2,4,7	44

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 HDE C 761 (B):

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
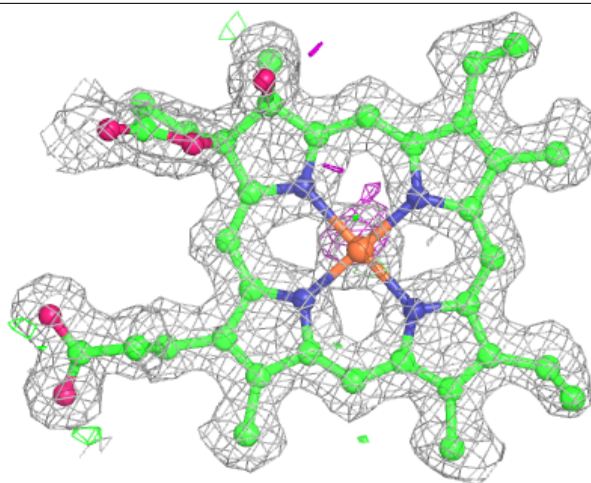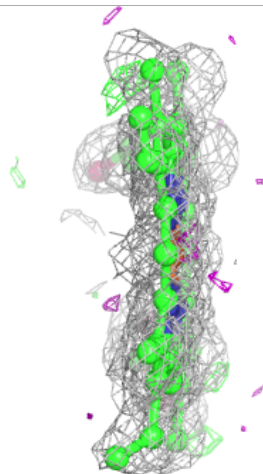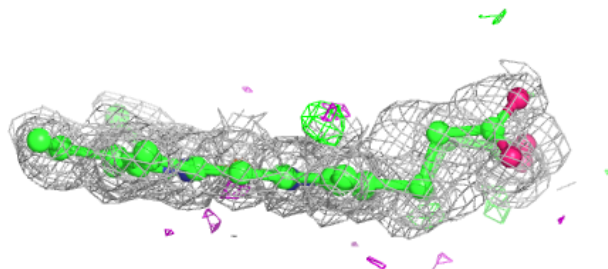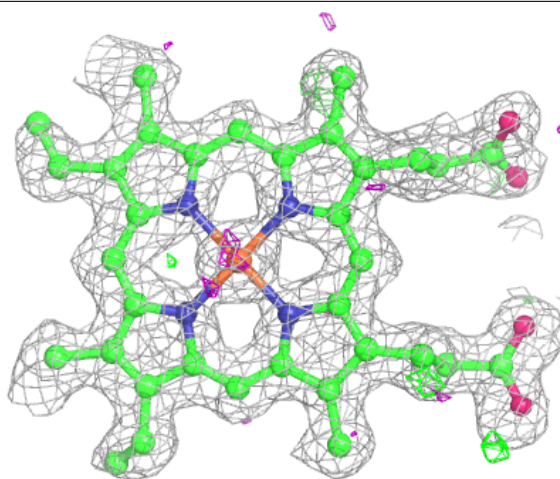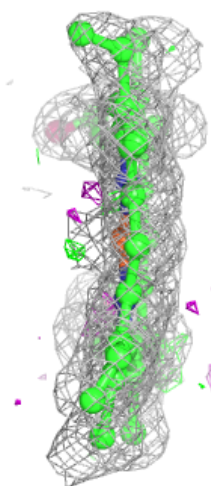