Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 03:59 PM EDT

PDB ID	:	1QF7 / pdb_00001qf7
Title	:	STRUCTURE OF THE MUTANT HIS392GLN OF CATALASE HPII FROM E. COLI
Authors	:	Mate, M.J.; Loewen, P.C.; Fita, I.
Deposited on	:	1999-03-26
Resolution	:	2.20 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:

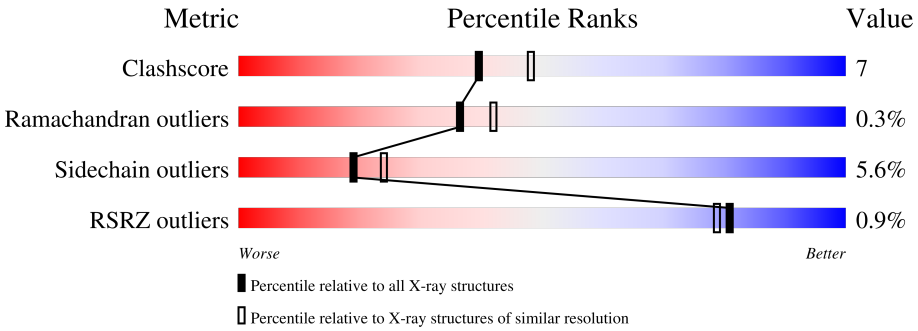
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	753	2% 72% 20%
1	B	753	73% 20%
1	C	753	% 71% 20% 5%
1	D	753	% 73% 20%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 25843 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.

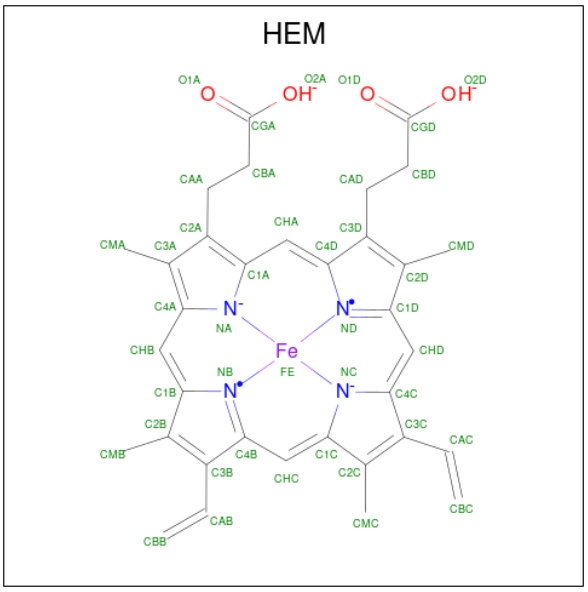
- Molecule 1 is a protein called PROTEIN (CATALASE HPII).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	1	0
			5748	3650	1004	1082	12			
1	B	727	Total	C	N	O	S	0	1	0
			5748	3650	1004	1082	12			
1	C	727	Total	C	N	O	S	0	1	0
			5748	3650	1004	1082	12			
1	D	727	Total	C	N	O	S	0	1	0
			5748	3650	1004	1082	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	392	GLN	HIS	engineered mutation	UNP P21179
B	392	GLN	HIS	engineered mutation	UNP P21179
C	392	GLN	HIS	engineered mutation	UNP P21179
D	392	GLN	HIS	engineered mutation	UNP P21179

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is water.

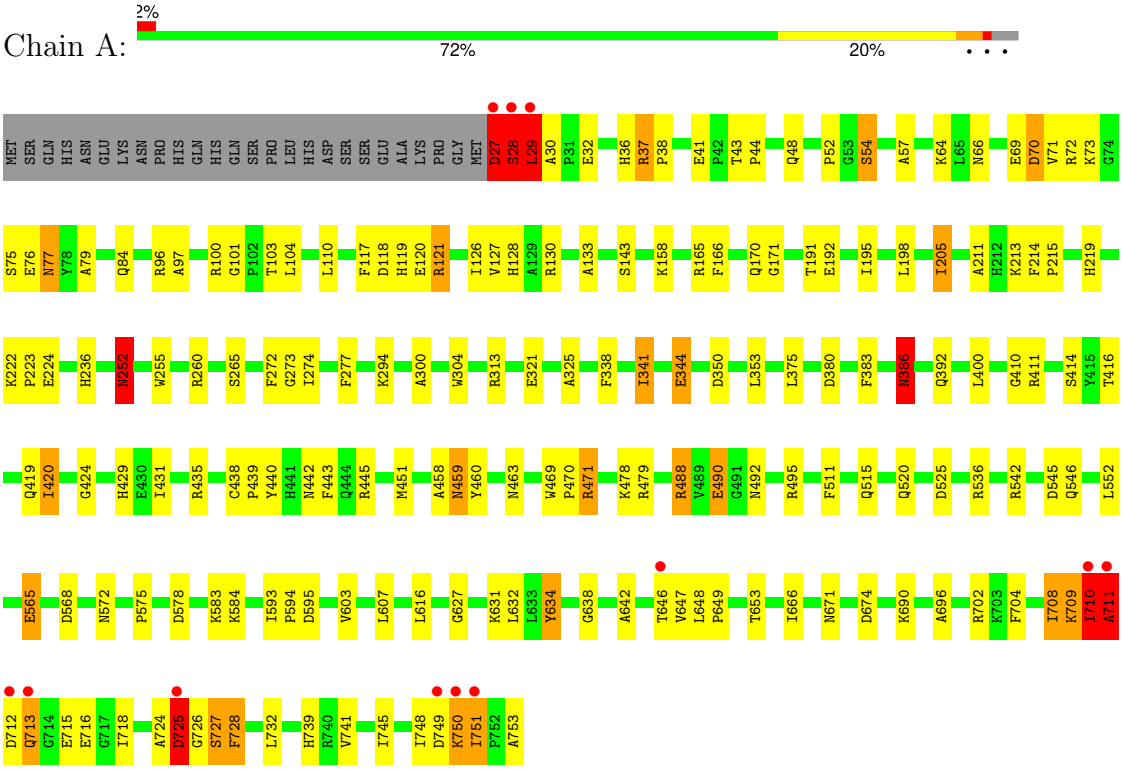
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	728	Total	O	0	0
			728	728		
3	B	625	Total	O	0	0
			625	625		
3	C	634	Total	O	0	0
			634	634		
3	D	692	Total	O	0	0
			692	692		

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.

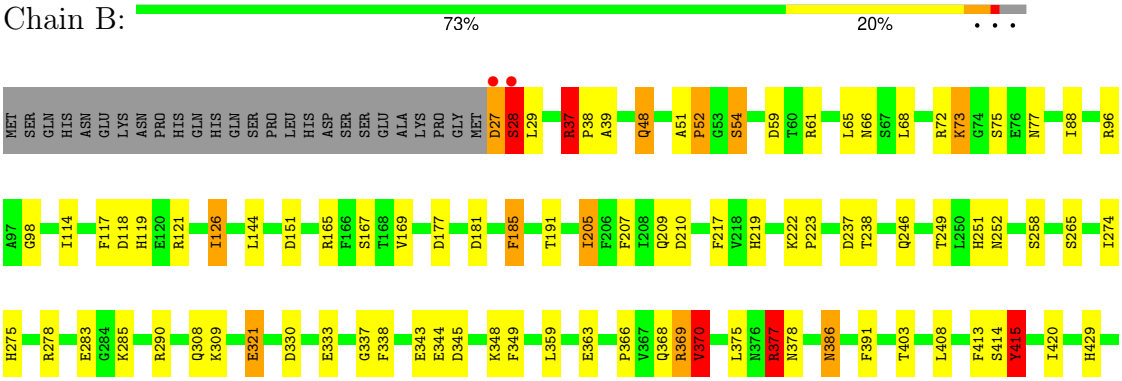
• Molecule 1: PROTEIN (CATALASE HPII)

Chain A:



• Molecule 1: PROTEIN (CATALASE HPII)

Chain B:

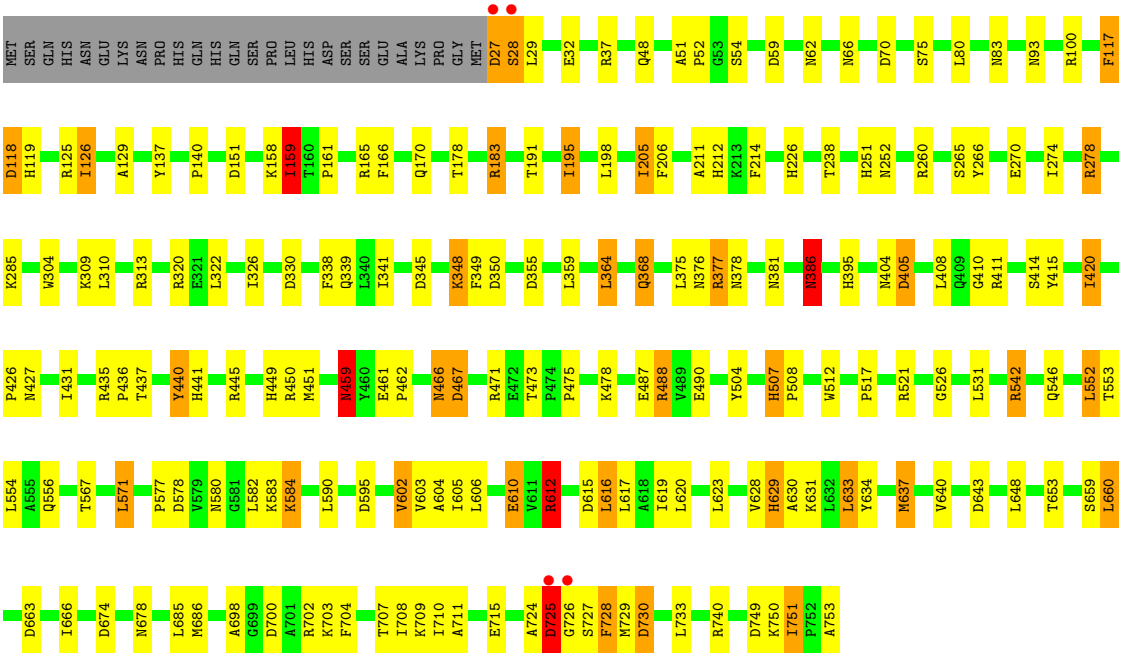




• Molecule 1: PROTEIN (CATALASE HPII)

Chain C:

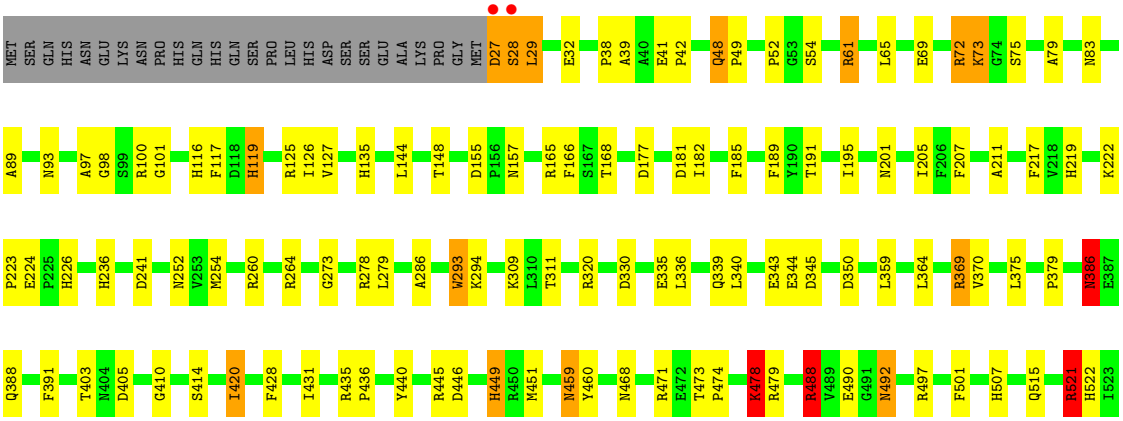


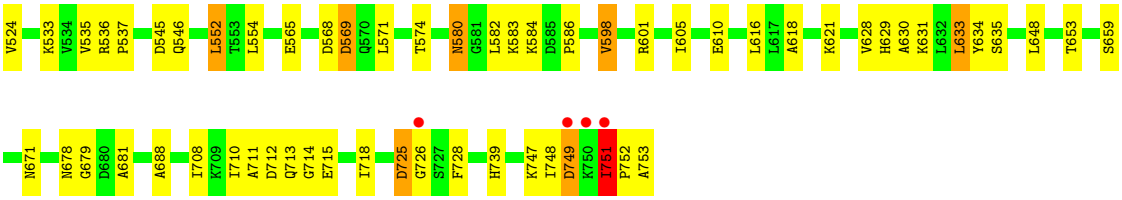


• Molecule 1: PROTEIN (CATALASE HPII)

Chain D:






V524
K533
V534
V535
R536
P537
D545
Q546
L552
T553
L554
E565
D568
D569
Q570
L571
T574
N580
G581
L582
K583
K584
D585
P586
V598
R601
I605
E610
L616
L617
A618
K621
V628
H629
A630
K631
L632
L633
Y634
S635
L648
T653
S659
M671
N678
G679
D680
A681
A688
I708
K709
I710
A711
D712
Q713
G714
E715
I718
D725
G726
S727
F728
H739
K747
I748
D749
K750
I751
P752
A753

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.40Å 132.92Å 121.67Å 90.00° 109.47° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.6 (20.00-2.20) 92.7 (20.00-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.99 (at 2.19Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.144 , 0.210 0.143 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	12.3	Xtriage
Anisotropy	0.485	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 62.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	25843	wwPDB-VP
Average B, all atoms (Å^2)	19.0	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.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.97	4/5907 (0.1%)	2.06	152/8032 (1.9%)
1	B	0.93	0/5907	1.90	112/8032 (1.4%)
1	C	0.95	4/5907 (0.1%)	1.94	125/8032 (1.6%)
1	D	0.94	0/5907	1.90	121/8032 (1.5%)
All	All	0.95	8/23628 (0.0%)	1.95	510/32128 (1.6%)

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	4
1	D	0	1
All	All	0	5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	725	ASP	CA-CB	8.29	1.67	1.53
1	A	29	LEU	N-CA	-7.56	1.36	1.46
1	C	725	ASP	N-CA	-5.84	1.38	1.46
1	A	710	ILE	N-CA	5.83	1.52	1.46
1	C	161	PRO	C-O	5.16	1.29	1.23
1	A	29	LEU	CA-CB	5.11	1.62	1.53
1	C	542	ARG	CD-NE	-5.09	1.39	1.46
1	A	30	ALA	N-CA	-5.02	1.39	1.45

