



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:32 PM UTC

PDB ID : 1CF9 / pdb_00001cf9
Title : Structure of the mutant VAL169CYS of catalase HP11 from Escherichia coli
Authors : Mate, M.J.; Loewen, P.C.; Fita, I.
Deposited on : 1999-03-24
Resolution : 1.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

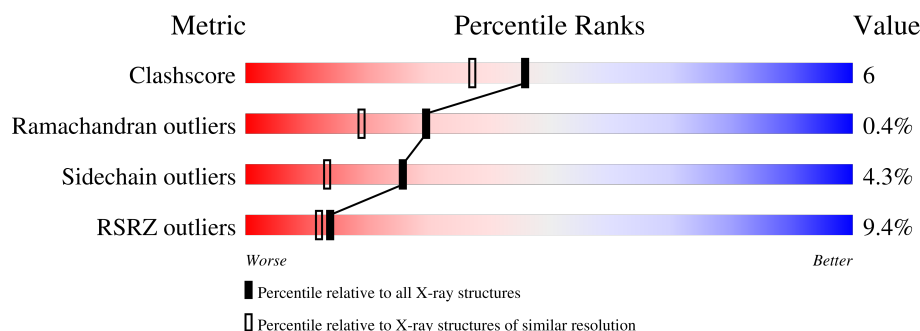
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	753	11% 75% 18% ...
1	B	753	8% 73% 21% ..
1	C	753	9% 74% 19% ...
1	D	753	8% 77% 16% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25850 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 HP11).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	1	0
			5748	3649	1005	1081	13			
1	B	727	Total	C	N	O	S	0	1	0
			5748	3649	1005	1081	13			
1	C	727	Total	C	N	O	S	0	1	0
			5748	3649	1005	1081	13			
1	D	727	Total	C	N	O	S	0	1	0
			5748	3649	1005	1081	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	169	CYS	VAL	engineered mutation	UNP P21179
B	169	CYS	VAL	engineered mutation	UNP P21179
C	169	CYS	VAL	engineered mutation	UNP P21179
D	169	CYS	VAL	engineered mutation	UNP P21179

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



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

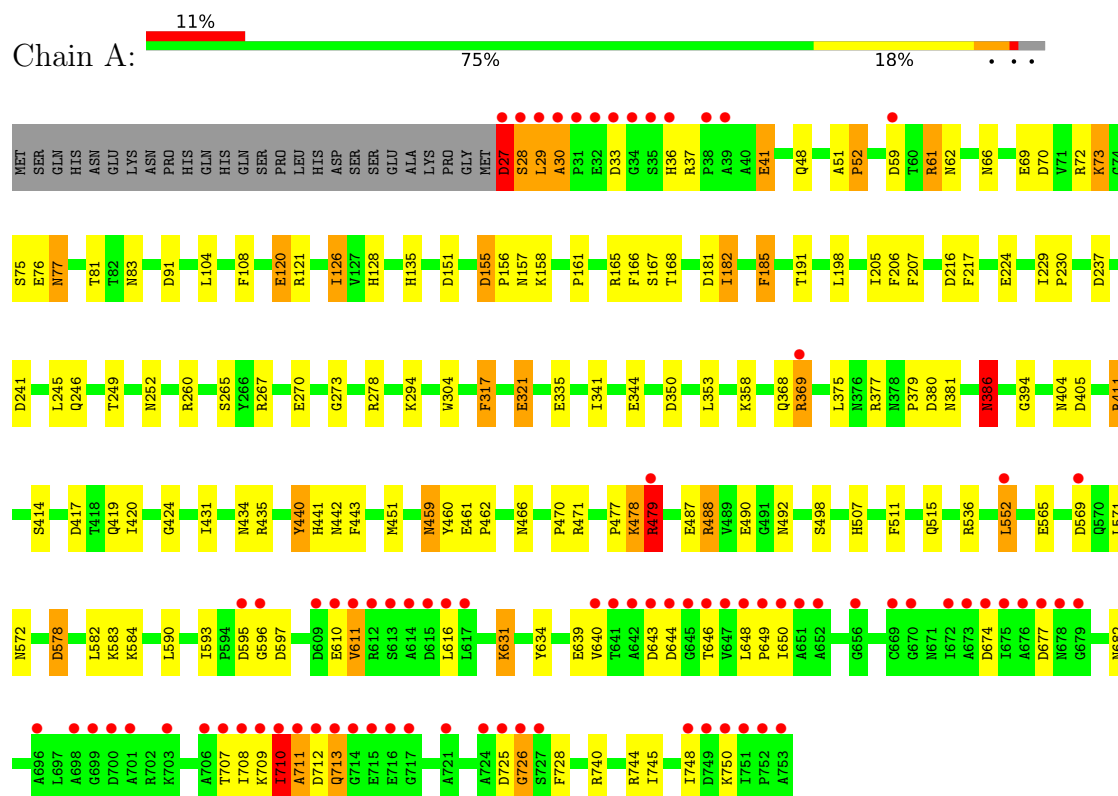
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	727	Total O 727 727	0	0
3	B	616	Total O 616 616	0	0
3	C	638	Total O 638 638	0	0
3	D	705	Total O 705 705	0	0