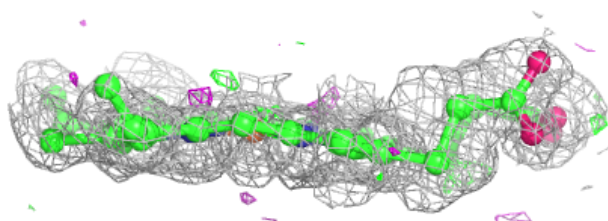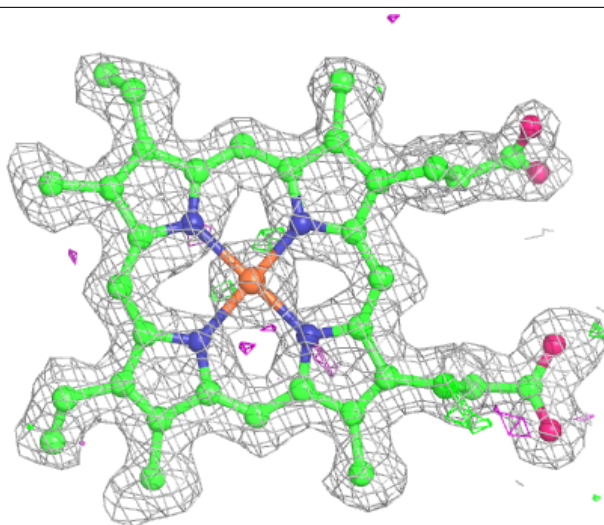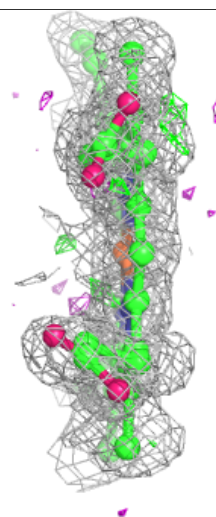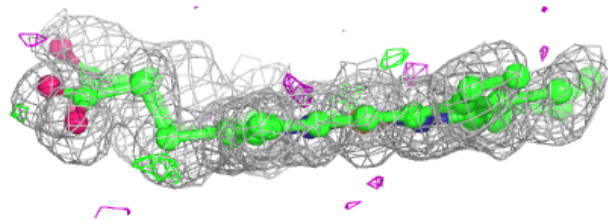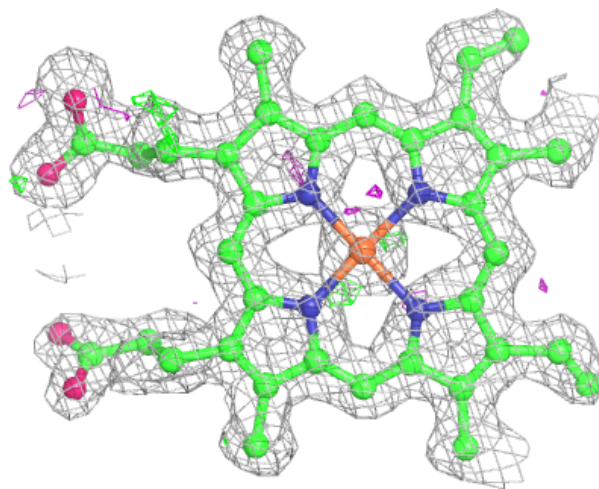$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
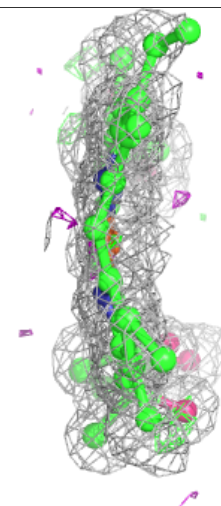