All (510) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	27	ASP	CA-CB-CG	45.77	158.37	112.60
1	C	542	ARG	CD-NE-CZ	36.82	175.94	124.40
1	C	725	ASP	N-CA-C	24.34	162.65	110.80
1	A	29	LEU	CA-C-O	24.25	155.19	120.51
1	D	488	ARG	CD-NE-CZ	24.10	158.14	124.40
1	C	27	ASP	CA-CB-CG	-24.00	88.60	112.60
1	A	710	ILE	CB-CA-C	23.84	148.84	110.69
1	D	61	ARG	CD-NE-CZ	23.21	156.90	124.40
1	D	449	HIS	CA-CB-CG	18.09	131.89	113.80
1	C	725	ASP	CA-CB-CG	16.43	129.03	112.60
1	B	707	THR	N-CA-CB	14.62	132.94	110.28
1	B	27	ASP	CA-CB-CG	-14.12	98.48	112.60
1	A	710	ILE	O-C-N	-13.62	108.43	123.00
1	A	710	ILE	CA-C-O	13.54	136.98	121.28
1	A	27	ASP	O-C-N	-13.44	101.49	123.00
1	A	29	LEU	CA-C-N	13.34	138.93	120.39
1	A	29	LEU	C-N-CA	13.34	138.93	120.39
1	A	712	ASP	CA-C-O	13.31	135.28	119.97
1	D	725	ASP	CA-CB-CG	13.19	125.79	112.60
1	A	712	ASP	CB-CA-C	13.02	135.66	110.67
1	A	28	SER	CA-C-N	-12.33	97.99	121.54
1	A	28	SER	C-N-CA	-12.33	97.99	121.54
1	B	28	SER	N-CA-CB	11.91	130.62	110.49
1	B	59	ASP	CA-CB-CG	-11.89	100.71	112.60
1	B	377	ARG	NE-CZ-NH2	11.65	129.68	119.20
1	A	713	GLN	N-CA-CB	-11.45	91.18	110.41
1	A	471	ARG	NE-CZ-NH2	11.27	129.34	119.20
1	D	28	SER	CA-C-N	-11.17	100.97	121.52
1	D	28	SER	C-N-CA	-11.17	100.97	121.52
1	A	414	SER	N-CA-C	11.03	123.30	111.28
1	A	712	ASP	N-CA-CB	-11.00	93.23	110.28
1	D	29	LEU	CB-CA-C	10.96	131.71	109.67
1	B	377	ARG	NE-CZ-NH1	-10.84	110.66	121.50
1	C	615	ASP	CA-CB-CG	10.82	123.42	112.60
1	B	612	ARG	CD-NE-CZ	10.61	139.25	124.40
1	A	712	ASP	O-C-N	-10.58	109.26	122.27
1	C	725	ASP	N-CA-CB	-10.47	92.80	110.49
1	B	391	PHE	CA-CB-CG	10.34	124.14	113.80
1	D	711	ALA	CA-C-O	10.20	132.46	121.44
1	C	28	SER	CA-C-N	-10.20	103.35	120.68
1	C	28	SER	C-N-CA	-10.20	103.35	120.68
1	A	709	LYS	CA-C-N	-10.19	106.49	122.69
1	A	709	LYS	C-N-CA	-10.19	106.49	122.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	753	ALA	CA-C-O	-10.16	103.52	120.80
1	C	725	ASP	CB-CA-C	-10.06	90.40	110.42
1	B	521	ARG	CD-NE-CZ	10.01	138.42	124.40
1	A	70	ASP	CA-CB-CG	10.00	122.60	112.60
1	C	29	LEU	CB-CA-C	9.51	129.79	110.38
1	B	29	LEU	CB-CA-C	9.51	128.78	109.67
1	A	121	ARG	CD-NE-CZ	9.49	137.69	124.40
1	A	29	LEU	N-CA-C	9.38	130.78	110.80
1	D	369	ARG	CD-NE-CZ	9.37	137.52	124.40
1	B	414	SER	N-CA-C	9.28	121.47	111.36
1	A	28	SER	CB-CA-C	-9.24	92.55	110.10
1	A	28	SER	CA-CB-OG	9.23	129.56	111.10
1	B	338	PHE	CA-CB-CG	9.20	123.00	113.80
1	B	753	ALA	CA-C-O	-9.15	105.25	120.80
1	D	414	SER	N-CA-C	9.14	121.25	111.28
1	D	28	SER	O-C-N	9.13	134.73	122.59
1	A	753	ALA	CA-C-O	-9.07	105.37	120.80
1	D	725	ASP	N-CA-C	9.02	130.02	110.80
1	C	674	ASP	CA-CB-CG	8.96	121.56	112.60
1	D	546	GLN	OE1-CD-NE2	-8.93	113.67	122.60
1	B	217	PHE	CA-CB-CG	-8.87	104.93	113.80
1	A	30	ALA	N-CA-C	-8.82	98.44	109.64
1	D	207	PHE	CA-CB-CG	8.79	122.59	113.80
1	B	601	ARG	CD-NE-CZ	8.71	136.60	124.40
1	D	678	ASN	OD1-CG-ND2	-8.68	113.92	122.60
1	A	711	ALA	CA-C-O	8.65	132.88	120.51
1	B	617	LEU	CB-CA-C	-8.63	97.33	110.88
1	C	678	ASN	CA-CB-CG	-8.58	104.02	112.60
1	B	77	ASN	CA-CB-CG	-8.58	104.02	112.60
1	D	189	PHE	CA-CB-CG	8.55	122.35	113.80
1	A	725	ASP	N-CA-C	8.52	128.94	110.80
1	A	479	ARG	CD-NE-CZ	8.48	136.28	124.40
1	C	414	SER	N-CA-C	8.45	120.49	111.28
1	B	321	GLU	CA-CB-CG	8.42	130.94	114.10
1	B	27	ASP	CA-C-O	8.37	135.03	120.80
1	D	536	ARG	NE-CZ-NH1	-8.34	113.16	121.50
1	A	69	GLU	CA-C-O	-8.32	110.69	120.10
1	C	355	ASP	CA-C-O	8.32	124.70	119.29
1	A	710	ILE	CA-CB-CG1	8.28	124.47	110.40
1	B	28	SER	O-C-N	8.21	133.51	122.59
1	C	27	ASP	N-CA-C	8.18	133.90	111.00
1	B	370	VAL	CB-CA-C	8.17	118.31	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	236	HIS	CA-CB-CG	8.10	121.90	113.80
1	D	598	VAL	N-CA-CB	-8.10	93.52	111.50
1	D	52	PRO	CA-C-N	8.10	129.10	120.03
1	D	52	PRO	C-N-CA	8.10	129.10	120.03
1	B	369	ARG	CA-C-O	-8.07	111.53	120.81
1	C	542	ARG	CA-CB-CG	8.06	130.22	114.10
1	A	728	PHE	CA-CB-CG	8.05	121.85	113.80
1	C	640	VAL	N-CA-CB	8.04	125.95	112.44
1	A	711	ALA	O-C-N	-8.02	111.92	122.59
1	A	568	ASP	CA-CB-CG	-8.02	104.58	112.60
1	C	338	PHE	CA-CB-CG	8.01	121.81	113.80
1	C	663	ASP	CA-CB-CG	-7.90	104.70	112.60
1	D	488	ARG	NE-CZ-NH1	7.88	129.38	121.50
1	B	73	LYS	CA-CB-CG	7.86	129.81	114.10
1	A	710	ILE	N-CA-CB	-7.83	97.44	111.93
1	B	463	ASN	OD1-CG-ND2	-7.81	114.79	122.60
1	D	264	ARG	CD-NE-CZ	7.79	135.31	124.40
1	C	159	ILE	CB-CA-C	7.75	121.90	110.98
1	A	520	GLN	OE1-CD-NE2	-7.74	114.86	122.60
1	A	704	PHE	CA-CB-CG	7.71	121.51	113.80
1	C	100	ARG	N-CA-CB	7.71	123.92	111.20
1	D	725	ASP	CA-C-O	-7.70	109.50	120.51
1	C	28	SER	O-C-N	7.70	132.83	122.59
1	B	28	SER	CA-C-N	-7.69	107.37	121.52
1	B	28	SER	C-N-CA	-7.69	107.37	121.52
1	C	471	ARG	NE-CZ-NH2	7.68	126.12	119.20
1	C	728	PHE	CA-CB-CG	7.68	121.48	113.80
1	D	32	GLU	CB-CG-CD	7.67	125.64	112.60
1	C	339	GLN	N-CA-CB	7.64	122.88	110.42
1	B	711	ALA	CA-C-O	7.61	129.66	121.44
1	A	77	ASN	CA-CB-CG	-7.61	104.99	112.60
1	B	682	ASN	CA-CB-CG	-7.58	105.02	112.60
1	C	753	ALA	CA-C-O	-7.54	107.98	120.80
1	D	278	ARG	NE-CZ-NH2	-7.51	112.44	119.20
1	B	725	ASP	N-CA-C	7.38	126.51	110.80
1	C	368	GLN	CB-CG-CD	7.37	125.13	112.60
1	C	441	HIS	CA-CB-CG	-7.37	106.43	113.80
1	A	525	ASP	CA-CB-CG	-7.35	105.25	112.60
1	A	28	SER	N-CA-CB	7.33	122.95	110.50
1	B	185	PHE	CA-CB-CG	7.30	121.10	113.80
1	A	751	ILE	N-CA-CB	7.29	116.86	110.08
1	D	728	PHE	CA-CB-CG	7.26	121.06	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	344	GLU	CA-CB-CG	7.25	128.60	114.10
1	A	572	ASN	CA-CB-CG	-7.22	105.38	112.60
1	A	542	ARG	NE-CZ-NH2	-7.21	112.71	119.20
1	A	674	ASP	CA-CB-CG	7.17	119.77	112.60
1	A	54	SER	CA-CB-OG	-7.16	96.78	111.10
1	A	420	ILE	CA-C-O	-7.15	112.92	120.57
1	D	61	ARG	CB-CG-CD	7.13	127.69	111.30
1	B	567	THR	CA-C-N	7.12	130.69	120.79
1	B	567	THR	C-N-CA	7.12	130.69	120.79
1	D	226	HIS	CA-C-O	-7.11	113.38	120.70
1	C	629	HIS	CA-CB-CG	-7.08	106.72	113.80
1	A	419	GLN	OE1-CD-NE2	-7.06	115.54	122.60
1	A	646	THR	CA-C-O	7.05	128.92	120.81
1	C	381	ASN	CA-CB-CG	7.02	119.62	112.60
1	A	642	ALA	CA-C-O	-7.02	113.87	121.94
1	D	168	THR	CA-C-N	-7.01	116.00	123.08
1	D	168	THR	C-N-CA	-7.01	116.00	123.08
1	B	29	LEU	N-CA-CB	-7.01	99.81	110.33
1	A	260	ARG	NE-CZ-NH2	-7.01	112.89	119.20
1	B	479	ARG	CD-NE-CZ	7.00	134.20	124.40
1	B	715	GLU	CB-CG-CD	6.98	124.47	112.60
1	B	728	PHE	CA-CB-CG	6.96	120.76	113.80
1	A	490	GLU	CB-CG-CD	6.94	124.40	112.60
1	C	666	ILE	O-C-N	-6.93	115.78	123.26
1	B	492	ASN	OD1-CG-ND2	-6.92	115.68	122.60
1	A	648	LEU	CB-CA-C	-6.91	102.20	110.15
1	B	609	ASP	CA-CB-CG	6.89	119.49	112.60
1	A	66	ASN	CA-C-O	-6.88	113.12	120.42
1	C	546	GLN	OE1-CD-NE2	-6.88	115.72	122.60
1	C	251	HIS	CA-C-O	-6.88	113.61	120.70
1	D	749	ASP	CA-CB-CG	-6.85	105.75	112.60
1	A	492	ASN	CA-C-O	-6.84	113.20	121.89
1	B	707	THR	CB-CA-C	-6.83	97.56	110.67
1	C	159	ILE	CB-CG1-CD1	-6.83	99.46	113.80
1	B	440	TYR	O-C-N	-6.83	115.05	123.44
1	A	386	ASN	OD1-CG-ND2	-6.78	115.82	122.60
1	D	181	ASP	CA-CB-CG	6.78	119.38	112.60
1	A	749	ASP	CA-CB-CG	-6.76	105.84	112.60
1	A	28	SER	O-C-N	6.75	133.81	123.00
1	D	29	LEU	N-CA-CB	-6.71	100.26	110.33
1	D	671	ASN	CA-CB-CG	6.71	119.31	112.60
1	D	580	ASN	CA-CB-CG	-6.70	105.90	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	255	TRP	CA-C-O	6.70	127.65	120.55
1	D	166	PHE	CA-C-O	-6.66	113.64	121.16
1	B	724	ALA	CA-C-N	6.65	134.25	121.54
1	B	724	ALA	C-N-CA	6.65	134.25	121.54
1	C	711	ALA	CA-C-O	6.62	128.57	121.55
1	D	155	ASP	CA-CB-CG	6.60	119.20	112.60
1	C	749	ASP	CA-CB-CG	-6.59	106.01	112.60
1	B	27	ASP	N-CA-C	6.59	129.46	111.00
1	B	486	GLN	CA-C-N	6.59	130.06	120.71
1	B	486	GLN	C-N-CA	6.59	130.06	120.71
1	A	166	PHE	CA-C-O	-6.58	113.52	121.28
1	A	380	ASP	CA-CB-CG	-6.57	106.03	112.60
1	A	383	PHE	CA-CB-CG	-6.56	107.24	113.80
1	D	217	PHE	CA-CB-CG	-6.56	107.24	113.80
1	A	442	ASN	CA-CB-CG	6.54	119.14	112.60
1	B	37	ARG	CA-CB-CG	6.52	127.14	114.10
1	D	521	ARG	NE-CZ-NH2	6.52	125.07	119.20
1	A	255	TRP	O-C-N	-6.49	115.24	122.12
1	A	575	PRO	CA-C-O	-6.49	116.23	120.90
1	A	458	ALA	CA-C-O	-6.47	113.64	121.28
1	B	66	ASN	CA-C-O	-6.47	113.56	120.42
1	A	304	TRP	N-CA-C	6.46	118.86	111.11
1	D	403	THR	N-CA-CB	6.45	122.07	111.31
1	C	100	ARG	N-CA-C	-6.44	104.04	112.41
1	B	167	SER	N-CA-CB	-6.43	101.56	111.46
1	B	377	ARG	CA-CB-CG	-6.41	101.28	114.10
1	B	565	GLU	CB-CG-CD	-6.41	101.71	112.60
1	D	739	HIS	CA-CB-CG	6.41	120.20	113.80
1	C	660	LEU	N-CA-CB	-6.40	100.02	110.14
1	B	98	GLY	N-CA-C	-6.38	104.76	112.48
1	B	37	ARG	CD-NE-CZ	6.37	133.31	124.40
1	C	29	LEU	CA-C-O	-6.37	112.28	119.79
1	D	474	PRO	N-CA-CB	6.35	106.75	103.19
1	A	41	GLU	CA-CB-CG	6.34	126.78	114.10
1	B	595	ASP	CA-CB-CG	6.34	118.94	112.60
1	C	54	SER	CB-CA-C	6.34	122.56	109.95
1	A	442	ASN	CA-C-O	-6.33	114.41	121.05
1	C	304	TRP	N-CA-C	6.31	118.68	111.11
1	D	522	HIS	CA-CB-CG	-6.31	107.49	113.80
1	C	48	GLN	OE1-CD-NE2	-6.30	116.30	122.60
1	D	116	HIS	CA-CB-CG	-6.29	107.51	113.80
1	B	38	PRO	CB-CA-C	-6.28	102.75	110.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	344	GLU	CB-CA-C	-6.28	97.07	110.32
1	D	712	ASP	N-CA-CB	6.28	119.11	110.01
1	D	479	ARG	NE-CZ-NH2	6.28	124.85	119.20
1	D	201	ASN	OD1-CG-ND2	-6.27	116.33	122.60
1	A	646	THR	N-CA-CB	6.26	119.18	109.85
1	A	712	ASP	N-CA-C	-6.25	104.57	111.82
1	C	473	THR	CA-C-N	6.23	124.21	119.66
1	C	473	THR	C-N-CA	6.23	124.21	119.66
1	A	627	GLY	CA-C-N	6.22	130.40	122.37
1	A	627	GLY	C-N-CA	6.22	130.40	122.37
1	C	376	ASN	OD1-CG-ND2	-6.22	116.38	122.60
1	D	679	GLY	CA-C-O	6.22	127.71	121.00
1	C	445	ARG	NE-CZ-NH1	6.16	127.66	121.50
1	A	724	ALA	CA-C-N	6.16	133.31	121.54
1	A	724	ALA	C-N-CA	6.16	133.31	121.54
1	D	388	GLN	OE1-CD-NE2	-6.16	116.44	122.60
1	A	130	ARG	NE-CZ-NH1	6.14	127.64	121.50
1	D	681	ALA	CA-C-O	-6.14	114.04	120.55
1	A	130	ARG	NH1-CZ-NH2	-6.13	111.34	119.30
1	B	620	LEU	CA-C-O	6.12	127.02	120.10
1	D	569	ASP	N-CA-CB	6.12	119.77	110.28
1	B	568	ASP	N-CA-CB	-6.12	100.52	109.82
1	D	224	GLU	CA-C-N	6.11	126.00	119.28
1	D	224	GLU	C-N-CA	6.11	126.00	119.28
1	A	649	PRO	N-CA-CB	6.10	108.99	103.19
1	A	338	PHE	CA-CB-CG	6.09	119.89	113.80
1	D	712	ASP	CB-CA-C	-6.09	101.33	110.88
1	C	637	MET	CA-C-N	-6.08	116.69	121.86
1	C	637	MET	C-N-CA	-6.08	116.69	121.86
1	D	751	ILE	N-CA-CB	-6.08	102.70	111.21
1	B	333	GLU	CA-C-O	6.07	127.64	120.66
1	B	749	ASP	N-CA-CB	-6.06	100.97	110.06
1	B	96	ARG	NE-CZ-NH1	-6.05	115.45	121.50
1	C	414	SER	CA-C-O	-6.04	114.14	120.55
1	A	96	ARG	NH1-CZ-NH2	6.04	127.15	119.30
1	D	445	ARG	CD-NE-CZ	6.04	132.85	124.40
1	A	575	PRO	O-C-N	6.03	124.08	121.31
1	D	260	ARG	NH1-CZ-NH2	6.03	127.14	119.30
1	B	309	LYS	CA-C-O	6.01	126.79	120.42
1	C	377	ARG	CD-NE-CZ	-6.01	115.98	124.40
1	D	177	ASP	CA-C-O	-6.01	114.12	120.55
1	B	501	PHE	CA-CB-CG	6.00	119.81	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	424	GLY	N-CA-C	5.98	123.91	115.30
1	D	678	ASN	CA-CB-CG	5.98	118.58	112.60