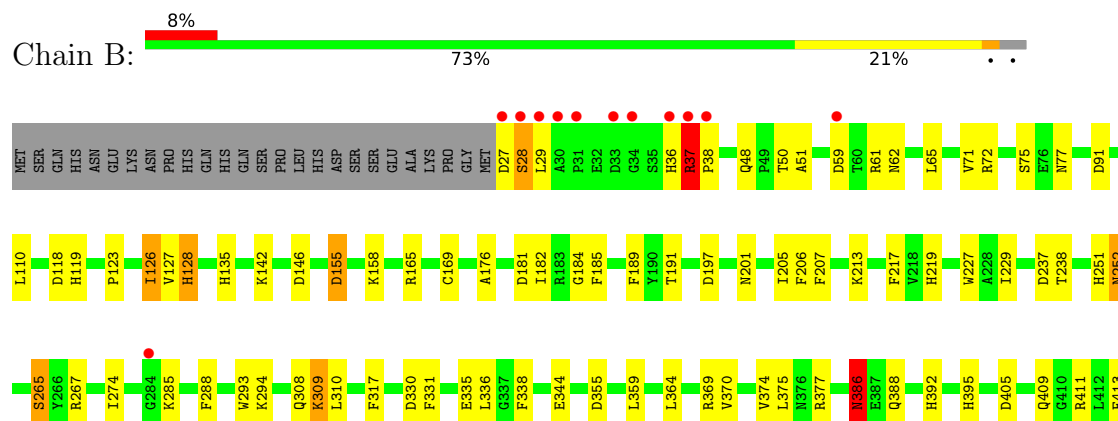
3 Residue-property plots

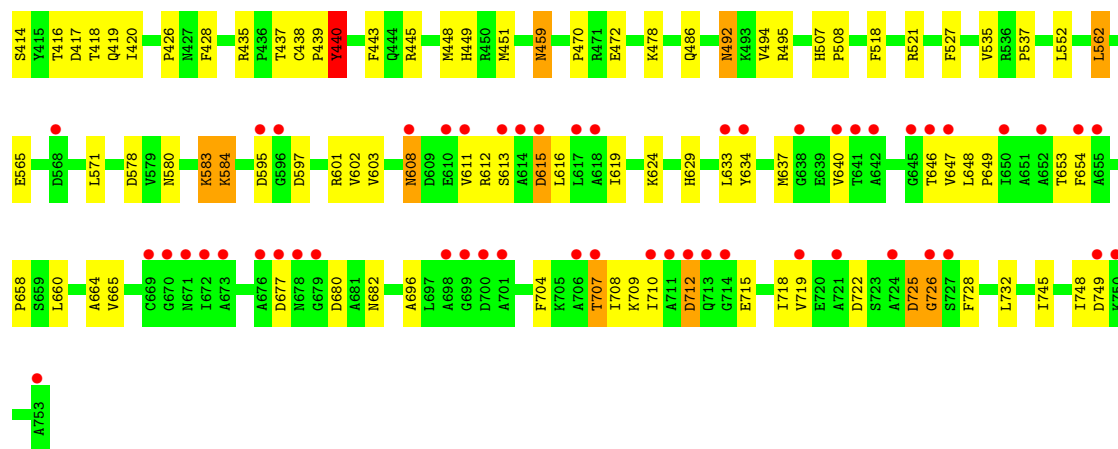
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: PROTEIN (CATALASE HP11)

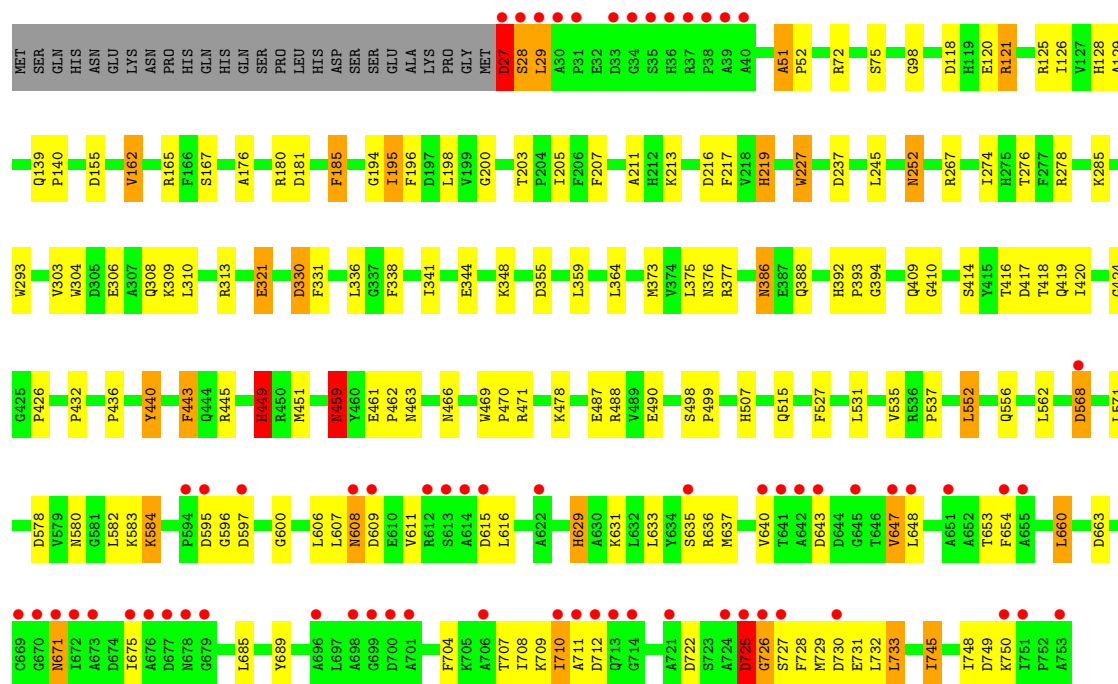
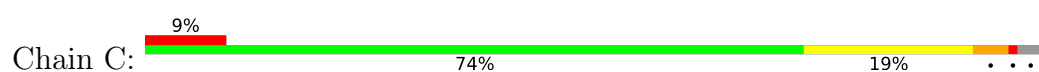


• Molecule 1: PROTEIN (CATALASE HP11)

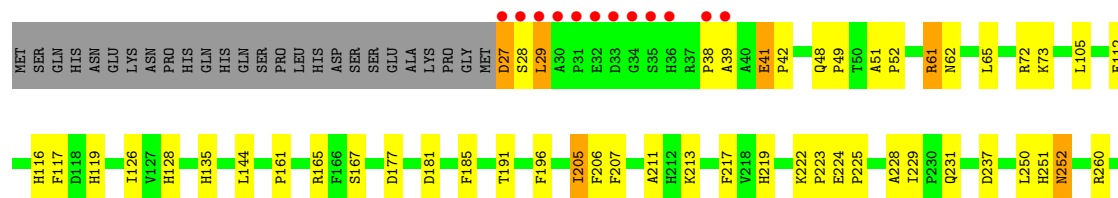
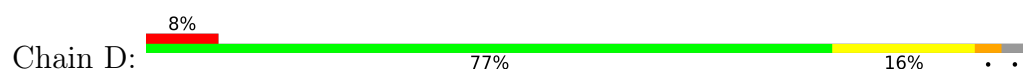