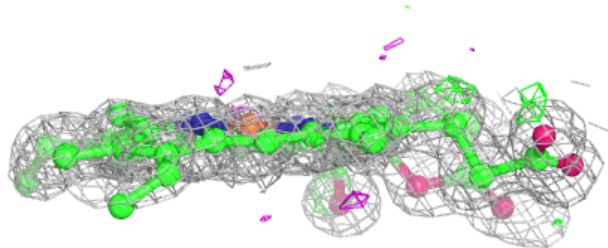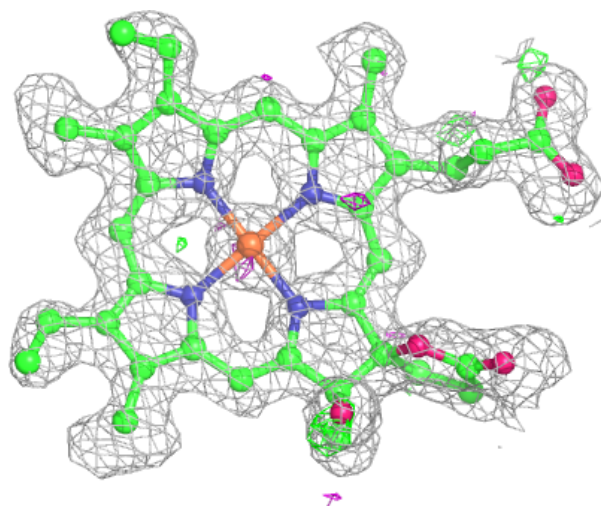
Electron density around HDE B 761 (B):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
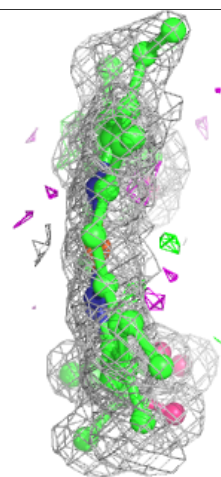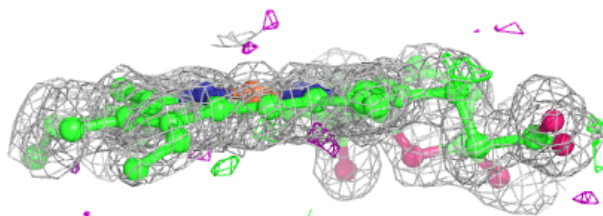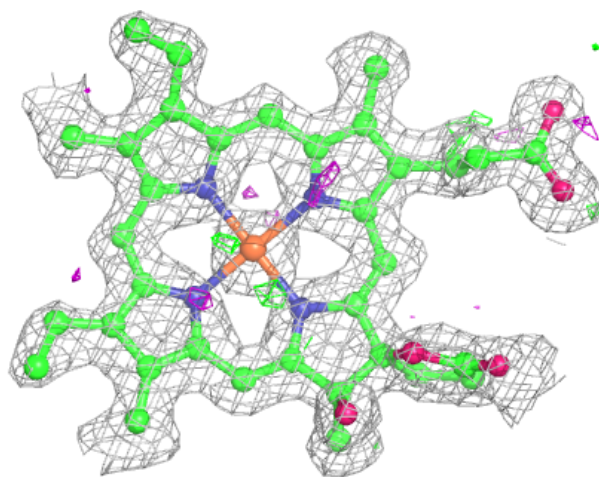
Electron density around HDE D 761 (B):