1	B	68	LEU	CA-C-O	5.98	126.76	119.11
1	C	386	ASN	OD1-CG-ND2	-5.95	116.65	122.60
1	B	474	PRO	O-C-N	-5.93	118.58	121.31
1	C	166	PHE	CA-C-O	-5.93	114.21	120.80
1	C	59	ASP	CA-CB-CG	-5.93	106.67	112.60
1	C	126[A]	ILE	CB-CA-C	-5.93	104.14	112.14
1	C	126[B]	ILE	CB-CA-C	-5.93	104.14	112.14
1	D	93	ASN	OD1-CG-ND2	-5.92	116.69	122.60
1	A	536	ARG	NE-CZ-NH2	5.91	124.52	119.20
1	B	403	THR	N-CA-CB	5.91	120.56	111.22
1	D	350	ASP	CB-CA-C	-5.91	98.19	109.95
1	B	290	ARG	N-CA-CB	5.91	121.02	110.80
1	D	119	HIS	CA-CB-CG	-5.91	107.89	113.80
1	A	224	GLU	CA-C-N	5.89	125.76	119.28
1	A	224	GLU	C-N-CA	5.89	125.76	119.28
1	C	521	ARG	NE-CZ-NH2	-5.89	113.90	119.20
1	C	378	ASN	N-CA-CB	-5.88	101.67	109.78
1	D	391	PHE	CA-CB-CG	5.87	119.67	113.80
1	A	727	SER	N-CA-CB	-5.87	100.84	110.40
1	A	171	GLY	N-CA-C	5.87	120.05	112.54
1	D	98	GLY	N-CA-C	-5.86	105.39	112.48
1	B	210	ASP	CA-CB-CG	5.85	118.45	112.60
1	B	527	PHE	CA-CB-CG	5.84	119.64	113.80
1	C	309	LYS	N-CA-CB	5.83	118.69	110.12
1	A	710	ILE	CA-C-N	5.82	132.65	121.54
1	A	710	ILE	C-N-CA	5.82	132.65	121.54
1	D	501	PHE	CA-CB-CG	5.82	119.61	113.80
1	C	140	PRO	CA-C-O	-5.78	114.81	121.86
1	C	265	SER	N-CA-CB	-5.78	102.60	111.56
1	B	52	PRO	CA-C-N	5.78	126.50	120.03
1	B	52	PRO	C-N-CA	5.78	126.50	120.03
1	D	293	TRP	N-CA-CB	5.77	119.83	110.77
1	C	170	GLN	N-CA-C	5.76	118.43	111.40
1	D	568	ASP	CA-C-O	-5.75	114.45	120.55
1	A	350	ASP	CA-CB-CG	5.75	118.35	112.60
1	D	345	ASP	CA-CB-CG	5.74	118.34	112.60
1	B	209	GLN	CA-C-O	-5.74	112.84	119.78
1	D	379	PRO	CB-CA-C	-5.73	102.10	111.56
1	A	488	ARG	NH1-CZ-NH2	5.73	126.75	119.30
1	C	666	ILE	CA-C-O	5.72	126.40	120.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	714	GLY	CA-C-O	-5.72	116.67	122.56
1	A	120	GLU	N-CA-C	5.71	117.58	111.36
1	C	48	GLN	CA-CB-CG	5.71	125.52	114.10
1	C	206	PHE	CA-CB-CG	-5.71	108.09	113.80
1	D	100	ARG	CD-NE-CZ	5.70	132.38	124.40
1	B	716	GLU	CA-C-O	-5.70	114.42	120.92
1	C	577	PRO	CB-CA-C	-5.68	102.64	111.22
1	A	27	ASP	CA-C-O	5.68	130.46	120.80
1	A	463	ASN	OD1-CG-ND2	-5.67	116.93	122.60
1	B	595	ASP	CA-C-N	5.67	126.10	120.31
1	B	595	ASP	C-N-CA	5.67	126.10	120.31
1	A	79	ALA	N-CA-CB	-5.67	102.01	110.17
1	C	459	ASN	OD1-CG-ND2	-5.64	116.96	122.60
1	C	408	LEU	CB-CA-C	-5.64	101.78	110.81
1	B	698	ALA	CA-C-O	5.64	127.06	120.80
1	C	612	ARG	CD-NE-CZ	5.64	132.29	124.40
1	C	158	LYS	CA-C-N	-5.63	114.85	122.91
1	C	158	LYS	C-N-CA	-5.63	114.85	122.91
1	A	546	GLN	OE1-CD-NE2	-5.62	116.98	122.60
1	D	681	ALA	O-C-N	5.62	128.08	122.12
1	C	93	ASN	OD1-CG-ND2	5.62	128.22	122.60
1	A	702	ARG	CD-NE-CZ	5.60	132.24	124.40
1	D	386	ASN	OD1-CG-ND2	-5.60	117.00	122.60
1	C	355	ASP	CA-CB-CG	5.59	118.19	112.60
1	D	343	GLU	CA-C-N	5.59	129.55	120.60
1	D	343	GLU	C-N-CA	5.59	129.55	120.60
1	B	668	PRO	CA-C-O	-5.59	114.77	122.15
1	D	339	GLN	N-CA-CB	5.59	119.56	110.17
1	A	431	ILE	CA-C-N	5.57	126.81	119.84
1	A	431	ILE	C-N-CA	5.57	126.81	119.84
1	D	125	ARG	NE-CZ-NH2	-5.57	114.19	119.20
1	C	526	GLY	N-CA-C	-5.57	106.04	112.50
1	A	325	ALA	N-CA-C	-5.57	105.13	111.14
1	C	70	ASP	CA-C-O	-5.57	112.75	119.49
1	A	671	ASN	N-CA-CB	-5.57	103.06	110.57
1	C	602	VAL	CB-CA-C	-5.57	100.75	110.71
1	D	100	ARG	CG-CD-NE	5.56	124.23	112.00
1	B	169	VAL	CA-C-O	5.55	125.74	120.80
1	A	751	ILE	CA-C-O	5.54	124.86	119.71
1	D	61	ARG	NE-CZ-NH1	5.52	127.02	121.50
1	A	54	SER	O-C-N	-5.52	114.37	122.43
1	C	740	ARG	CA-C-N	5.52	126.84	121.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	740	ARG	C-N-CA	5.52	126.84	121.65
1	C	93	ASN	N-CA-C	5.52	117.78	109.23
1	D	586	PRO	N-CA-CB	5.52	109.00	103.48
1	A	64	LYS	CD-CE-NZ	5.52	129.55	111.90
1	B	521	ARG	NH1-CZ-NH2	-5.52	112.13	119.30
1	C	151	ASP	CA-C-O	-5.52	113.87	120.10
1	D	536	ARG	NH1-CZ-NH2	5.52	126.47	119.30
1	D	471	ARG	N-CA-C	5.51	118.72	109.95
1	C	320	ARG	CB-CA-C	-5.51	102.23	110.88
1	D	420	ILE	CA-C-O	-5.51	115.22	120.95
1	B	151	ASP	CA-CB-CG	5.51	118.11	112.60
1	B	370	VAL	N-CA-CB	-5.51	103.09	111.57
1	D	473	THR	CA-C-N	5.50	123.67	119.66
1	D	473	THR	C-N-CA	5.50	123.67	119.66
1	A	741	VAL	CA-C-N	5.50	128.19	120.28
1	A	741	VAL	C-N-CA	5.50	128.19	120.28
1	C	517	PRO	O-C-N	-5.49	115.92	122.24
1	D	69	GLU	CA-C-O	-5.49	114.73	120.55
1	A	133	ALA	N-CA-C	5.49	118.03	109.52
1	D	273	GLY	N-CA-C	-5.48	107.87	114.66
1	B	363	GLU	N-CA-CB	5.48	118.65	110.22
1	C	405	ASP	CB-CA-C	5.47	117.87	109.60
1	A	479	ARG	CG-CD-NE	5.47	124.03	112.00
1	B	688	ALA	CB-CA-C	-5.46	101.72	110.79
1	C	212	HIS	CA-CB-CG	-5.46	108.34	113.80
1	D	431	ILE	N-CA-C	-5.46	103.94	109.02
1	A	255	TRP	CA-C-N	5.46	127.59	120.28
1	A	255	TRP	C-N-CA	5.46	127.59	120.28
1	D	601	ARG	NE-CZ-NH1	5.45	126.95	121.50
1	C	278	ARG	CA-C-O	-5.45	114.96	121.11
1	C	420	ILE	CA-C-O	-5.44	114.75	120.57
1	B	366	PRO	CB-CA-C	-5.44	104.27	111.23
1	B	715	GLU	CA-CB-CG	5.44	124.97	114.10
1	C	80	LEU	O-C-N	-5.44	116.24	122.93
1	C	326	ILE	CA-C-O	-5.44	115.30	120.95
1	D	446	ASP	CA-CB-CG	5.43	118.03	112.60
1	C	66	ASN	OD1-CG-ND2	-5.42	117.18	122.60
1	D	711	ALA	O-C-N	-5.42	115.89	122.82
1	B	707	THR	CA-C-O	-5.42	113.74	119.97
1	C	466	ASN	CA-CB-CG	-5.41	107.19	112.60
1	B	246	GLN	CA-C-N	5.41	125.08	119.56
1	B	246	GLN	C-N-CA	5.41	125.08	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	343	GLU	O-C-N	-5.41	116.39	122.12
1	D	168	THR	CA-C-O	-5.41	114.74	121.55
1	C	350	ASP	CA-CB-CG	-5.40	107.20	112.60
1	C	198	LEU	CA-C-N	-5.40	116.25	122.95
1	C	198	LEU	C-N-CA	-5.40	116.25	122.95
1	D	492	ASN	OD1-CG-ND2	-5.39	117.20	122.60
1	C	364	LEU	O-C-N	-5.39	114.36	122.28
1	B	177	ASP	CA-C-O	-5.39	114.26	120.24
1	B	601	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	B	237	ASP	N-CA-C	5.38	117.84	111.33
1	B	636	ARG	CA-C-O	-5.38	115.70	121.45
1	B	691	HIS	CA-CB-CG	-5.37	108.43	113.80
1	B	628	VAL	CA-C-O	-5.37	114.64	120.71
1	A	445	ARG	NE-CZ-NH2	5.37	124.03	119.20
1	D	286	ALA	O-C-N	-5.36	117.21	123.27
1	A	130	ARG	CA-C-O	-5.36	114.42	120.43
1	A	712	ASP	CA-C-N	5.36	132.02	121.58
1	A	712	ASP	C-N-CA	5.36	132.02	121.58
1	A	392	GLN	CG-CD-NE2	5.35	124.43	116.40
1	A	400	LEU	CA-C-O	-5.35	115.20	121.46
1	B	167	SER	CA-C-O	-5.34	115.72	121.38
1	B	337	GLY	O-C-N	-5.34	118.67	123.37
1	C	214	PHE	O-C-N	-5.34	115.69	120.71
1	B	444	GLN	CB-CG-CD	5.33	121.67	112.60
1	A	631	LYS	CA-CB-CG	5.33	124.76	114.10
1	A	277	PHE	CA-CB-CG	5.32	119.12	113.80
1	D	618	ALA	N-CA-CB	5.32	117.73	110.01
1	A	647	VAL	CB-CA-C	-5.31	104.86	111.08
1	A	745	ILE	O-C-N	-5.31	117.02	120.42
1	A	265	SER	N-CA-CB	-5.31	103.33	111.56
1	C	118	ASP	CA-CB-CG	5.30	117.90	112.60
1	C	553	THR	N-CA-C	-5.30	105.59	111.36
1	B	54	SER	CB-CA-C	5.29	121.06	109.99
1	C	467	ASP	CA-CB-CG	-5.29	107.31	112.60
1	A	647	VAL	N-CA-CB	5.29	116.88	110.95
1	C	643	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	495	ARG	CD-NE-CZ	5.29	131.81	124.40
1	C	411	ARG	NE-CZ-NH1	5.29	126.79	121.50
1	A	471	ARG	NE-CZ-NH1	-5.29	116.21	121.50
1	C	698	ALA	CA-C-O	5.29	126.19	120.43
1	A	37	ARG	NE-CZ-NH2	-5.28	114.44	119.20
1	C	339	GLN	N-CA-C	-5.28	100.13	108.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	569	ASP	CA-C-O	-5.28	113.90	119.97
1	A	565	GLU	N-CA-CB	-5.27	102.43	110.65
1	C	631	LYS	N-CA-CB	5.27	119.36	110.77
1	D	72	ARG	N-CA-CB	5.27	117.71	109.97
1	A	718	ILE	N-CA-CB	5.26	118.09	111.46
1	A	57	ALA	CA-C-N	5.26	125.07	119.28
1	A	57	ALA	C-N-CA	5.26	125.07	119.28
1	C	405	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	578	ASP	CA-CB-CG	-5.26	107.34	112.60
1	A	711	ALA	CA-C-N	5.26	128.30	120.31
1	A	711	ALA	C-N-CA	5.26	128.30	120.31
1	B	73	LYS	CA-C-N	5.26	128.33	122.55
1	B	73	LYS	C-N-CA	5.26	128.33	122.55
1	D	747	LYS	CA-C-O	-5.25	112.94	119.18
1	B	181	ASP	CA-CB-CG	5.24	117.84	112.60
1	B	265	SER	O-C-N	-5.24	117.81	123.42
1	D	678	ASN	CA-C-N	5.24	125.76	119.94
1	D	678	ASN	C-N-CA	5.24	125.76	119.94
1	D	254	MET	N-CA-CB	5.24	117.82	110.12
1	C	730	ASP	CA-CB-CG	-5.24	107.36	112.60
1	D	478	LYS	CA-CB-CG	5.23	124.55	114.10
1	A	542	ARG	CA-C-O	-5.23	115.01	120.55
1	D	182	ILE	N-CA-C	-5.23	104.35	110.05
1	D	515	GLN	CA-C-O	-5.23	115.46	121.47
1	A	272	PHE	CA-C-O	-5.22	114.12	120.54
1	B	65	LEU	CA-C-O	-5.22	115.02	120.55
1	A	713	GLN	CB-CG-CD	-5.21	103.74	112.60
1	D	311	THR	N-CA-CB	5.21	118.24	110.22
1	A	595	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	716	GLU	CA-CB-CG	5.19	124.48	114.10
1	C	62	ASN	N-CA-CB	5.19	119.45	111.46
1	B	415	TYR	CA-C-O	-5.18	114.93	120.42
1	C	183	ARG	CG-CD-NE	5.18	123.39	112.00
1	B	169	VAL	CG1-CB-CG2	-5.16	99.44	110.80
1	B	546	GLN	N-CA-CB	5.16	117.71	110.12
1	C	100	ARG	CG-CD-NE	5.15	123.34	112.00
1	A	252	ASN	OD1-CG-ND2	-5.15	117.45	122.60
1	A	545	ASP	CA-CB-CG	-5.15	107.45	112.60
1	C	117	PHE	CA-C-N	5.15	127.70	120.28
1	C	117	PHE	C-N-CA	5.15	127.70	120.28
1	A	96	ARG	NE-CZ-NH1	-5.15	116.35	121.50
1	D	254	MET	CB-CA-C	-5.13	102.28	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	405	ASP	CA-CB-CG	5.13	117.73	112.60
1	D	335	GLU	CA-C-O	5.13	125.85	120.36
1	D	420	ILE	CB-CA-C	-5.13	105.22	112.14
1	C	628	VAL	CA-C-O	-5.12	114.92	120.71
1	A	416	THR	N-CA-CB	5.11	117.72	110.16
1	B	114	ILE	CB-CA-C	-5.10	105.19	112.22
1	A	70	ASP	CB-CG-OD2	5.09	130.12	118.40
1	C	507	HIS	CA-CB-CG	-5.09	108.71	113.80
1	C	427	ASN	OD1-CG-ND2	5.09	127.69	122.60
1	A	170	GLN	N-CA-C	5.09	116.64	111.14
1	C	437	THR	N-CA-C	-5.09	107.12	113.38
1	D	497	ARG	CD-NE-CZ	5.09	131.53	124.40
1	A	727	SER	CB-CA-C	5.08	120.61	109.99
1	B	349	PHE	CA-CB-CG	-5.08	108.72	113.80
1	B	413	PHE	CA-C-O	5.08	125.98	120.55
1	C	431	ILE	N-CA-C	-5.08	103.43	108.96
1	D	628	VAL	N-CA-CB	5.07	116.25	110.72
1	B	88	ILE	CB-CG1-CD1	5.07	124.45	113.80
1	A	236	HIS	CA-CB-CG	5.07	118.87	113.80
1	A	638	GLY	CA-C-O	-5.07	116.18	120.64
1	C	29	LEU	N-CA-CB	-5.07	102.50	110.30
1	A	634	TYR	CA-C-O	-5.06	116.00	121.36
1	A	273	GLY	N-CA-C	-5.05	108.39	114.66
1	C	504	TYR	N-CA-CB	-5.05	103.91	110.88
1	A	143	SER	CB-CA-C	-5.05	102.02	109.90
1	C	567	THR	CA-CB-OG1	-5.05	102.03	109.60
1	B	675	ILE	CA-C-O	5.04	123.77	119.38
1	C	349	PHE	CA-CB-CG	-5.04	108.76	113.80
1	D	545	ASP	CA-CB-CG	-5.04	107.56	112.60
1	D	79	ALA	CA-C-N	5.04	128.49	121.24
1	D	79	ALA	C-N-CA	5.04	128.49	121.24
1	D	241	ASP	N-CA-C	-5.04	105.70	111.14
1	A	642	ALA	N-CA-CB	-5.03	103.24	110.44
1	C	195	ILE	CA-C-O	-5.03	115.12	120.85
1	A	103	THR	CA-CB-CG2	5.02	119.04	110.50
1	D	428	PHE	O-C-N	-5.02	115.70	122.43
1	A	72	ARG	N-CA-CB	5.02	117.35	109.97
1	C	475	PRO	CB-CA-C	-5.02	104.64	111.12
1	D	488	ARG	CA-C-O	5.01	126.41	120.69
1	C	659	SER	CA-C-N	5.01	127.70	120.38
1	C	659	SER	C-N-CA	5.01	127.70	120.38
1	C	226	HIS	CA-CB-CG	5.01	118.81	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	42	PRO	O-C-N	-5.01	117.25	123.01
1	B	72	ARG	CA-C-N	-5.00	115.43	122.94
1	B	72	ARG	C-N-CA	-5.00	115.43	122.94
1	C	595	ASP	CA-C-N	5.00	124.72	119.92
1	C	595	ASP	C-N-CA	5.00	124.72	119.92