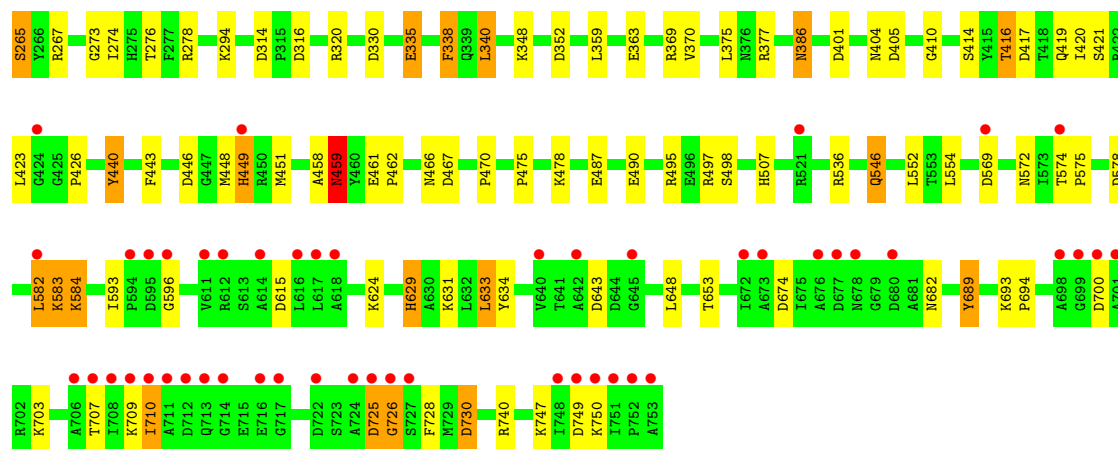


• Molecule 1: PROTEIN (CATALASE HP1I)



• Molecule 1: PROTEIN (CATALASE HP1I)





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.47Å 133.04Å 122.22Å 90.00° 109.64° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 20.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	88.3 (20.00-1.80) 83.4 (20.00-1.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	9.00	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.60 (at 1.77Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.181 , 0.237 0.179 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	15.2	Xtriage
Anisotropy	0.416	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 63.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.028 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25850	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.96	3/5908 (0.1%)	1.88	136/8033 (1.7%)
1	B	0.93	1/5908 (0.0%)	1.75	87/8033 (1.1%)
1	C	0.93	1/5908 (0.0%)	1.77	100/8033 (1.2%)
1	D	0.92	0/5908	1.71	78/8033 (1.0%)
All	All	0.94	5/23632 (0.0%)	1.78	401/32132 (1.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	4
1	C	1	2
1	D	0	2
All	All	3	8

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	28	SER	N-CA	-8.93	1.35	1.45
1	A	29	LEU	CA-C	-7.68	1.45	1.53
1	C	200	GLY	N-CA	5.73	1.49	1.44
1	B	184	GLY	CA-C	5.27	1.58	1.52
1	A	28	SER	C-N	5.24	1.39	1.33