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
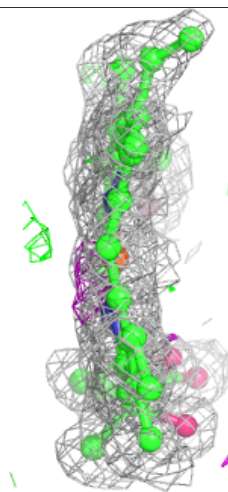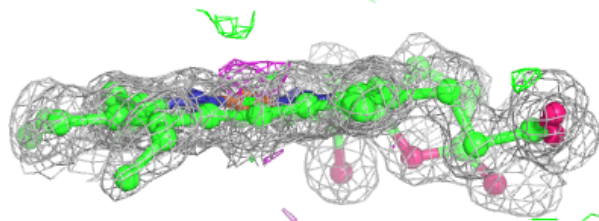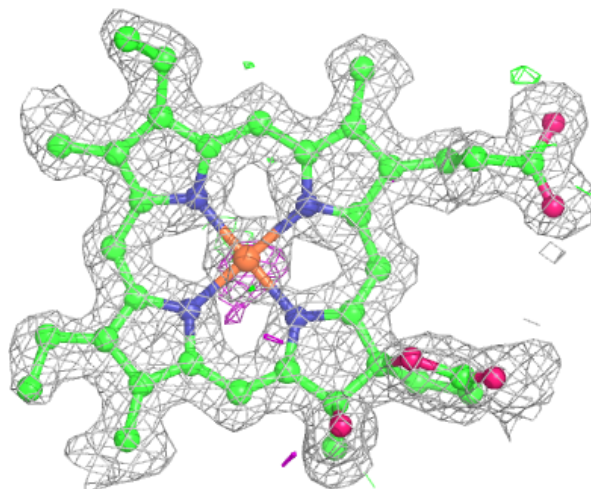
Electron density around HEM C 754 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
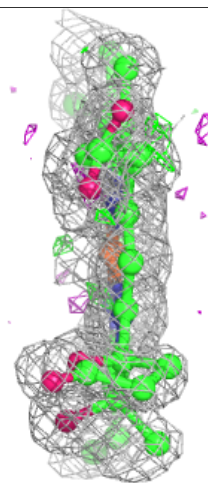mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
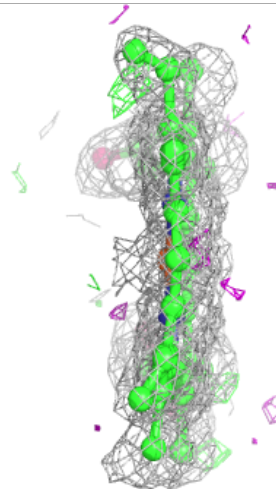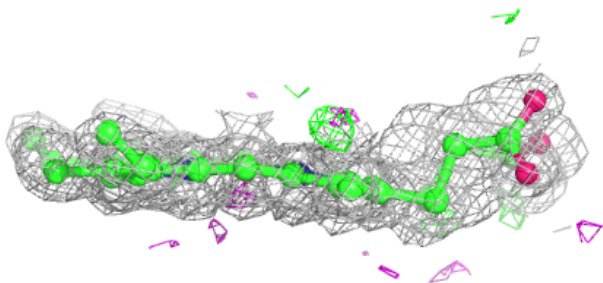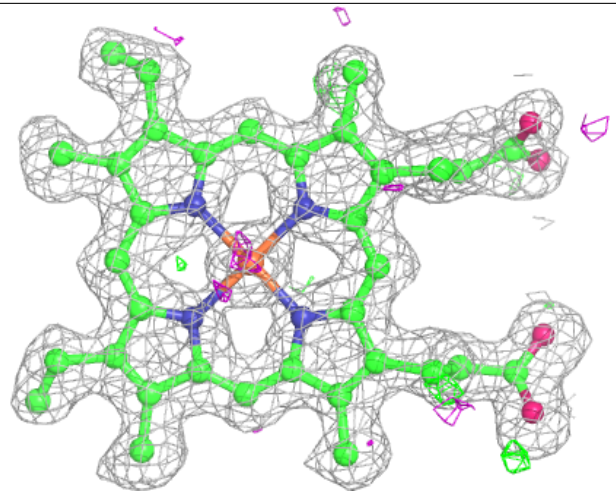
Electron density around HEM A 754 (A):