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	27	ASP	Peptide,Mainchain
1	A	28	SER	Mainchain
1	A	711	ALA	Mainchain
1	D	157	ASN	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5748	0	5586	82	0
1	B	5748	0	5586	88	0
1	C	5748	0	5586	92	0
1	D	5748	0	5586	87	1
2	A	43	0	30	4	0
2	B	43	0	30	6	0
2	C	43	0	30	4	0
2	D	43	0	30	5	0
3	A	728	0	0	8	2
3	B	625	0	0	14	0
3	C	634	0	0	13	1
3	D	692	0	0	11	2
All	All	25843	0	22464	307	3

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 7.

All (307) 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:451:MET:HE2	1:C:451:MET:HE2	1.34	1.10
1:C:725:ASP:HB2	1:C:728:PHE:HB3	1.30	1.08
1:B:451:MET:HE2	1:D:451:MET:HE2	1.36	1.01
1:B:583:LYS:HE2	1:B:583:LYS:H	1.25	0.98
1:C:724:ALA:O	1:C:725:ASP:HB3	1.65	0.96
1:B:415:TYR:HB2	3:B:1378:HOH:O	1.64	0.95
1:D:369:ARG:HB2	3:D:1392:HOH:O	1.76	0.86
1:A:126[B]:ILE:HD12	1:A:127:VAL:HG22	1.58	0.84
1:A:726:GLY:HA3	3:A:1398:HOH:O	1.77	0.84
1:D:126[B]:ILE:HD11	2:D:754:HEM:CMD	2.08	0.84
1:B:368:GLN:HB2	3:B:1245:HOH:O	1.78	0.83
1:B:126[A]:ILE:HD11	1:C:118:ASP:O	1.80	0.82
1:B:583:LYS:H	1:B:583:LYS:CE	1.91	0.82
1:D:710:ILE:HD13	1:D:718:ILE:HG13	1.62	0.82
1:D:126[B]:ILE:HD11	2:D:754:HEM:HMD1	1.66	0.77
1:C:126[B]:ILE:HD11	2:C:754:HEM:CMD	2.14	0.77
1:C:386:ASN:HD22	1:C:386:ASN:C	1.94	0.75
1:B:552:LEU:HD21	1:B:571:LEU:HD12	1.68	0.75
1:B:377:ARG:NH1	3:B:1296:HOH:O	2.13	0.74
1:C:126[B]:ILE:HD11	2:C:754:HEM:HMD1	1.69	0.74
1:D:605:ILE:HD12	1:D:630:ALA:HB1	1.70	0.73
1:A:27:ASP:CB	1:A:28:SER:HA	2.19	0.72
1:A:386:ASN:C	1:A:386:ASN:HD22	1.98	0.72
1:D:28:SER:H	1:D:29:LEU:HD23	1.55	0.71
2:D:754:HEM:HMB2	2:D:754:HEM:HBB2	1.71	0.71
1:D:39:ALA:H	1:D:48:GLN:NE2	1.89	0.70
1:B:126[B]:ILE:HD11	2:B:754:HEM:CMD	2.21	0.70
1:A:28:SER:O	1:A:29:LEU:CB	2.39	0.70
1:B:710:ILE:HD13	1:B:718:ILE:HG13	1.73	0.70
1:A:709:LYS:HE3	1:A:709:LYS:HA	1.74	0.69
1:D:726:GLY:O	3:D:1205:HOH:O	2.11	0.69
1:A:469:TRP:CE3	1:A:471:ARG:HG3	2.27	0.69
1:A:708:ILE:O	1:A:710:ILE:HB	1.93	0.69
1:B:369:ARG:HG2	3:B:1115:HOH:O	1.91	0.69
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.75	0.68
1:D:552:LEU:HD11	1:D:571:LEU:HD23	1.74	0.68
1:A:27:ASP:N	3:A:1362:HOH:O	2.26	0.67
1:C:488:ARG:HH21	1:D:492:ASN:ND2	1.93	0.67
1:D:126[B]:ILE:HD11	2:D:754:HEM:HMD2	1.76	0.67
1:A:70:ASP:OD1	1:A:71:VAL:HG13	1.95	0.67
1:B:583:LYS:HE2	1:B:583:LYS:N	2.05	0.66
3:B:904:HOH:O	1:C:126[A]:ILE:HD11	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:ASN:C	1:B:386:ASN:HD22	2.03	0.66
1:B:117:PHE:CE2	1:C:126[B]:ILE:HD12	2.31	0.65
1:C:704:PHE:O	1:C:707:THR:HG22	1.96	0.65
1:D:165:ARG:HE	1:D:386:ASN:HD21	1.46	0.64
1:D:38:PRO:HA	1:D:48:GLN:HE21	1.61	0.63
3:B:924:HOH:O	1:D:73:LYS:HE2	1.97	0.63
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.14	0.63
1:A:751:ILE:HD12	1:A:751:ILE:O	1.98	0.63
1:A:73:LYS:NZ	1:C:440:TYR:OH	2.30	0.62
1:B:330:ASP:OD2	1:B:629:HIS:HE1	1.82	0.62
1:A:126[B]:ILE:HD13	1:D:117:PHE:CE2	2.34	0.62
1:B:37:ARG:HD2	3:B:1319:HOH:O	1.98	0.62
1:D:386:ASN:C	1:D:386:ASN:HD22	2.06	0.62
1:A:488:ARG:NE	1:A:490:GLU:OE2	2.26	0.62
1:D:330:ASP:OD2	1:D:629:HIS:HE1	1.84	0.61
1:D:28:SER:H	1:D:29:LEU:CD2	2.12	0.61
1:A:126[B]:ILE:CD1	1:A:127:VAL:HG22	2.29	0.61
1:B:449:HIS:HB2	1:D:449:HIS:CE1	2.35	0.61
1:C:266:TYR:HB2	3:C:1191:HOH:O	2.00	0.61
1:D:27:ASP:HB2	1:D:29:LEU:HD21	1.83	0.61
1:B:126[B]:ILE:HD11	2:B:754:HEM:HMD1	1.82	0.60
3:A:1472:HOH:O	1:D:126[A]:ILE:HD11	2.01	0.60
1:C:552:LEU:HD13	1:C:556:GLN:NE2	2.16	0.60
1:A:214:PHE:HB3	1:A:215:PRO:HD3	1.85	0.59
1:C:345:ASP:HA	1:C:348:LYS:HD3	1.85	0.59
1:B:165:ARG:HE	1:B:386:ASN:HD21	1.48	0.59
1:C:27:ASP:CG	3:C:873:HOH:O	2.46	0.59
1:A:341:ILE:HD12	1:A:353:LEU:HD21	1.85	0.59
1:B:126[B]:ILE:HD11	2:B:754:HEM:HMD2	1.84	0.58
1:A:435:ARG:NH1	3:A:1137:HOH:O	2.25	0.58
3:B:1136:HOH:O	1:D:451:MET:HE1	2.04	0.57
1:D:631:LYS:HE2	3:D:1261:HOH:O	2.04	0.57
1:B:126[B]:ILE:HD13	1:C:118:ASP:HA	1.86	0.57
1:C:126[B]:ILE:HD11	2:C:754:HEM:HMD2	1.86	0.57
1:D:631:LYS:HG3	1:D:633:LEU:HD13	1.85	0.57
1:A:443:PHE:CZ	1:A:470:PRO:HD2	2.39	0.57
1:D:144:LEU:HD11	1:D:370:VAL:HG13	1.86	0.57
1:B:27:ASP:CG	1:D:468:ASN:HD22	2.13	0.57
1:C:435:ARG:HD3	3:C:1120:HOH:O	2.05	0.57
1:D:751:ILE:HD13	1:D:752:PRO:HD2	1.85	0.57
1:A:750:LYS:HZ3	1:A:750:LYS:C	2.13	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126[B]:ILE:CD1	2:D:754:HEM:HMD1	2.34	0.56
1:B:751:ILE:HD12	1:B:753:ALA:HB2	1.86	0.56
1:A:28:SER:C	1:A:29:LEU:CG	2.79	0.56
1:A:37:ARG:NH2	1:C:466:ASN:HA	2.20	0.56
1:B:562:LEU:HA	1:C:637:MET:HB2	1.87	0.56
1:B:344:GLU:CD	1:B:344:GLU:H	2.14	0.56
1:B:725:ASP:OD1	1:B:726:GLY:N	2.39	0.56
1:B:278:ARG:HH22	1:B:487:GLU:CD	2.14	0.56
1:C:330:ASP:OD2	1:C:629:HIS:HE1	1.89	0.56
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.21	0.56
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.37	0.55
1:B:118:ASP:HA	1:C:126[B]:ILE:HD13	1.87	0.55
1:C:178:THR:HG21	1:C:310:LEU:HD23	1.88	0.55
1:B:345:ASP:HA	1:B:348:LYS:HD2	1.89	0.55
1:D:583:LYS:HB2	1:D:583:LYS:NZ	2.21	0.55
1:C:709:LYS:HD2	1:C:709:LYS:N	2.22	0.55
1:C:604:ALA:HB1	1:C:633:LEU:HD22	1.89	0.55
1:A:118:ASP:HA	1:D:126[B]:ILE:HD13	1.89	0.55
1:D:211:ALA:CB	1:D:410:GLY:HA3	2.37	0.55
1:A:710:ILE:HG12	1:A:715:GLU:OE1	2.07	0.54
1:B:27:ASP:OD2	1:D:468:ASN:ND2	2.39	0.54
1:B:39:ALA:N	1:B:48:GLN:OE1	2.34	0.54
1:A:583:LYS:O	1:A:584:LYS:HB3	2.07	0.54
1:B:451:MET:HE2	1:D:451:MET:CE	2.25	0.54
1:C:725:ASP:O	1:C:725:ASP:CG	2.48	0.54
1:B:126[A]:ILE:HD13	3:C:1387:HOH:O	2.08	0.54
1:B:749:ASP:OD2	1:B:750:LYS:HE2	2.08	0.54
1:A:165:ARG:HE	1:A:386:ASN:HD21	1.56	0.53
1:B:377:ARG:NH2	3:B:1296:HOH:O	2.40	0.53
1:B:438:CYS:HB2	1:B:439:PRO:HD2	1.91	0.53
1:C:629:HIS:HD2	3:C:1054:HOH:O	1.91	0.53
1:C:195:ILE:HD11	1:C:436:PRO:HA	1.90	0.53
1:A:725:ASP:CG	1:A:726:GLY:H	2.16	0.53
1:B:359:LEU:H	1:B:507:HIS:HD2	1.57	0.53
1:A:28:SER:O	1:A:29:LEU:CG	2.57	0.52
1:B:377:ARG:NH1	1:B:378:ASN:O	2.42	0.52
1:A:126[B]:ILE:HD11	2:A:754:HEM:CMD	2.40	0.52
1:D:574:THR:HG22	3:D:1363:HOH:O	2.09	0.52
1:A:211:ALA:CB	1:A:410:GLY:HA3	2.40	0.52
1:A:76:GLU:O	1:A:77:ASN:HB2	2.08	0.52
1:B:126[B]:ILE:HD12	1:C:117:PHE:CE2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:ARG:HG2	3:C:1381:HOH:O	2.08	0.52
1:C:488:ARG:HH21	1:D:492:ASN:HD21	1.54	0.52
1:C:700:ASP:O	1:C:703:LYS:HG3	2.10	0.52
1:B:207:PHE:O	1:B:249:THR:HA	2.10	0.51
1:A:690:LYS:HG3	1:A:751:ILE:HD11	1.90	0.51
1:A:28:SER:C	1:A:29:LEU:HG	2.36	0.51
1:B:443:PHE:CZ	1:B:470:PRO:HD2	2.46	0.51
1:B:578:ASP:HB3	1:B:582:LEU:O	2.10	0.51
1:A:725:ASP:CG	1:A:726:GLY:N	2.65	0.50
1:A:36:HIS:CD2	1:A:36:HIS:H	2.29	0.50
1:B:377:ARG:CZ	3:B:1296:HOH:O	2.58	0.50
1:B:451:MET:HE1	3:D:1135:HOH:O	2.11	0.50
1:D:751:ILE:HD13	1:D:752:PRO:CD	2.41	0.50
1:B:634:TYR:O	1:B:653:THR:HA	2.11	0.50
1:D:435:ARG:HD3	3:D:1135:HOH:O	2.11	0.50
3:A:919:HOH:O	1:C:52:PRO:HG3	2.12	0.50
1:C:552:LEU:HD21	1:C:571:LEU:HD12	1.93	0.50
1:B:629:HIS:HD2	3:B:1059:HOH:O	1.94	0.49
3:C:1104:HOH:O	1:D:488:ARG:HD2	2.11	0.49
1:D:629:HIS:HD2	3:D:1068:HOH:O	1.95	0.49
1:C:322:LEU:HB2	3:C:1191:HOH:O	2.11	0.49
1:C:725:ASP:O	1:C:725:ASP:OD1	2.29	0.49