All (401) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	725	ASP	CA-CB-CG	30.72	143.32	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	479	ARG	NE-CZ-NH2	-26.89	95.00	119.20
1	B	377	ARG	CD-NE-CZ	22.06	155.28	124.40
1	A	27	ASP	CA-CB-CG	21.54	134.14	112.60
1	A	710	ILE	CB-CA-C	19.10	138.40	110.90
1	A	29	LEU	N-CA-C	17.23	133.58	109.11
1	C	725	ASP	N-CA-CB	17.00	139.23	110.49
1	A	479	ARG	NE-CZ-NH1	16.59	138.09	121.50
1	A	28	SER	CA-C-N	-16.48	100.71	122.79
1	A	28	SER	C-N-CA	-16.48	100.71	122.79
1	A	27	ASP	O-C-N	-15.35	98.44	123.00
1	B	61	ARG	CD-NE-CZ	14.69	144.97	124.40
1	D	61	ARG	CD-NE-CZ	13.23	142.92	124.40
1	C	449	HIS	CA-CB-CG	-13.19	100.61	113.80
1	D	449	HIS	CA-CB-CG	11.45	125.25	113.80
1	B	338	PHE	CA-CB-CG	11.31	125.11	113.80
1	A	644	ASP	CA-CB-CG	11.11	123.71	112.60
1	C	194	GLY	CA-C-O	11.10	130.44	122.45
1	A	61	ARG	NE-CZ-NH1	-10.96	110.53	121.50
1	A	414	SER	N-CA-C	10.63	122.95	111.36
1	A	597	ASP	CA-CB-CG	10.61	123.21	112.60
1	A	712	ASP	CB-CA-C	10.25	128.28	110.85
1	C	725	ASP	CA-C-O	-10.24	105.87	120.51
1	A	709	LYS	CA-C-N	-10.19	105.75	122.57
1	A	709	LYS	C-N-CA	-10.19	105.75	122.57
1	A	155	ASP	CA-CB-CG	-10.14	102.46	112.60
1	A	344	GLU	CA-CB-CG	10.01	134.12	114.10
1	A	728	PHE	CA-CB-CG	9.99	123.79	113.80
1	C	27	ASP	CA-CB-CG	-9.83	102.77	112.60
1	C	393	PRO	CA-C-N	9.66	132.49	120.22
1	C	393	PRO	C-N-CA	9.66	132.49	120.22
1	A	712	ASP	N-CA-CB	-9.25	96.47	110.16
1	C	636	ARG	CD-NE-CZ	9.11	137.15	124.40
1	A	61	ARG	CD-NE-CZ	-8.95	111.87	124.40
1	B	597	ASP	CA-CB-CG	8.83	121.43	112.60
1	A	30	ALA	N-CA-C	-8.77	99.05	109.93
1	B	677	ASP	CA-CB-CG	8.59	121.19	112.60
1	C	338	PHE	CA-CB-CG	8.57	122.37	113.80
1	B	229	ILE	N-CA-C	-8.56	102.17	109.19
1	A	507	HIS	CA-CB-CG	-8.37	105.43	113.80
1	A	265	SER	N-CA-CB	-8.35	98.62	111.56
1	A	344	GLU	CB-CG-CD	8.32	126.74	112.60
1	A	386	ASN	CA-CB-CG	8.30	120.90	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	217	PHE	CA-CB-CG	-8.26	105.54	113.80
1	A	479	ARG	CB-CA-C	-8.24	98.49	111.51
1	A	28	SER	N-CA-C	8.22	123.40	110.17
1	B	414	SER	N-CA-C	8.21	120.31	111.36
1	C	341	ILE	CA-C-O	8.15	124.18	119.94
1	D	728	PHE	CA-CB-CG	8.13	121.93	113.80
1	A	33	ASP	CA-CB-CG	8.12	120.72	112.60
1	B	77	ASN	CA-CB-CG	-8.01	104.59	112.60
1	C	128	HIS	CA-CB-CG	-7.98	105.82	113.80
1	A	350	ASP	CB-CA-C	7.95	124.52	110.37
1	C	643	ASP	CA-CB-CG	7.91	120.51	112.60
1	C	217	PHE	CA-CB-CG	-7.91	105.89	113.80
1	C	414	SER	N-CA-C	7.86	119.93	111.36
1	D	377	ARG	NE-CZ-NH2	-7.83	112.15	119.20
1	B	615	ASP	CA-CB-CG	7.79	120.39	112.60
1	D	414	SER	N-CA-C	7.75	119.81	111.36
1	D	265	SER	N-CA-CB	-7.73	99.58	111.56
1	B	185	PHE	CA-CB-CG	7.72	121.52	113.80
1	C	155	ASP	CA-CB-CG	7.71	120.31	112.60
1	D	629	HIS	CA-CB-CG	-7.70	106.10	113.80
1	B	386	ASN	CA-CB-CG	7.69	120.29	112.60
1	D	377	ARG	NH1-CZ-NH2	7.67	129.27	119.30
1	B	578	ASP	CA-CB-CG	-7.65	104.95	112.60
1	C	237	ASP	N-CA-C	7.62	120.25	111.11
1	C	308	GLN	OE1-CD-NE2	7.62	130.22	122.60
1	D	237	ASP	N-CA-C	7.58	119.54	111.28
1	A	270	GLU	CA-C-N	7.47	127.36	121.61
1	A	270	GLU	C-N-CA	7.47	127.36	121.61
1	B	409	GLN	OE1-CD-NE2	-7.34	115.26	122.60
1	C	463	ASN	CB-CG-ND2	7.31	127.36	116.40
1	A	713	GLN	N-CA-CB	-7.30	99.00	110.46
1	C	710	ILE	CB-CA-C	-7.30	100.98	111.34
1	B	527	PHE	CA-CB-CG	7.26	121.06	113.80
1	A	72	ARG	N-CA-CB	7.20	120.55	109.97
1	C	180	ARG	NE-CZ-NH1	7.17	128.67	121.50
1	A	711	ALA	CA-C-O	7.17	130.76	120.51
1	B	51	ALA	N-CA-CB	-7.17	103.58	111.10
1	B	612	ARG	CB-CA-C	7.13	123.10	111.05
1	C	728	PHE	CA-CB-CG	7.12	120.92	113.80
1	A	267	ARG	CD-NE-CZ	7.05	134.27	124.40
1	B	207	PHE	O-C-N	-7.05	114.12	122.15
1	A	611	VAL	CB-CA-C	-7.01	100.16	111.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	709	LYS	CB-CA-C	-7.01	100.65	111.66
1	C	745	ILE	N-CA-CB	6.99	115.91	110.45
1	B	492	ASN	CA-CB-CG	-6.99	105.61	112.60
1	C	121	ARG	CD-NE-CZ	6.98	134.17	124.40
1	D	61	ARG	CB-CG-CD	6.92	127.21	111.30
1	A	369	ARG	CD-NE-CZ	6.89	134.05	124.40
1	C	216	ASP	CA-CB-CG	-6.89	105.71	112.60
1	D	466	ASN	OD1-CG-ND2	-6.87	115.73	122.60
1	B	317	PHE	N-CA-C	6.86	119.34	111.11
1	A	646	THR	N-CA-CB	6.83	120.02	109.85
1	B	59	ASP	N-CA-CB	6.81	121.16	110.46
1	A	648	LEU	CB-CA-C	-6.79	102.34	110.15
1	B	748	ILE	CA-C-N	6.79	129.68	120.38