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
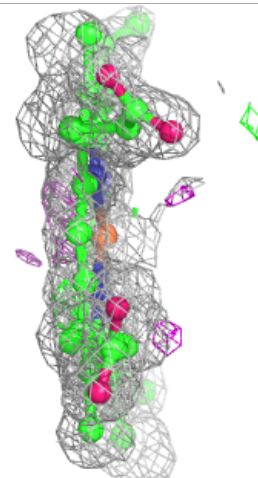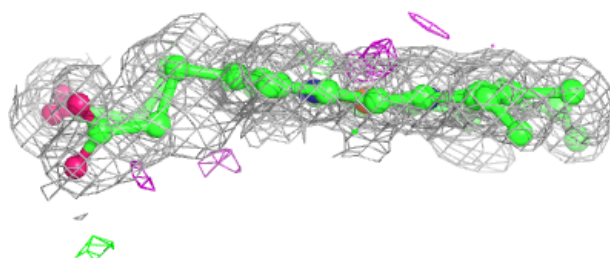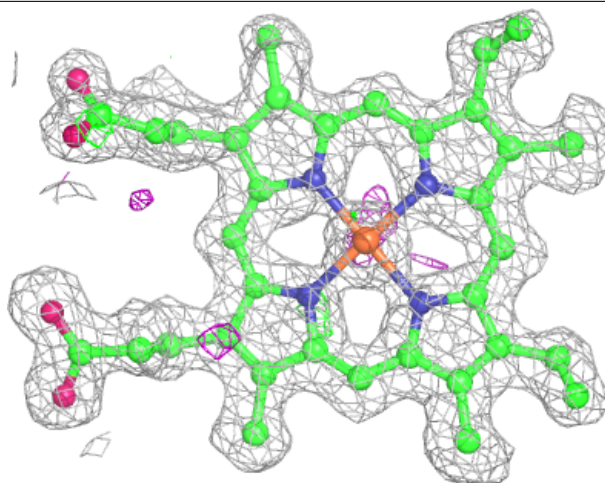
Electron density around HEM D 754 (A):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
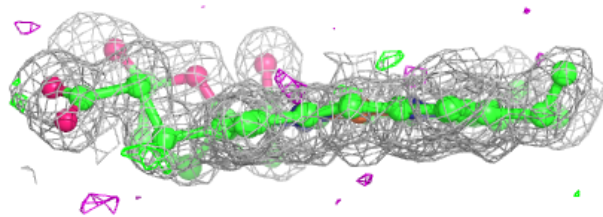mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
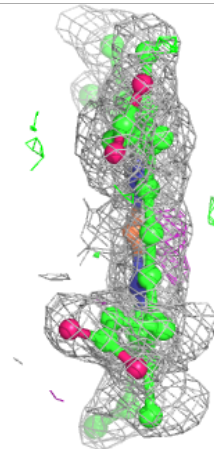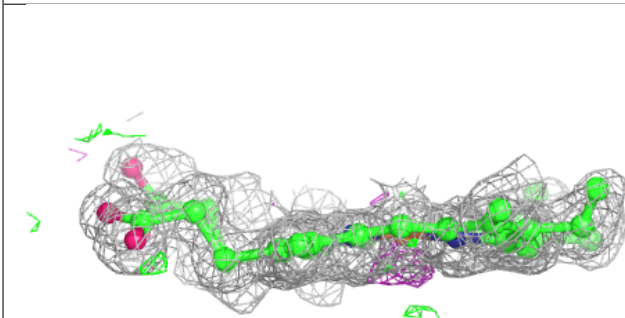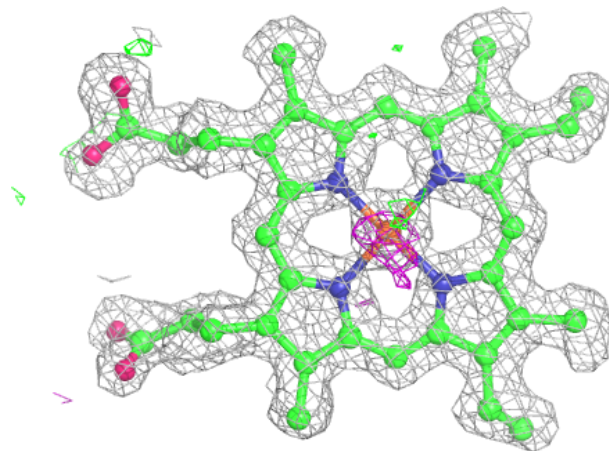