1:C:490:GLU:HG3	1:D:490:GLU:HG3	1.94	0.49
1:A:121:ARG:HG2	1:D:126[A]:ILE:HD13	1.95	0.49
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.27	0.49
1:B:583:LYS:H	1:B:583:LYS:CD	2.26	0.48
1:D:710:ILE:CD1	1:D:718:ILE:HG13	2.38	0.48
1:C:619:ILE:O	1:C:623:LEU:HG	2.14	0.48
1:C:583:LYS:O	1:C:584:LYS:HB3	2.12	0.48
1:B:27:ASP:CG	1:D:468:ASN:ND2	2.72	0.48
1:C:205:ILE:HD13	1:C:205:ILE:H	1.78	0.48
1:B:274:ILE:HD12	2:B:754:HEM:HMB1	1.95	0.47
1:C:602:VAL:HG12	1:C:603:VAL:N	2.30	0.47
2:B:754:HEM:HBB2	2:B:754:HEM:CMB	2.45	0.47
1:C:364:LEU:HD11	1:C:580:ASN:HB2	1.96	0.47
1:D:748:ILE:O	1:D:751:ILE:HG22	2.14	0.47
1:A:84:GLN:HG3	1:C:395:HIS:CD2	2.50	0.47
1:B:507:HIS:N	1:B:508:PRO:HD2	2.29	0.47
1:C:238:THR:HB	1:D:460:TYR:CE1	2.49	0.47
1:C:616:LEU:HD22	1:C:620:LEU:HG	1.96	0.47
1:A:27:ASP:OD1	1:A:28:SER:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:ARG:HE	1:B:386:ASN:ND2	2.12	0.47
1:C:274:ILE:HD12	2:C:754:HEM:HMB1	1.96	0.47
1:D:533:LYS:NZ	3:D:1366:HOH:O	2.48	0.47
1:A:117:PHE:CE2	1:D:126[B]:ILE:HD12	2.50	0.46
1:D:459:ASN:HD22	1:D:459:ASN:H	1.62	0.46
1:A:127:VAL:O	1:A:128:HIS:HB2	2.15	0.46
1:A:420:ILE:HG21	1:C:119:HIS:CE1	2.51	0.46
1:B:386:ASN:C	1:B:386:ASN:ND2	2.73	0.46
1:D:659:SER:HB2	1:D:688:ALA:HB2	1.97	0.46
1:A:411:ARG:HG2	2:A:754:HEM:C2C	2.51	0.46
1:C:552:LEU:HD22	1:C:556:GLN:HG3	1.97	0.46
1:B:583:LYS:O	1:B:584:LYS:HB3	2.16	0.46
1:C:449:HIS:HB2	3:C:1285:HOH:O	2.14	0.46
1:A:607:LEU:HD11	1:A:632:LEU:HB3	1.98	0.46
1:D:359:LEU:H	1:D:507:HIS:HD2	1.64	0.46
1:B:308:GLN:OE1	1:C:313:ARG:NH1	2.48	0.46
1:B:368:GLN:NE2	3:B:1141:HOH:O	2.45	0.46
1:D:708:ILE:HG13	1:D:710:ILE:HD12	1.97	0.46
1:A:459:ASN:HD22	1:A:459:ASN:C	2.24	0.45
1:B:607:LEU:HD22	1:B:611:VAL:HG21	1.98	0.45
1:D:293:TRP:CZ3	1:D:336:LEU:HB2	2.52	0.45
1:A:593:ILE:HA	1:A:594:PRO:HD2	1.86	0.45
1:A:52:PRO:HG3	3:C:961:HOH:O	2.17	0.45
1:C:578:ASP:HB2	1:C:582:LEU:O	2.17	0.45
1:A:126[A]:ILE:HD11	3:D:1446:HOH:O	2.17	0.45
1:A:488:ARG:HA	1:B:492:ASN:HD22	1.81	0.45
1:B:469:TRP:CE3	1:B:471:ARG:HG3	2.52	0.45
1:C:686:MET:HB3	1:C:751:ILE:HD11	1.99	0.45
1:A:435:ARG:HD3	3:A:1137:HOH:O	2.16	0.45
1:B:258:SER:HA	1:B:523:ILE:HG12	1.99	0.45
1:C:727:SER:HA	1:C:730:ASP:OD2	2.16	0.45
1:B:461:GLU:HA	1:B:462:PRO:C	2.42	0.44
1:C:507:HIS:N	1:C:508:PRO:HD2	2.32	0.44
1:B:275:HIS:CD2	1:B:408:LEU:HB2	2.52	0.44
1:C:278:ARG:HH22	1:C:487:GLU:CD	2.26	0.44
1:A:488:ARG:HA	1:B:492:ASN:ND2	2.33	0.44
1:C:165:ARG:HE	1:C:386:ASN:HD21	1.65	0.44
1:B:359:LEU:H	1:B:507:HIS:CD2	2.34	0.44
1:C:507:HIS:N	1:C:508:PRO:CD	2.80	0.44
1:A:603:VAL:HG11	1:A:666:ILE:CD1	2.48	0.44
1:D:631:LYS:HG3	1:D:633:LEU:CD1	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:HIS:CD2	1:C:83:ASN:HB3	2.53	0.44
1:A:438:CYS:HB2	1:A:439:PRO:CD	2.48	0.44
1:A:119:HIS:CE1	1:C:420:ILE:HG21	2.53	0.43
1:C:725:ASP:OD2	1:C:729:MET:N	2.23	0.43
1:A:29:LEU:HA	1:C:467:ASP:OD1	2.18	0.43
3:A:1137:HOH:O	1:C:451:MET:HE1	2.17	0.43
1:C:386:ASN:C	1:C:386:ASN:ND2	2.66	0.43
1:D:708:ILE:CD1	1:D:710:ILE:HD12	2.49	0.43
1:D:725:ASP:O	3:D:1207:HOH:O	2.21	0.43
1:C:461:GLU:HB2	1:C:462:PRO:HA	1.99	0.43
1:A:252:ASN:HD22	1:A:252:ASN:HA	1.72	0.43
1:A:696:ALA:HB1	1:A:728:PHE:CZ	2.53	0.43
1:B:435:ARG:HD3	3:B:1136:HOH:O	2.18	0.43
1:C:610:GLU:HG3	1:C:610:GLU:O	2.18	0.43
1:D:97:ALA:O	1:D:101:GLY:HA3	2.19	0.43
1:A:748:ILE:O	1:A:751:ILE:HG13	2.18	0.43
1:C:725:ASP:OD2	1:C:726:GLY:O	2.37	0.43
1:D:222:LYS:HB3	1:D:223:PRO:HD2	2.00	0.43
1:A:104:LEU:HB3	3:C:775:HOH:O	2.19	0.43
1:C:552:LEU:HD22	1:C:552:LEU:O	2.18	0.43
1:D:583:LYS:O	1:D:584:LYS:HB3	2.18	0.43
2:A:754:HEM:HBC2	2:A:754:HEM:CMC	2.48	0.43
1:D:222:LYS:HB3	1:D:223:PRO:CD	2.49	0.43
1:D:320:ARG:HD3	3:D:916:HOH:O	2.18	0.43
1:D:478:LYS:HZ3	1:D:478:LYS:HG3	1.65	0.43
1:A:313:ARG:NH2	1:D:309:LYS:HD2	2.34	0.43
1:B:121:ARG:HG2	1:C:126[A]:ILE:HD13	2.01	0.43
1:C:702:ARG:HE	1:C:702:ARG:HB2	1.66	0.43
1:A:73:LYS:HZ3	1:C:450:ARG:NH2	2.17	0.43
1:A:386:ASN:C	1:A:386:ASN:ND2	2.68	0.42
1:A:603:VAL:HG11	1:A:666:ILE:HD12	2.01	0.42
1:A:725:ASP:OD1	1:A:726:GLY:N	2.52	0.42
1:A:205:ILE:HD13	1:A:205:ILE:H	1.83	0.42
1:C:260:ARG:HD3	1:C:590:LEU:HD21	2.01	0.42
1:A:37:ARG:HA	1:A:38:PRO:HD3	1.91	0.42
1:B:251:HIS:CE1	1:B:507:HIS:HB3	2.54	0.42
1:B:655:ALA:HB3	3:B:1324:HOH:O	2.20	0.42
1:C:359:LEU:C	1:C:359:LEU:HD12	2.44	0.42
1:A:511:PHE:O	1:A:515:GLN:HG2	2.18	0.42
1:B:377:ARG:HH11	1:B:377:ARG:HD2	1.37	0.42
1:B:536:ARG:HA	1:B:537:PRO:HD3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:512:TRP:CZ3	1:C:554:LEU:HD13	2.54	0.42
1:C:602:VAL:HG21	3:C:1312:HOH:O	2.20	0.42
1:A:36:HIS:HE1	3:A:1329:HOH:O	2.01	0.42
1:D:583:LYS:HB2	1:D:583:LYS:HZ3	1.84	0.42
1:A:222:LYS:HB3	1:A:223:PRO:HD2	2.00	0.42
1:C:341:ILE:HD12	1:C:341:ILE:N	2.35	0.42
1:C:724:ALA:O	1:C:725:ASP:CB	2.49	0.42
1:C:51:ALA:HB1	1:C:52:PRO:HD2	2.01	0.42
1:B:222:LYS:HB3	1:B:223:PRO:HD2	2.01	0.42
1:B:705:LYS:HE3	1:B:710:ILE:HG22	2.02	0.42
1:B:51:ALA:HB1	1:B:52:PRO:HD2	2.01	0.42
1:C:126[A]:ILE:HG12	3:C:899:HOH:O	2.20	0.42
1:D:386:ASN:C	1:D:386:ASN:ND2	2.75	0.42
1:A:43:THR:HB	1:A:44:PRO:HD2	2.02	0.41
1:B:126[B]:ILE:CD1	2:B:754:HEM:HMD1	2.50	0.41
1:C:404:ASN:O	1:C:405:ASP:C	2.62	0.41
1:D:535:VAL:O	1:D:537:PRO:HD3	2.19	0.41
1:B:596:GLY:HA3	1:B:737:ALA:O	2.20	0.41
1:C:125:ARG:HB2	1:C:129:ALA:HA	2.01	0.41
1:D:72:ARG:HH11	1:D:72:ARG:HD2	1.64	0.41
1:D:195:ILE:HD11	1:D:436:PRO:HA	2.01	0.41
1:B:440:TYR:CD1	1:B:440:TYR:C	2.98	0.41
1:D:359:LEU:H	1:D:507:HIS:CD2	2.37	0.41
1:B:27:ASP:CB	1:D:468:ASN:HD22	2.33	0.41
1:B:119:HIS:CE1	1:D:420:ILE:HG21	2.55	0.41
1:C:260:ARG:NH1	1:C:270:GLU:OE1	2.45	0.41
1:D:48:GLN:HB3	1:D:49:PRO:HD2	2.01	0.41
1:A:460:TYR:CE1	1:B:238:THR:HB	2.55	0.41
1:D:27:ASP:HB2	1:D:29:LEU:CD2	2.49	0.41
1:A:158:LYS:HE2	1:A:192:GLU:OE1	2.19	0.41
1:C:623:LEU:HD21	1:C:729:MET:HE1	2.03	0.41
1:D:165:ARG:HE	1:D:386:ASN:ND2	2.14	0.41
1:A:126[B]:ILE:HD13	1:D:117:PHE:CZ	2.55	0.41
1:A:300:ALA:HB1	1:A:739:HIS:CE1	2.56	0.41
1:A:634:TYR:O	1:A:653:THR:HA	2.20	0.41
1:B:473:THR:O	1:D:89:ALA:HA	2.21	0.41
1:B:725:ASP:HB2	1:B:726:GLY:H	1.55	0.41
1:C:634:TYR:O	1:C:653:THR:HA	2.20	0.41
1:D:65:LEU:HD21	1:D:135:HIS:CG	2.55	0.41
1:D:126[B]:ILE:HD13	1:D:126[B]:ILE:HG21	1.85	0.41
1:D:521:ARG:HH21	1:D:524:VAL:HG11	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ALA:O	1:A:101:GLY:HA3	2.20	0.41
1:C:359:LEU:H	1:C:507:HIS:CD2	2.39	0.41
1:C:605:ILE:HD12	1:C:630:ALA:HB1	2.03	0.41
1:D:148:THR:HB	1:D:279:LEU:HB3	2.01	0.41
1:D:634:TYR:O	1:D:653:THR:HA	2.21	0.41
1:D:634:TYR:CG	1:D:635:SER:N	2.89	0.41
1:B:420:ILE:HG21	1:D:119:HIS:CE1	2.57	0.40
1:D:364:LEU:HD11	1:D:580:ASN:HB2	2.03	0.40
1:B:275:HIS:CG	1:B:408:LEU:HB2	2.56	0.40
1:C:211:ALA:CB	1:C:410:GLY:HA3	2.50	0.40
1:C:490:GLU:OE2	1:D:488:ARG:NH2	2.54	0.40
1:A:126[B]:ILE:HD12	1:A:127:VAL:N	2.36	0.40
1:A:274:ILE:HD12	2:A:754:HEM:HMB1	2.04	0.40
1:B:144:LEU:HD21	1:B:370:VAL:HG22	2.03	0.40
1:B:205:ILE:HD13	1:B:205:ILE:H	1.86	0.40
1:B:516:THR:HB	1:B:517:PRO:CD	2.52	0.40
1:A:709:LYS:O	1:A:710:ILE:CB	2.60	0.40
1:B:429:HIS:CG	1:D:83:ASN:HB3	2.56	0.40
1:C:612:ARG:NH1	1:C:612:ARG:HB2	2.37	0.40