1	B	748	ILE	C-N-CA	6.79	129.68	120.38
1	D	128	HIS	CA-CB-CG	-6.76	107.04	113.80
1	C	120	GLU	N-CA-C	6.76	119.66	111.82
1	C	306	GLU	CA-CB-CG	6.76	127.62	114.10
1	C	376	ASN	OD1-CG-ND2	-6.75	115.85	122.60
1	A	441	HIS	CA-CB-CG	-6.74	107.06	113.80
1	A	492	ASN	CA-CB-CG	-6.74	105.86	112.60
1	A	712	ASP	CA-C-O	6.73	127.55	120.42
1	D	643	ASP	CA-CB-CG	6.72	119.32	112.60
1	B	728	PHE	CA-CB-CG	6.70	120.50	113.80
1	D	490	GLU	CB-CG-CD	6.69	123.98	112.60
1	A	711	ALA	CA-C-N	6.69	129.79	120.29
1	A	711	ALA	C-N-CA	6.69	129.79	120.29
1	A	168	THR	N-CA-C	-6.68	99.38	109.79
1	C	471	ARG	NE-CZ-NH2	6.66	125.20	119.20
1	B	37	ARG	CD-NE-CZ	6.62	133.68	124.40
1	C	445	ARG	NE-CZ-NH1	6.60	128.10	121.50
1	A	128	HIS	CA-CB-CG	-6.59	107.21	113.80
1	C	608	ASN	CA-CB-CG	6.59	119.19	112.60
1	B	355	ASP	CA-C-O	6.58	123.57	119.29
1	B	595	ASP	CA-CB-CG	6.53	119.13	112.60
1	D	231	GLN	OE1-CD-NE2	-6.51	116.09	122.60
1	A	182	ILE	CA-CB-CG1	-6.51	99.34	110.40
1	A	304	TRP	N-CA-C	6.50	118.92	111.11
1	C	663	ASP	CA-CB-CG	-6.50	106.10	112.60
1	B	128	HIS	CA-CB-CG	-6.49	107.31	113.80
1	A	151	ASP	CA-CB-CG	-6.49	106.11	112.60
1	D	497	ARG	CD-NE-CZ	6.48	133.48	124.40
1	A	595	ASP	CA-CB-CG	6.45	119.05	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	475	PRO	N-CA-C	-6.44	101.75	111.41
1	B	227	TRP	O-C-N	6.43	129.79	122.20
1	D	749	ASP	CA-CB-CG	-6.43	106.17	112.60
1	C	609	ASP	CA-CB-CG	6.41	119.01	112.60
1	D	615	ASP	CA-CB-CG	6.39	118.99	112.60
1	A	639	GLU	CB-CG-CD	6.38	123.44	112.60
1	B	707	THR	N-CA-CB	6.38	120.16	110.28
1	B	518	PHE	CA-CB-CG	6.37	120.17	113.80
1	A	420	ILE	N-CA-CB	6.37	118.00	110.55
1	C	631	LYS	N-CA-CB	6.36	120.76	110.77
1	A	466	ASN	OD1-CG-ND2	-6.36	116.25	122.60
1	A	377	ARG	CA-CB-CG	-6.35	101.40	114.10
1	D	467	ASP	CA-C-O	6.34	128.90	121.54
1	D	419	GLN	OE1-CD-NE2	6.30	128.91	122.60
1	A	677	ASP	CA-CB-CG	-6.30	106.30	112.60
1	B	181	ASP	CA-CB-CG	6.30	118.90	112.60
1	A	572	ASN	CA-CB-CG	-6.29	106.31	112.60
1	C	443	PHE	O-C-N	6.29	129.89	122.34
1	C	647	VAL	N-CA-CB	6.29	117.57	110.72
1	B	602	VAL	CB-CA-C	-6.28	100.82	110.50
1	D	207	PHE	O-C-N	-6.28	114.55	122.27
1	B	640	VAL	N-CA-CB	6.27	123.00	112.47
1	C	420	ILE	CB-CA-C	-6.27	103.95	111.97
1	A	181	ASP	CA-CB-CG	6.24	118.84	112.60
1	C	162	VAL	CA-C-O	6.22	127.78	121.63
1	D	335	GLU	CB-CG-CD	-6.21	102.04	112.60
1	A	28	SER	CA-C-O	6.21	128.61	121.28
1	B	411	ARG	NE-CZ-NH2	6.21	124.78	119.20
1	B	440	TYR	O-C-N	-6.21	115.34	123.28
1	D	224	GLU	CB-CA-C	6.19	119.24	109.27
1	A	83	ASN	OD1-CG-ND2	-6.18	116.42	122.60
1	A	569	ASP	CA-CB-CG	-6.17	106.44	112.60
1	C	596	GLY	N-CA-C	6.16	120.58	110.97
1	A	420	ILE	CB-CA-C	-6.14	104.11	111.97
1	C	355	ASP	CA-CB-CG	6.13	118.73	112.60
1	D	62	ASN	CA-CB-CG	6.12	118.72	112.60
1	D	205	ILE	CA-C-O	-6.12	115.64	121.64
1	C	72	ARG	NE-CZ-NH2	-6.11	113.70	119.20
1	C	459	ASN	OD1-CG-ND2	-6.11	116.49	122.60
1	B	331	PHE	CA-CB-CG	6.10	119.90	113.80
1	D	260	ARG	NE-CZ-NH2	-6.09	113.72	119.20
1	C	377	ARG	NE-CZ-NH1	-6.09	115.41	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	72	ARG	N-CA-CB	6.09	118.92	109.97
1	D	459	ASN	CA-CB-CG	6.07	118.67	112.60
1	D	596	GLY	N-CA-C	6.06	120.43	110.97
1	D	217	PHE	CA-CB-CG	-6.05	107.75	113.80
1	A	246	GLN	O-C-N	-6.04	116.03	121.17
1	B	59	ASP	CB-CA-C	-6.03	98.14	109.72
1	A	368	GLN	OE1-CD-NE2	-6.03	116.57	122.60
1	C	424	GLY	N-CA-C	6.00	123.60	115.32
1	C	176	ALA	N-CA-C	6.00	119.36	110.48
1	C	185	PHE	O-C-N	-5.98	116.64	123.40
1	C	419	GLN	OE1-CD-NE2	5.97	128.57	122.60
1	C	388	GLN	OE1-CD-NE2	-5.97	116.63	122.60
1	B	680	ASP	CA-CB-CG	-5.95	106.65	112.60
1	C	445	ARG	CA-C-O	-5.94	114.86	121.51
1	D	416	THR	CA-CB-CG2	5.93	120.58	110.50
1	D	631	LYS	CA-CB-CG	5.92	125.94	114.10
1	D	185	PHE	CA-CB-CG	5.89	119.69	113.80
1	A	498	SER	O-C-N	-5.88	115.40	121.28
1	B	435	ARG	O-C-N	5.88	128.02	121.43
1	A	206	PHE	CA-CB-CG	-5.87	107.93	113.80
1	D	112	GLU	OE1-CD-OE2	5.87	136.98	122.90
1	B	495	ARG	NE-CZ-NH1	5.87	127.37	121.50
1	C	98	GLY	CA-C-O	-5.87	117.30	121.88
1	B	206	PHE	CA-CB-CG	-5.85	107.95	113.80
1	B	155	ASP	CA-CB-CG	5.85	118.45	112.60
1	C	654	PHE	CA-CB-CG	5.83	119.63	113.80
1	A	61	ARG	CB-CG-CD	-5.82	97.91	111.30
1	A	712	ASP	O-C-N	-5.82	115.52	122.15
1	B	207	PHE	CA-C-O	5.82	126.59	120.42
1	A	479	ARG	NH1-CZ-NH2	5.82	126.86	119.30