Electron density around HDD A 760 (D):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
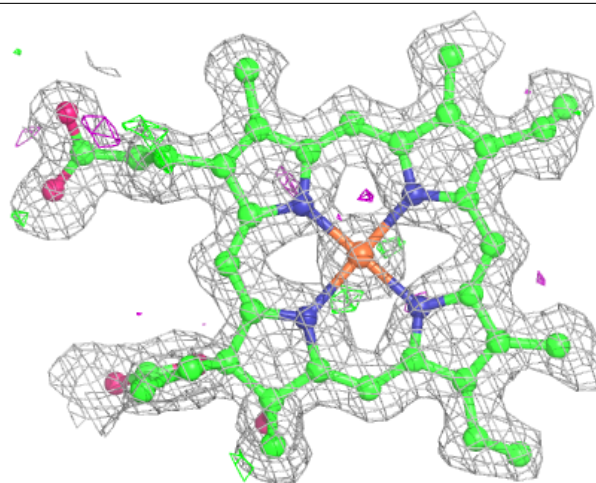and green (positive)
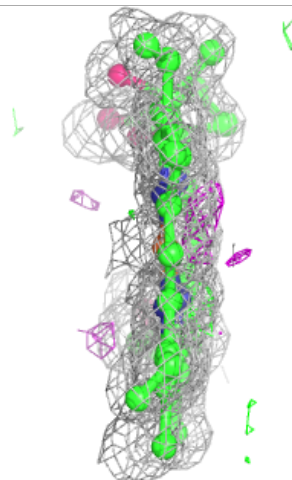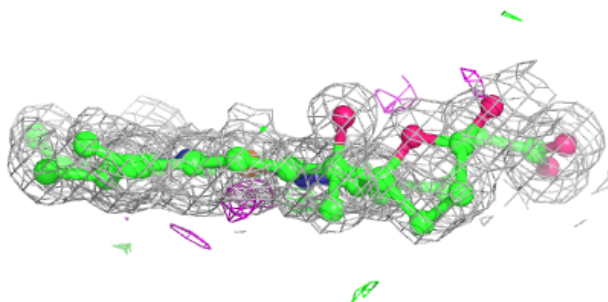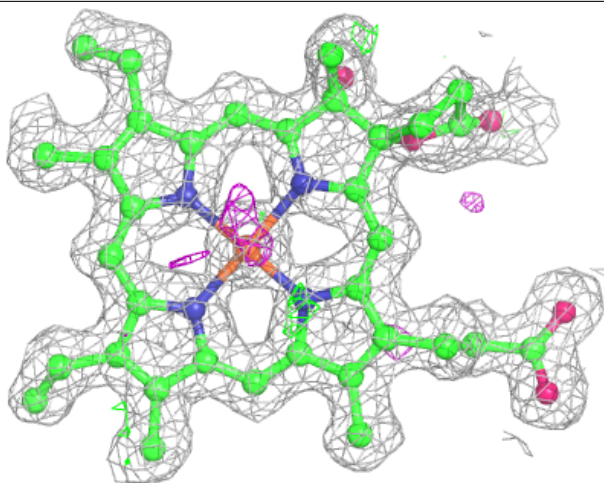
Electron density around HDD C 760 (D):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
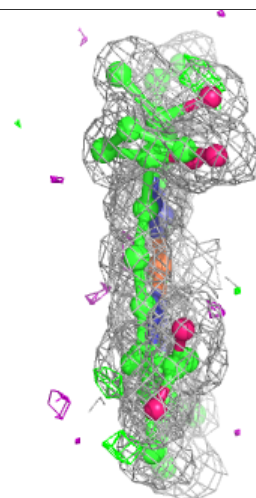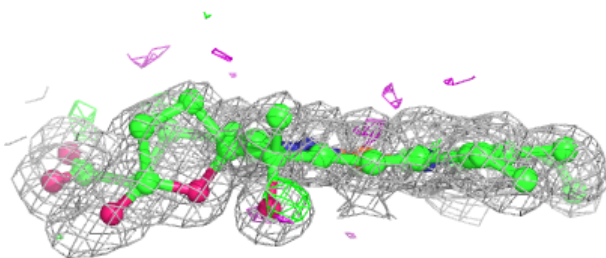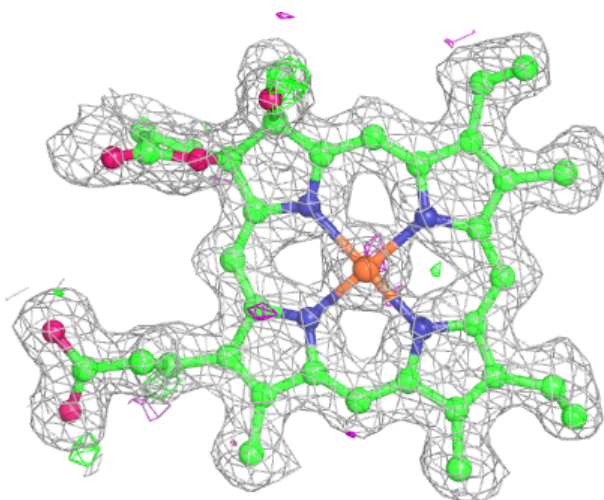
Electron density around HEM D 755 (C):