All (3) 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)
3:A:1360:HOH:O	3:D:1418:HOH:O[1_455]	2.06	0.14
1:D:28:SER:CA	3:C:1326:HOH:O[2_555]	2.07	0.13
3:A:1133:HOH:O	3:D:1418:HOH:O[1_455]	2.12	0.08

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	726/753 (96%)	703 (97%)	19 (3%)	4 (1%)	21	23
1	B	726/753 (96%)	701 (97%)	22 (3%)	3 (0%)	30	34
1	C	726/753 (96%)	705 (97%)	19 (3%)	2 (0%)	36	42
1	D	726/753 (96%)	700 (96%)	25 (3%)	1 (0%)	48	57
All	All	2904/3012 (96%)	2809 (97%)	85 (3%)	10 (0%)	36	42

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	725	ASP
1	A	711	ALA
1	B	725	ASP
1	C	75	SER
1	A	75	SER
1	B	75	SER
1	C	28	SER
1	D	75	SER
1	A	29	LEU
1	B	28	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	613/636 (96%)	582 (95%)	31 (5%)	21	27
1	B	613/636 (96%)	578 (94%)	35 (6%)	18	23
1	C	613/636 (96%)	576 (94%)	37 (6%)	17	21
1	D	613/636 (96%)	578 (94%)	35 (6%)	18	23
All	All	2452/2544 (96%)	2314 (94%)	138 (6%)	19	24

All (138) 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	32	GLU
1	A	48	GLN
1	A	54	SER
1	A	100	ARG
1	A	110	LEU
1	A	191	THR
1	A	195	ILE
1	A	198	LEU
1	A	205	ILE
1	A	213	LYS
1	A	252	ASN
1	A	294	LYS
1	A	321	GLU
1	A	341	ILE
1	A	344	GLU
1	A	375	LEU
1	A	386	ASN
1	A	440	TYR
1	A	459	ASN
1	A	478	LYS
1	A	552	LEU
1	A	565	GLU
1	A	616	LEU
1	A	708	ILE
1	A	710	ILE
1	A	713	GLN
1	A	727	SER
1	A	732	LEU
1	A	750	LYS
1	B	28	SER
1	B	37	ARG
1	B	48	GLN
1	B	54	SER
1	B	61	ARG
1	B	73	LYS
1	B	126[A]	ILE
1	B	126[B]	ILE
1	B	185	PHE
1	B	191	THR
1	B	205	ILE
1	B	252	ASN

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Mol	Chain	Res	Type
1	B	283	GLU
1	B	285	LYS
1	B	321	GLU
1	B	370	VAL
1	B	375	LEU
1	B	377	ARG
1	B	386	ASN
1	B	415	TYR
1	B	440	TYR
1	B	459	ASN
1	B	478	LYS
1	B	562	LEU
1	B	566	LEU
1	B	568	ASP
1	B	571	LEU
1	B	583	LYS
1	B	584	LYS
1	B	610	GLU
1	B	633	LEU
1	B	639	GLU
1	B	703	LYS
1	B	709	LYS
1	B	751	ILE
1	C	32	GLU
1	C	37	ARG
1	C	159	ILE
1	C	191	THR
1	C	205	ILE
1	C	252	ASN
1	C	285	LYS
1	C	348	LYS
1	C	368	GLN
1	C	375	LEU
1	C	377	ARG
1	C	386	ASN
1	C	415	TYR
1	C	426	PRO
1	C	440	TYR
1	C	459	ASN
1	C	478	LYS
1	C	488	ARG
1	C	531	LEU

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Mol	Chain	Res	Type
1	C	542	ARG
1	C	552	LEU
1	C	571	LEU
1	C	584	LYS
1	C	606	LEU
1	C	610	GLU
1	C	612	ARG
1	C	616	LEU
1	C	617	LEU
1	C	633	LEU
1	C	648	LEU
1	C	660	LEU
1	C	685	LEU
1	C	715	GLU
1	C	725	ASP
1	C	733	LEU
1	C	750	LYS
1	C	751	ILE
1	D	27	ASP
1	D	41	GLU
1	D	48	GLN
1	D	54	SER
1	D	61	ARG
1	D	73	LYS
1	D	127	VAL
1	D	185	PHE
1	D	191	THR
1	D	205	ILE
1	D	252	ASN
1	D	294	LYS
1	D	340	LEU
1	D	375	LEU
1	D	386	ASN
1	D	440	TYR
1	D	459	ASN
1	D	478	LYS
1	D	488	ARG
1	D	521	ARG
1	D	552	LEU
1	D	554	LEU
1	D	565	GLU
1	D	569	ASP

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Mol	Chain	Res	Type
1	D	582	LEU
1	D	598	VAL
1	D	610	GLU
1	D	616	LEU
1	D	621	LYS
1	D	633	LEU
1	D	648	LEU
1	D	713	GLN
1	D	715	GLU
1	D	749	ASP
1	D	751	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	66	ASN
1	A	246	GLN
1	A	252	ASN
1	A	386	ASN
1	A	449	HIS
1	A	459	ASN
1	A	556	GLN
1	B	157	ASN
1	B	252	ASN
1	B	368	GLN
1	B	386	ASN
1	B	459	ASN
1	B	507	HIS
1	B	629	HIS
1	C	77	ASN
1	C	252	ASN
1	C	386	ASN
1	C	459	ASN
1	C	507	HIS
1	C	556	GLN
1	C	629	HIS
1	D	48	GLN
1	D	252	ASN
1	D	386	ASN
1	D	459	ASN
1	D	492	ASN

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Mol	Chain	Res	Type
1	D	507	HIS
1	D	546	GLN
1	D	629	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEM	D	754	1	50,50,50	1.44	8 (16%)	67,82,82	1.02	3 (4%)
2	HEM	C	754	1	50,50,50	1.51	13 (26%)	67,82,82	1.10	2 (2%)
2	HEM	A	754	1	50,50,50	1.40	9 (18%)	67,82,82	0.94	3 (4%)
2	HEM	B	754	1	50,50,50	1.49	8 (16%)	67,82,82	1.08	2 (2%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	D	754	1	-	2/14/54/54	-
2	HEM	C	754	1	-	2/14/54/54	-
2	HEM	A	754	1	-	2/14/54/54	-
2	HEM	B	754	1	-	2/14/54/54	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	754	HEM	CAB-C3B	3.36	1.56	1.47
2	C	754	HEM	CMB-C2B	3.30	1.57	1.50
2	D	754	HEM	FE-ND	3.17	2.04	1.94
2	B	754	HEM	CAB-C3B	3.08	1.55	1.47
2	B	754	HEM	FE-ND	3.00	2.04	1.94
2	C	754	HEM	FE-NC	2.98	2.05	1.95
2	D	754	HEM	CAC-C3C	2.97	1.55	1.47
2	B	754	HEM	CAC-C3C	2.96	1.55	1.47
2	D	754	HEM	FE-NC	2.95	2.04	1.95
2	A	754	HEM	CMB-C2B	2.91	1.56	1.50
2	A	754	HEM	FE-NB	2.89	2.03	1.94
2	A	754	HEM	CMD-C2D	2.88	1.56	1.50
2	D	754	HEM	CMB-C2B	2.85	1.56	1.50
2	A	754	HEM	FE-NC	2.82	2.04	1.95
2	B	754	HEM	FE-NC	2.76	2.04	1.95
2	C	754	HEM	CAC-C3C	2.70	1.54	1.47
2	A	754	HEM	CAC-C3C	2.69	1.54	1.47
2	C	754	HEM	CAB-C3B	2.65	1.54	1.47
2	B	754	HEM	CMC-C2C	2.64	1.56	1.50
2	A	754	HEM	CAB-C3B	2.61	1.54	1.47
2	C	754	HEM	CMA-C3A	2.54	1.56	1.50
2	C	754	HEM	C3B-C2B	-2.54	1.32	1.37
2	B	754	HEM	FE-NA	2.48	2.03	1.95
2	C	754	HEM	FE-ND	2.47	2.02	1.94
2	B	754	HEM	C3D-C2D	-2.44	1.31	1.36
2	D	754	HEM	CMD-C2D	2.40	1.55	1.50
2	A	754	HEM	CMC-C2C	2.39	1.55	1.50
2	C	754	HEM	CAD-C3D	2.36	1.57	1.51
2	C	754	HEM	CMC-C2C	2.24	1.55	1.50
2	D	754	HEM	FE-NB	2.20	2.01	1.94
2	A	754	HEM	FE-NA	2.19	2.02	1.95
2	C	754	HEM	O2A-CGA	-2.19	1.23	1.30
2	B	754	HEM	CAD-C3D	2.19	1.57	1.51
2	D	754	HEM	FE-NA	2.11	2.02	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	754	HEM	C2A-C3A	-2.09	1.33	1.38
2	C	754	HEM	C3D-C2D	-2.08	1.32	1.36
2	A	754	HEM	FE-ND	2.02	2.01	1.94
2	C	754	HEM	FE-NB	2.02	2.01	1.94

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	754	HEM	O1A-CGA-CBA	-3.48	112.07	123.09
2	C	754	HEM	O2A-CGA-O1A	3.04	131.16	123.33
2	C	754	HEM	O1A-CGA-CBA	-2.58	114.92	123.09
2	A	754	HEM	CHD-C4C-NC	2.56	127.24	124.45
2	D	754	HEM	CHD-C4C-NC	2.47	127.14	124.45
2	A	754	HEM	O1A-CGA-CBA	-2.36	115.61	123.09
2	A	754	HEM	CBC-CAC-C3C	-2.14	116.82	127.53
2	D	754	HEM	C3B-C4B-NB	-2.10	107.96	109.47
2	B	754	HEM	CMD-C2D-C1D	-2.05	121.84	125.03
2	D	754	HEM	CHD-C1D-ND	2.03	126.61	124.42

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	754	HEM	CAA-CBA-CGA-O2A
2	D	754	HEM	CAA-CBA-CGA-O2A
2	B	754	HEM	CAA-CBA-CGA-O1A
2	C	754	HEM	CAA-CBA-CGA-O2A
2	A	754	HEM	CAA-CBA-CGA-O1A
2	C	754	HEM	CAA-CBA-CGA-O1A
2	B	754	HEM	CAA-CBA-CGA-O2A
2	D	754	HEM	CAA-CBA-CGA-O1A

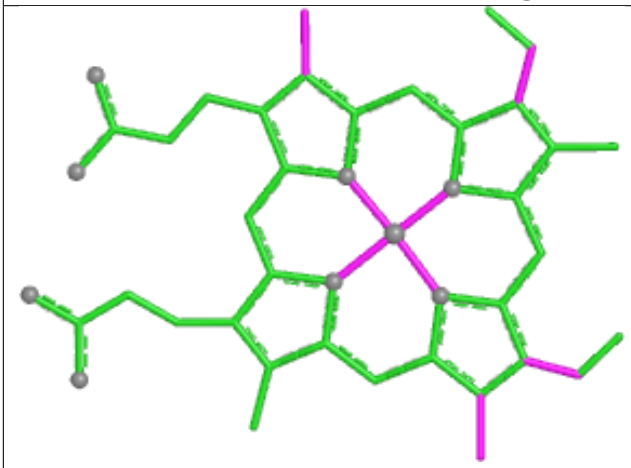
There are no ring outliers.