1	A	61	ARG	NH1-CZ-NH2	5.81	126.86	119.30
1	A	674	ASP	CA-CB-CG	5.81	118.41	112.60
1	B	201	ASN	OD1-CG-ND2	-5.81	116.79	122.60
1	C	629	HIS	CA-CB-CG	-5.80	108.00	113.80
1	C	725	ASP	CA-CB-CG	-5.80	106.80	112.60
1	B	601	ARG	CA-CB-CG	5.80	125.69	114.10
1	B	725	ASP	N-CA-CB	-5.80	100.69	110.49
1	D	196	PHE	CA-CB-CG	5.79	119.59	113.80
1	B	182	ILE	N-CA-C	-5.78	103.75	110.05
1	C	219	HIS	CA-CB-CG	-5.76	108.04	113.80
1	D	177	ASP	N-CA-C	5.76	117.36	111.14
1	B	189	PHE	CA-CB-CG	5.76	119.56	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	565	GLU	CB-CA-C	-5.75	100.76	110.19
1	C	671	ASN	CA-CB-CG	-5.73	106.87	112.60
1	B	486	GLN	OE1-CD-NE2	-5.72	116.88	122.60
1	C	636	ARG	NE-CZ-NH2	-5.72	114.05	119.20
1	A	237	ASP	N-CA-C	5.72	117.97	111.11
1	D	29	LEU	N-CA-CB	-5.72	100.60	110.32
1	C	409	GLN	OE1-CD-NE2	-5.71	116.89	122.60
1	A	273	GLY	N-CA-C	-5.71	106.75	115.66
1	A	708	ILE	CA-C-N	5.71	132.44	121.54
1	A	708	ILE	C-N-CA	5.71	132.44	121.54
1	C	640	VAL	N-CA-CB	5.71	122.06	112.47
1	D	229	ILE	N-CA-C	-5.70	104.51	109.19
1	A	108	PHE	CA-C-N	5.70	127.85	120.56
1	A	108	PHE	C-N-CA	5.70	127.85	120.56
1	A	411	ARG	NE-CZ-NH2	5.69	124.32	119.20
1	A	419	GLN	OE1-CD-NE2	5.69	128.29	122.60
1	B	388	GLN	OE1-CD-NE2	-5.69	116.91	122.60
1	C	377	ARG	NH1-CZ-NH2	5.68	126.69	119.30
1	A	135	HIS	CA-CB-CG	5.68	119.48	113.80
1	A	488	ARG	CD-NE-CZ	-5.68	116.45	124.40
1	C	196	PHE	CA-CB-CG	5.68	119.48	113.80
1	D	459	ASN	OD1-CG-ND2	-5.66	116.94	122.60
1	C	51	ALA	N-CA-CB	-5.66	104.17	111.35
1	C	331	PHE	CA-CB-CG	5.66	119.46	113.80
1	D	467	ASP	CA-CB-CG	-5.65	106.95	112.60
1	A	48	GLN	CA-CB-CG	5.64	125.39	114.10
1	C	712	ASP	CA-CB-CG	5.64	118.25	112.60
1	A	536	ARG	CA-C-O	5.64	122.96	119.29
1	B	374	VAL	CA-C-O	-5.64	114.38	120.36
1	B	445	ARG	NH1-CZ-NH2	-5.64	111.97	119.30
1	C	711	ALA	CA-C-N	5.64	127.83	120.28
1	C	711	ALA	C-N-CA	5.64	127.83	120.28
1	B	71	VAL	CA-C-O	-5.63	113.43	119.35
1	D	338	PHE	CA-CB-CG	5.62	119.42	113.80
1	B	608	ASN	CA-CB-CG	5.62	118.22	112.60
1	D	495	ARG	NE-CZ-NH1	5.62	127.12	121.50
1	D	228	ALA	CA-C-N	5.62	129.60	121.68
1	D	228	ALA	C-N-CA	5.62	129.60	121.68
1	B	288	PHE	CA-CB-CG	5.62	119.42	113.80
1	D	497	ARG	NE-CZ-NH1	5.61	127.11	121.50
1	B	472	GLU	O-C-N	5.60	129.30	122.75
1	C	463	ASN	OD1-CG-ND2	-5.60	117.00	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	419	GLN	CA-CB-CG	-5.59	102.91	114.10
1	D	572	ASN	CA-CB-CG	-5.59	107.01	112.60
1	A	596	GLY	N-CA-C	5.58	119.68	110.97
1	D	27	ASP	CA-CB-CG	-5.58	107.02	112.60
1	B	417	ASP	N-CA-CB	-5.58	101.92	110.01
1	C	711	ALA	CA-C-O	5.58	128.01	121.87
1	B	176	ALA	N-CA-C	5.57	118.73	110.48
1	B	127	VAL	CA-C-O	-5.57	115.82	121.67
1	C	181	ASP	CA-CB-CG	5.56	118.16	112.60
1	C	685	LEU	CA-C-O	-5.54	114.54	120.42
1	B	725	ASP	CB-CA-C	-5.54	99.40	110.42
1	C	330	ASP	CA-CB-CG	5.53	118.13	112.60
1	D	316	ASP	CA-CB-CG	-5.53	107.07	112.60
1	D	740	ARG	NE-CZ-NH1	5.53	127.03	121.50
1	C	355	ASP	CA-C-O	5.53	124.00	119.36
1	C	426	PRO	CA-C-N	-5.52	114.95	123.17
1	C	426	PRO	C-N-CA	-5.52	114.95	123.17
1	C	376	ASN	CB-CG-ND2	5.51	124.67	116.40
1	A	157	ASN	CA-CB-CG	-5.51	107.09	112.60
1	A	649	PRO	N-CA-CB	5.50	108.42	103.19
1	C	653	THR	N-CA-CB	5.50	118.98	110.46
1	B	61	ARG	NE-CZ-NH2	-5.49	114.26	119.20
1	C	490	GLU	CB-CG-CD	5.49	121.94	112.60
1	D	320	ARG	CD-NE-CZ	5.49	132.09	124.40
1	B	414	SER	O-C-N	-5.49	115.89	122.15
1	D	421	SER	N-CA-CB	5.47	118.25	110.16
1	A	358	LYS	CA-C-O	-5.45	114.82	120.70
1	C	730	ASP	CA-CB-CG	-5.43	107.17	112.60
1	A	185	PHE	CA-CB-CG	5.43	119.23	113.80
1	B	237	ASP	N-CA-C	5.43	117.90	111.33
1	D	401	ASP	CA-CB-CG	5.43	118.03	112.60
1	A	381	ASN	CA-CB-CG	-5.42	107.18	112.60
1	A	77	ASN	CA-CB-CG	-5.42	107.18	112.60
1	C	167	SER	N-CA-CB	-5.42	103.12	111.46
1	C	568	ASP	N-CA-CB	5.42	118.18	110.16
1	B	749	ASP	N-CA-CB	-5.42	101.94	110.06
1	A	713	GLN	CB-CA-C	5.41	120.12	109.72
1	C	207	PHE	O-C-N	-5.41	115.99	122.15
1	D	440	TYR	N-CA-CB	5.41	119.58	110.77
1	B	405	ASP	CA-CB-CG	5.40	118.00	112.60
1	D	167	SER	N-CA-CB	-5.40	103.03	111.56
1	D	536	ARG	O-C-N	-5.39	115.12	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	446	ASP	CB-CA-C	-5.39	108.80	116.34
1	A	712	ASP	N-CA-C	-5.38	105.49	111.36
1	A	498	SER	CA-C-O	5.38	125.18	119.80
1	A	27	ASP	CA-C-N	-5.37	113.50	122.64