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
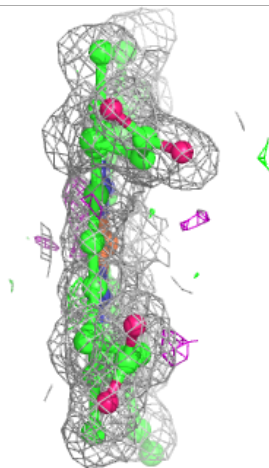$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
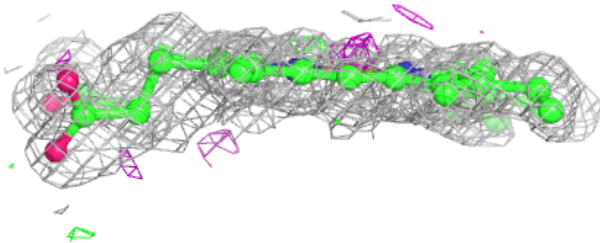and green (positive)
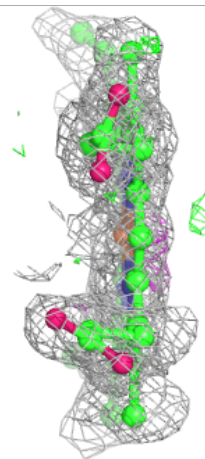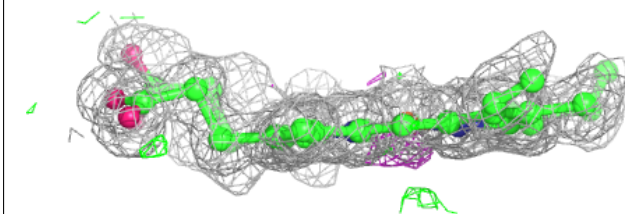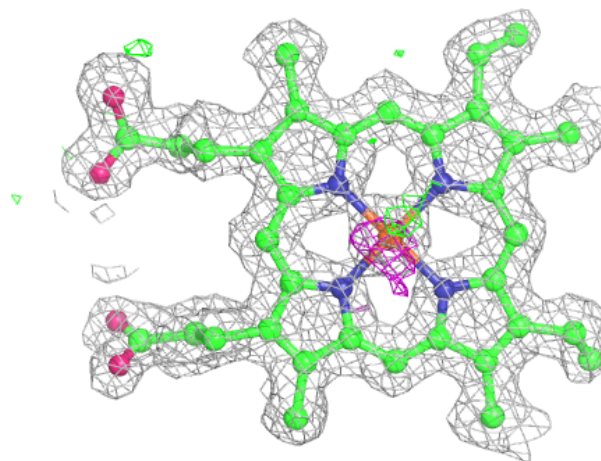
Electron density around HDD D 760 (D):