4 monomers are involved in 19 short contacts:

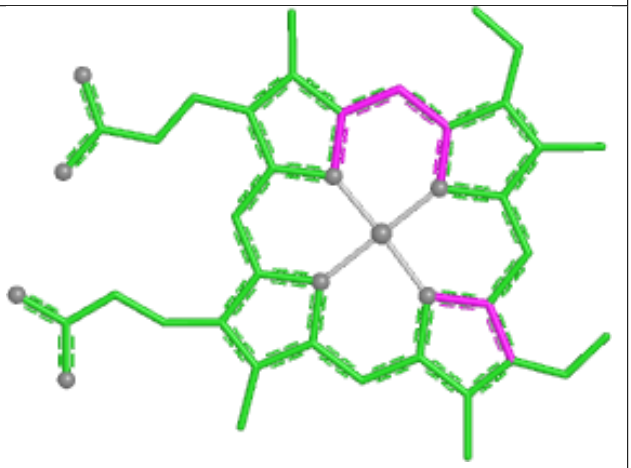
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	754	HEM	5	0
2	C	754	HEM	4	0
2	A	754	HEM	4	0
2	B	754	HEM	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

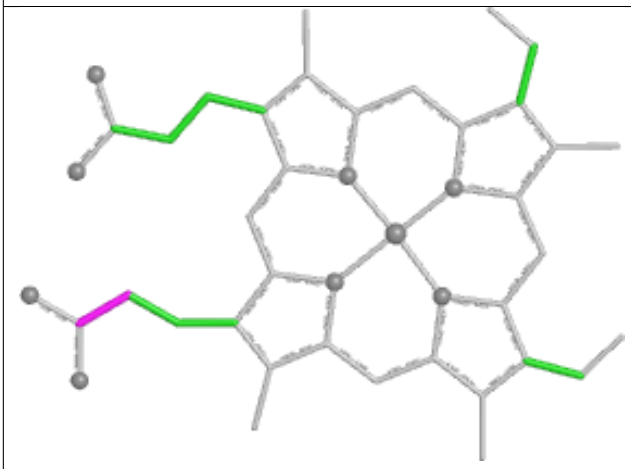
Ligand HEM D 754



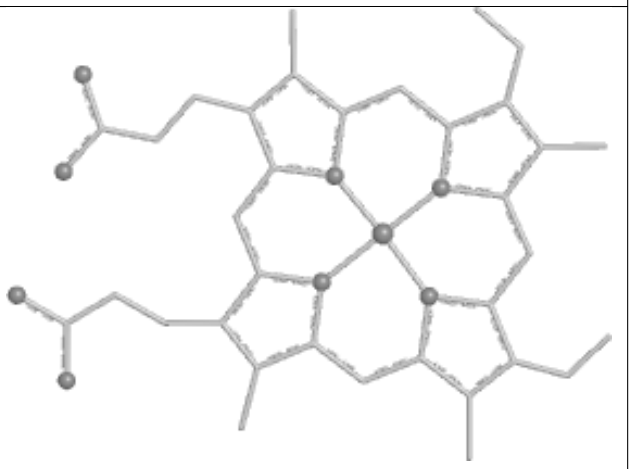
Bond lengths



Bond angles

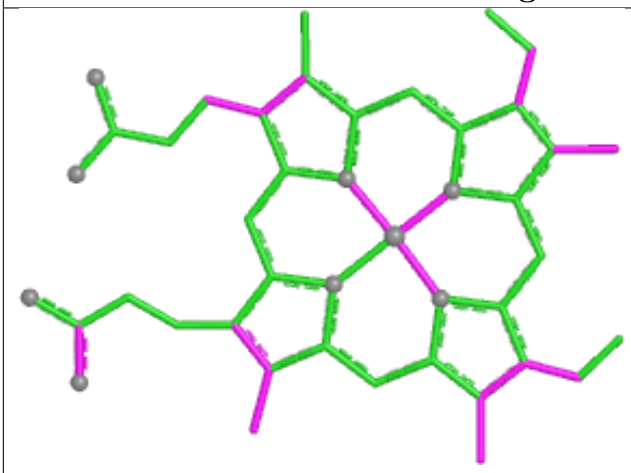


Torsions

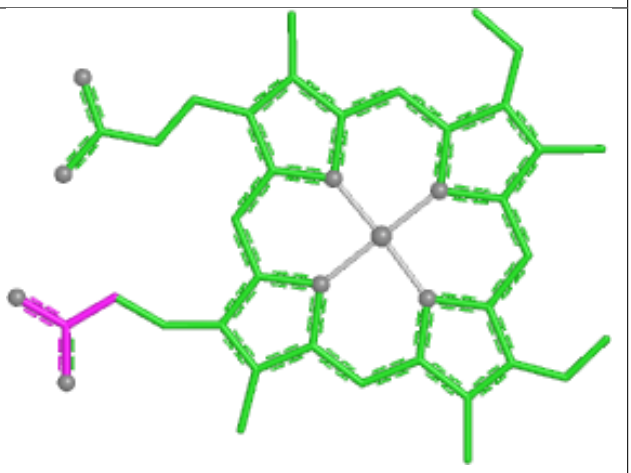


Rings

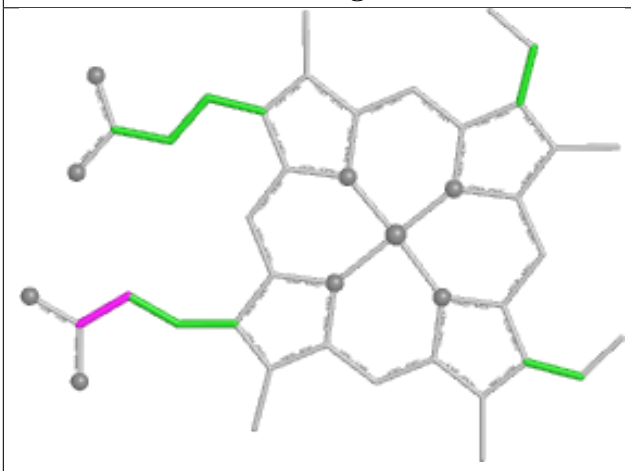
Ligand HEM C 754



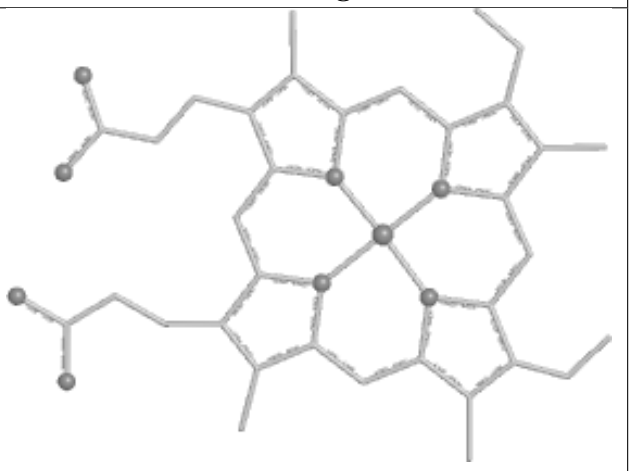
Bond lengths



Bond angles

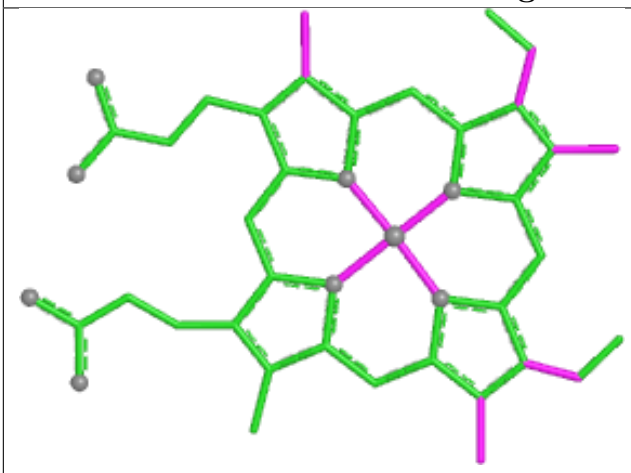


Torsions

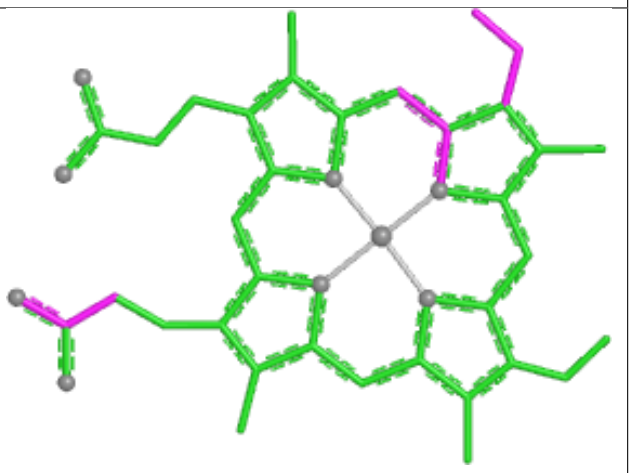


Rings

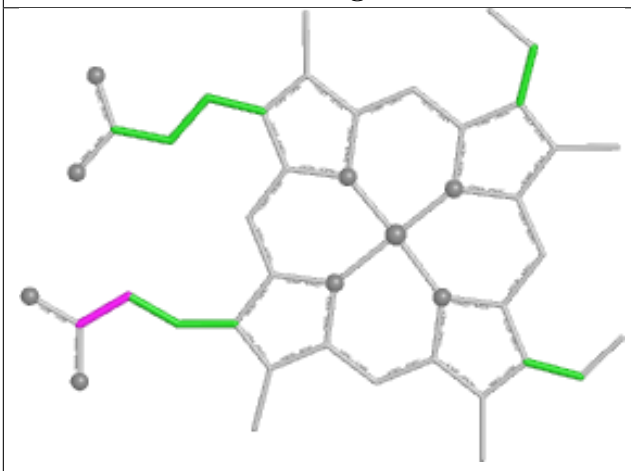
Ligand HEM A 754



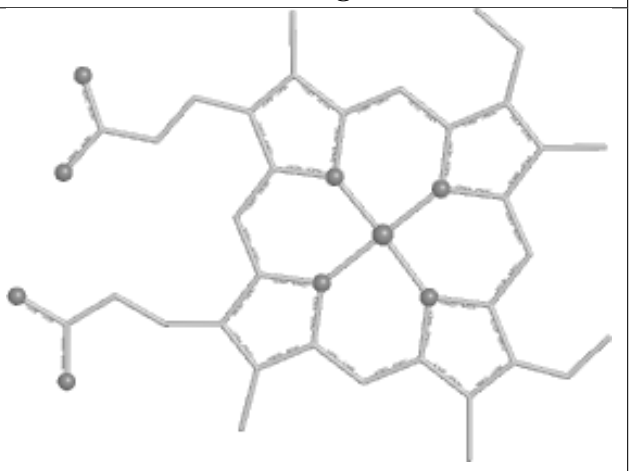
Bond lengths



Bond angles

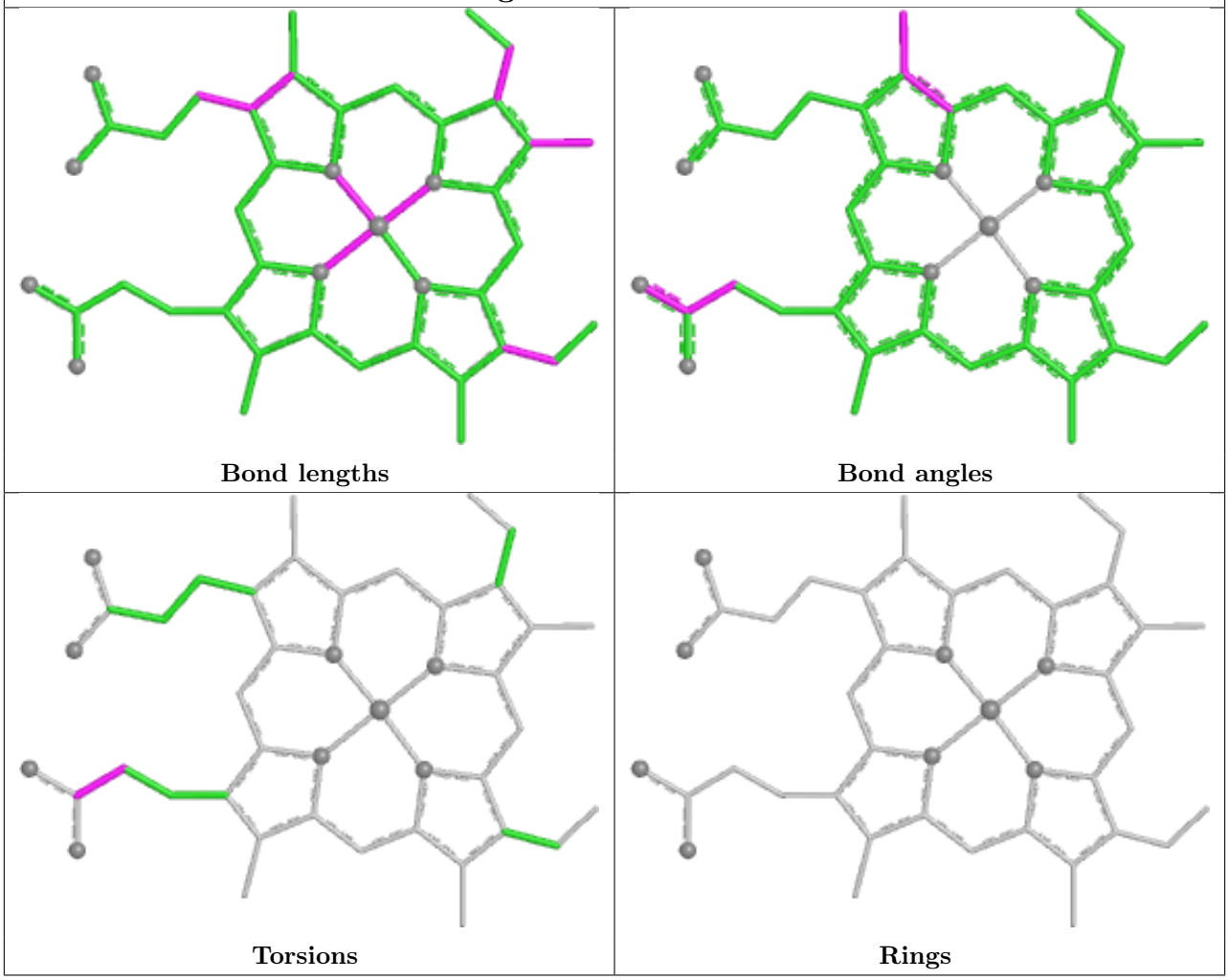


Torsions



Rings

Ligand HEM B 754



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	727/753 (96%)	-0.62	12 (1%)	69	66	8, 16, 34, 64	1 (0%)
1	B	727/753 (96%)	-0.62	3 (0%)	88	87	9, 17, 35, 63	1 (0%)
1	C	727/753 (96%)	-0.64	4 (0%)	85	83	9, 17, 35, 63	1 (0%)
1	D	727/753 (96%)	-0.70	6 (0%)	82	80	10, 16, 34, 62	1 (0%)
All	All	2908/3012 (96%)	-0.64	25 (0%)	81	79	8, 16, 35, 64	4 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	28	SER	10.4
1	A	27	ASP	5.6
1	B	27	ASP	5.5
1	D	27	ASP	4.8
1	C	27	ASP	4.5
1	A	713	GLN	4.2