1	A	27	ASP	C-N-CA	-5.37	113.50	122.64
1	D	72	ARG	CA-C-O	-5.37	114.64	120.81
1	C	203	THR	O-C-N	-5.36	117.19	121.80
1	D	314	ASP	CA-CB-CG	-5.36	107.24	112.60
1	A	41	GLU	CA-CB-CG	5.36	124.81	114.10
1	D	740	ARG	NE-CZ-NH2	-5.36	114.38	119.20
1	B	428	PHE	CA-CB-CG	-5.35	108.45	113.80
1	A	224	GLU	CB-CA-C	5.34	117.87	109.27
1	C	377	ARG	CA-CB-CG	-5.34	103.41	114.10
1	C	615	ASP	CA-CB-CG	5.33	117.93	112.60
1	A	442	ASN	OD1-CG-ND2	5.32	127.92	122.60
1	C	185	PHE	CA-C-O	5.32	126.86	120.27
1	A	317	PHE	N-CA-C	5.31	117.49	111.11
1	A	59	ASP	CA-CB-CG	5.31	117.91	112.60
1	B	62	ASN	CA-C-O	-5.31	115.55	121.23
1	A	41	GLU	CB-CA-C	-5.31	102.70	109.92
1	A	81	THR	O-C-N	5.30	129.65	122.96
1	A	380	ASP	CA-CB-CG	-5.30	107.30	112.60
1	C	595	ASP	CA-CB-CG	5.30	117.91	112.60
1	A	431	ILE	CA-C-N	5.30	124.75	119.24
1	A	431	ILE	C-N-CA	5.30	124.75	119.24
1	A	479	ARG	CA-CB-CG	5.30	124.70	114.10
1	A	69	GLU	CB-CG-CD	5.29	121.60	112.60
1	A	471	ARG	N-CA-C	5.29	118.37	109.95
1	D	225	PRO	CA-C-N	-5.29	112.78	120.29
1	D	225	PRO	C-N-CA	-5.29	112.78	120.29
1	B	61	ARG	NE-CZ-NH1	5.28	126.78	121.50
1	D	206	PHE	CA-CB-CG	-5.26	108.54	113.80
1	D	466	ASN	CB-CG-ND2	5.26	124.30	116.40
1	D	546	GLN	OE1-CD-NE2	-5.26	117.34	122.60
1	B	123	PRO	CA-C-O	-5.26	115.60	121.23
1	A	216	ASP	CA-CB-CG	-5.25	107.34	112.60
1	B	217	PHE	CA-CB-CG	-5.25	108.55	113.80
1	A	411	ARG	CD-NE-CZ	-5.25	117.06	124.40
1	A	435	ARG	NE-CZ-NH1	-5.25	116.25	121.50
1	D	689	TYR	O-C-N	-5.24	116.67	122.07
1	C	515	GLN	CA-C-O	-5.24	115.44	121.47
1	D	417	ASP	CA-C-O	5.23	126.31	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	265	SER	N-CA-CB	-5.23	103.61	111.56
1	C	304	TRP	N-CA-C	5.23	117.38	111.11
1	A	640	VAL	CA-C-O	-5.23	115.22	121.28
1	B	309	LYS	CB-CG-CD	5.22	123.31	111.30
1	D	730	ASP	CA-CB-CG	-5.21	107.39	112.60
1	C	140	PRO	CA-C-O	-5.21	115.50	121.86
1	A	414	SER	N-CA-CB	-5.21	102.45	110.16
1	D	377	ARG	CA-CB-CG	-5.20	103.70	114.10
1	C	392	HIS	CA-CB-CG	5.20	119.00	113.80
1	D	689	TYR	CA-C-O	5.20	126.27	120.82
1	A	419	GLN	CA-CB-CG	-5.19	103.71	114.10
1	A	490	GLU	CB-CG-CD	5.19	121.42	112.60
1	B	437	THR	N-CA-C	-5.19	107.12	113.50
1	B	709	LYS	N-CA-C	5.19	118.75	111.90
1	C	722	ASP	CA-CB-CG	-5.18	107.42	112.60
1	A	66	ASN	CA-CB-CG	-5.18	107.42	112.60
1	C	471	ARG	NE-CZ-NH1	-5.17	116.33	121.50
1	A	161	PRO	CA-C-N	-5.17	115.35	122.69
1	A	161	PRO	C-N-CA	-5.17	115.35	122.69
1	C	29	LEU	N-CA-C	5.16	118.36	111.75
1	B	712	ASP	CA-CB-CG	-5.16	107.44	112.60
1	B	665	VAL	CB-CA-C	-5.16	103.46	110.42
1	A	424	GLY	N-CA-C	5.14	122.19	115.36
1	A	710	ILE	CA-C-O	5.13	127.81	121.75
1	B	654	PHE	CA-CB-CG	5.13	118.93	113.80
1	B	704	PHE	CA-CB-CG	-5.13	108.67	113.80
1	A	479	ARG	CG-CD-NE	-5.13	100.72	112.00
1	A	744	ARG	NE-CZ-NH1	-5.12	116.38	121.50
1	C	597	ASP	CA-CB-CG	5.12	117.72	112.60
1	C	227	TRP	CA-CB-CG	5.12	123.32	113.60
1	D	498	SER	O-C-N	-5.11	116.03	121.30
1	D	276	THR	O-C-N	-5.11	116.73	123.02
1	A	710	ILE	O-C-N	-5.11	117.50	122.97
1	A	417	ASP	N-CA-CB	-5.11	102.61	110.01
1	D	29	LEU	CB-CA-C	5.11	121.09	110.32
1	D	161	PRO	CA-C-O	-5.10	115.64	121.56
1	A	241	ASP	CA-C-O	5.10	126.18	120.82
1	C	443	PHE	CA-C-O	-5.10	113.59	119.56
1	C	440	TYR	N-CA-CB	5.10	119.08	110.77
1	A	166	PHE	CA-C-O	-5.09	115.27	121.28
1	A	740	ARG	NE-CZ-NH2	-5.09	114.62	119.20
1	D	674	ASP	CA-CB-CG	5.09	117.69	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	469	TRP	CA-C-O	-5.09	116.02	120.60
1	A	434	ASN	CA-CB-CG	-5.08	107.52	112.60
1	A	440	TYR	N-CA-CB	5.08	119.05	110.77
1	B	440	TYR	N-CA-CB	5.07	119.04	110.77
1	A	120	GLU	N-CA-C	5.07	117.70	111.82
1	C	303	VAL	CA-C-O	-5.07	114.96	121.40
1	A	52	PRO	CB-CA-C	-5.07	105.13	111.56
1	C	139	GLN	CA-CB-CG	5.06	124.23	114.10
1	D	181	ASP	O-C-N	-5.06	118.50	123.26
1	A	321	GLU	N-CA-CB	-5.06	102.69	110.12
1	D	458	ALA	CB-CA-C	-5.06	100.95	109.50
1	B	494	VAL	CB-CA-C	-5.05	101.68	110.71
1	A	62	ASN	OD1-CG-ND2	5.04	127.64	122.60
1	A	379	PRO	O-C-N	5.04	129.10	122.86
1	B	110	LEU	N-CA-CB	-5.04	102.72	110.12
1	C	276	THR	CA-CB-OG1	-5.03	102.05	109.60
1	B	658	PRO	CB-CA-C	5.03	117.61	111.12
1	A	167	SER	N-CA-CB	-5.03	103.62	111.56
1	B	338	PHE	CA-C-O	-5.02	114.94	120.36
1	C	488	ARG	CA-CB-CG	5.01	124.12	114.10
1	A	578	ASP	CA-CB-CG	5.01	117.61	112.60
1	D	633	LEU	N-CA-C	5.00	118.23	110.17