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
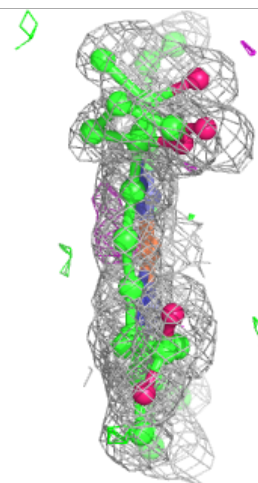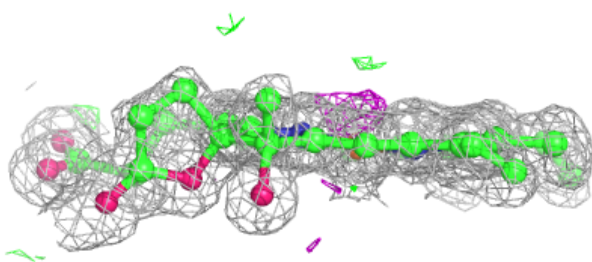
Electron density around HEM C 755 (C):

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

Electron density around HEM B 754 (A):

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

Electron density around HEM B 755 (C):

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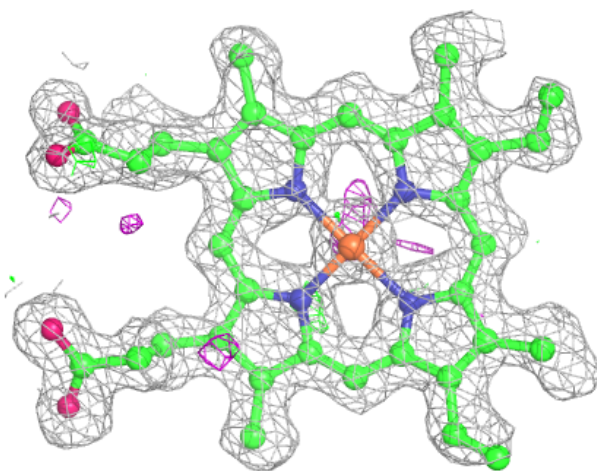mF_o-DF_c (at 3 rmsd) in purple (negative)
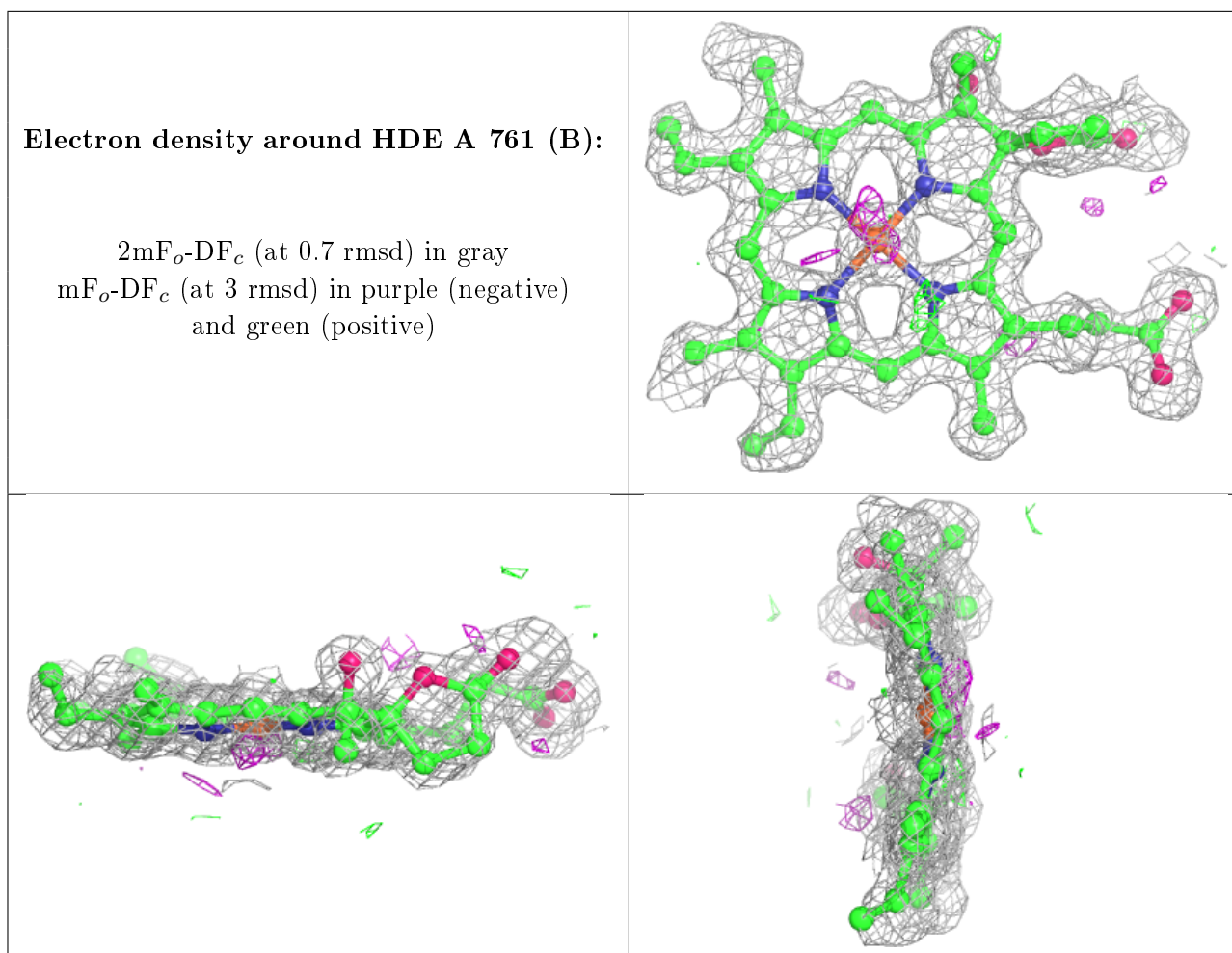and green (positive)

Electron density around HDD B 760 (D):

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

Electron density around HEM A 755 (C):

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

Electron density around HDE A 761 (B):

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

6.5 Other polymers ⓘ

There are no such residues in this entry.