1	D	726	GLY	4.2
1	C	725	ASP	3.6
1	B	28	SER	3.6
1	A	712	ASP	3.4
1	C	28	SER	3.4
1	D	28	SER	3.4
1	C	726	GLY	3.2
1	A	710	ILE	3.0
1	D	751	ILE	2.7
1	D	749	ASP	2.5
1	A	725	ASP	2.4
1	A	711	ALA	2.3
1	D	750	LYS	2.3
1	A	750	LYS	2.3
1	A	751	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	29	LEU	2.2
1	A	646	THR	2.1
1	A	749	ASP	2.1
1	B	724	ALA	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)

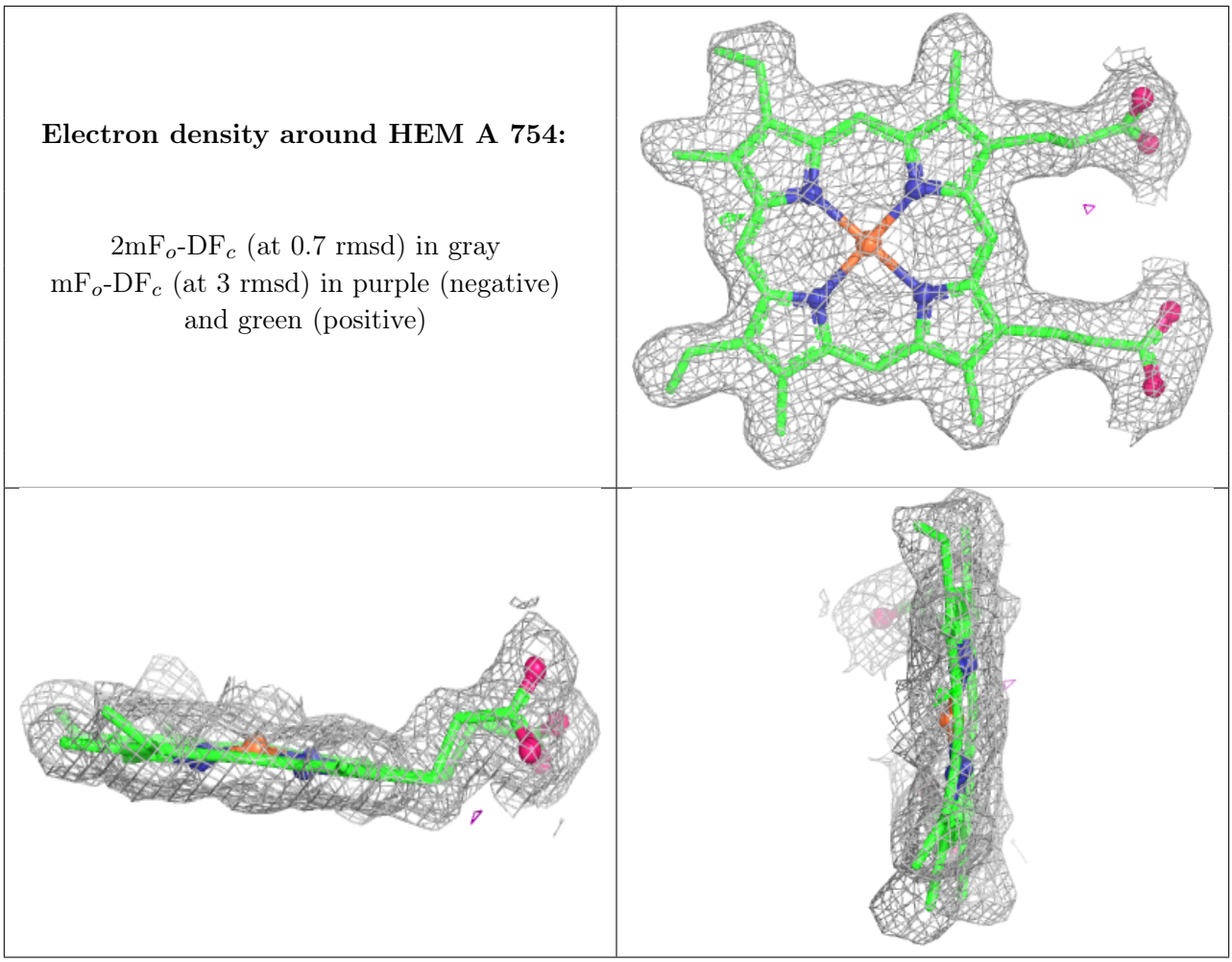
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEM	A	754	43/43	0.98	0.05	11,14,19,28	0
2	HEM	B	754	43/43	0.98	0.06	10,15,19,27	0
2	HEM	C	754	43/43	0.98	0.06	10,15,19,27	0
2	HEM	D	754	43/43	0.98	0.05	11,14,19,28	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

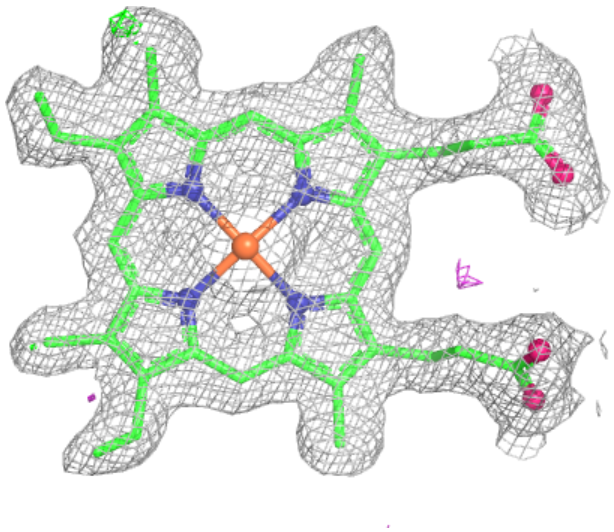
Electron density around HEM A 754:

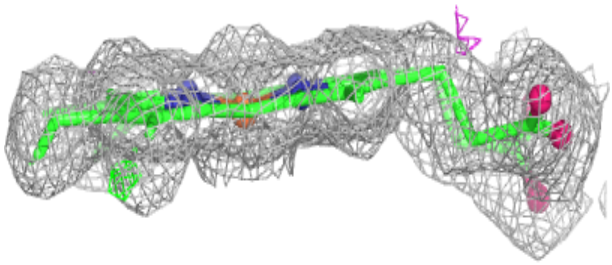
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

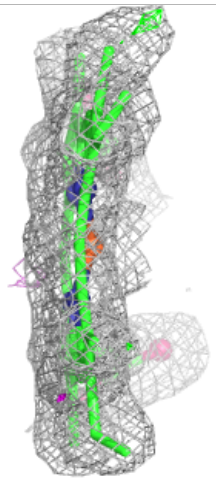


Electron density around HEM B 754:

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

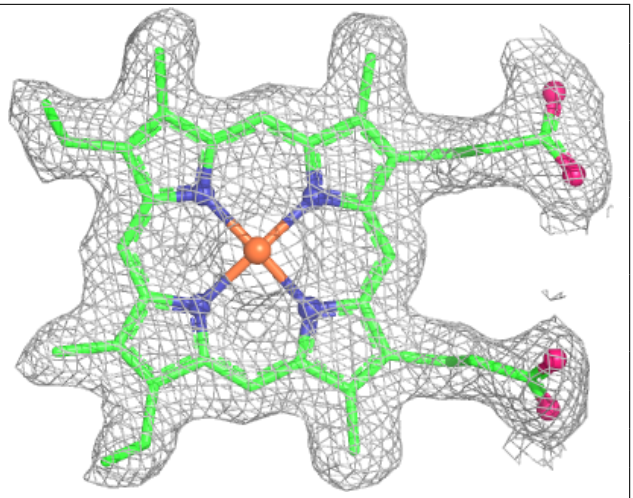


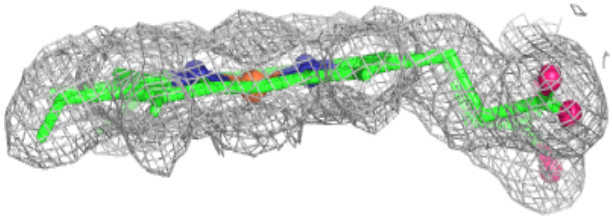


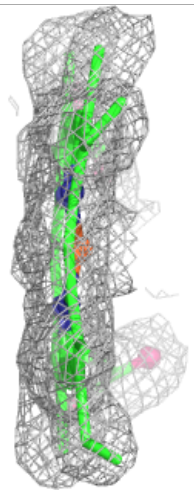


Electron density around HEM C 754:

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

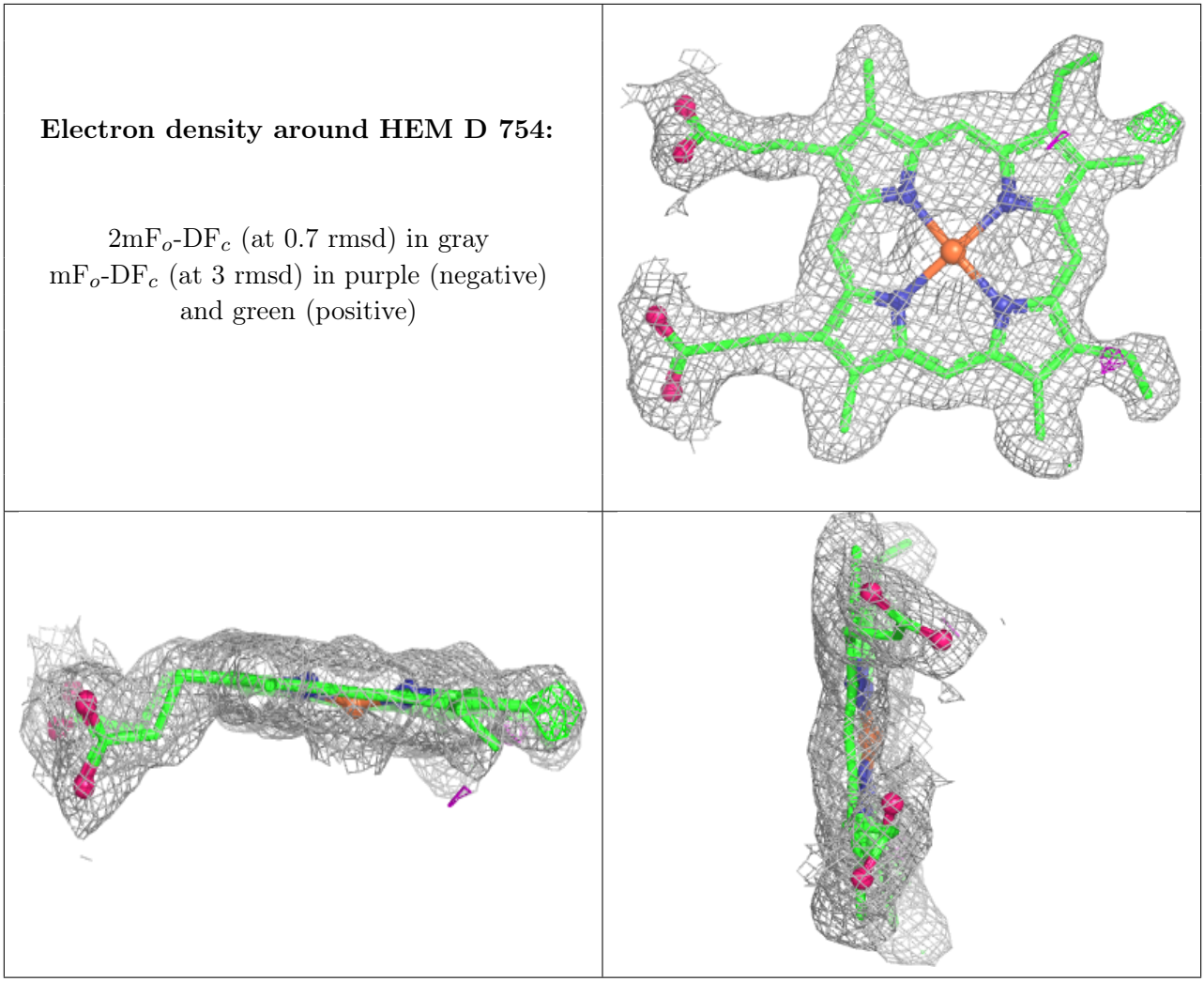






Electron density around HEM D 754:

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



6.5 Other polymers

There are no such residues in this entry.