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	28	SER	CA
1	A	29	LEU	CA
1	C	725	ASP	CA

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	27	ASP	Mainchain,Peptide
1	A	394	GLY	Mainchain
1	A	710	ILE	Mainchain
1	C	394	GLY	Mainchain
1	C	725	ASP	Mainchain
1	D	273	GLY	Mainchain
1	D	423	LEU	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5748	0	5580	67	5
1	B	5748	0	5580	95	1
1	C	5748	0	5580	68	0
1	D	5748	0	5580	67	0
2	A	43	0	30	3	0
2	B	43	0	30	4	0
2	C	43	0	30	3	0
2	D	43	0	30	4	0
3	A	727	0	0	10	0
3	B	616	0	0	17	5
3	C	638	0	0	6	1
3	D	705	0	0	10	0
All	All	25850	0	22440	263	6

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 6.

All (263) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126[B]:ILE:HD12	2:B:754:HEM:HMD1	1.43	0.99
1:C:126[B]:ILE:HD12	2:C:754:HEM:HMD1	1.48	0.96
1:D:39:ALA:H	1:D:48:GLN:HE21	1.16	0.93
1:A:451:MET:HE2	1:C:451:MET:HE2	1.50	0.92
1:B:451:MET:HE2	1:D:451:MET:HE2	1.58	0.85
1:B:710:ILE:HD13	1:B:718:ILE:HG13	1.59	0.84
1:A:28:SER:O	1:A:29:LEU:HG	1.77	0.84
1:D:39:ALA:H	1:D:48:GLN:NE2	1.77	0.81
1:B:583:LYS:HE2	1:B:583:LYS:H	1.45	0.81
1:C:27:ASP:O	1:C:28:SER:HB2	1.80	0.81
1:D:267:ARG:HG3	3:D:1243:HOH:O	1.83	0.79
1:B:309:LYS:HG3	3:B:1353:HOH:O	1.83	0.78
1:C:310:LEU:HD13	1:C:660:LEU:HB3	1.65	0.77
1:A:126[A]:ILE:HD12	1:D:117:PHE:CZ	2.20	0.76
1:B:126[A]:ILE:HD13	1:C:121:ARG:NH2	2.00	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:ARG:HH12	1:C:600:GLY:HA3	1.51	0.75
1:C:527:PHE:O	1:C:531:LEU:HD13	1.87	0.74
1:B:267:ARG:HG3	3:B:1361:HOH:O	1.87	0.74
1:B:310:LEU:HD13	1:B:660:LEU:HB3	1.70	0.74
1:B:603:VAL:HG22	1:B:664:ALA:HB3	1.69	0.74
1:D:386:ASN:C	1:D:386:ASN:HD22	1.95	0.73
1:A:479:ARG:NH1	1:A:479:ARG:HG2	2.05	0.71
1:A:488:ARG:HH11	1:B:492:ASN:ND2	1.88	0.71
1:A:29:LEU:HD23	1:A:30:ALA:O	1.91	0.71
1:A:51:ALA:HB1	1:A:52:PRO:HD2	1.71	0.70
1:B:386:ASN:C	1:B:386:ASN:HD22	1.98	0.70
1:C:267:ARG:HD2	3:C:998:HOH:O	1.89	0.70
1:A:611:VAL:HG23	3:A:1053:HOH:O	1.92	0.69
1:D:725:ASP:O	3:D:1208:HOH:O	2.11	0.69
1:A:726:GLY:HA3	3:A:1399:HOH:O	1.94	0.68
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.76	0.68
1:B:449:HIS:ND1	3:B:1357:HOH:O	2.26	0.67
1:B:309:LYS:HG2	1:B:660:LEU:HD11	1.76	0.66
1:C:386:ASN:HD22	1:C:386:ASN:C	2.04	0.66
1:C:309:LYS:HE2	3:C:1387:HOH:O	1.97	0.65
1:A:245:LEU:HD22	1:D:29:LEU:HD13	1.79	0.65
1:D:448:MET:HG2	3:D:1457:HOH:O	1.97	0.65
1:B:448:MET:HE3	3:B:1358:HOH:O	1.96	0.64
1:B:37:ARG:HD2	3:B:1367:HOH:O	1.99	0.63
1:C:552:LEU:HD22	1:C:556:GLN:HG3	1.80	0.63
1:D:126[A]:ILE:HG22	2:D:754:HEM:HMD1	1.81	0.62
1:C:607:LEU:HD22	1:C:611:VAL:HG21	1.82	0.62
1:A:488:ARG:HH11	1:B:492:ASN:HD21	1.46	0.62
1:B:583:LYS:H	1:B:583:LYS:CE	2.13	0.62
1:B:710:ILE:HG23	1:B:715:GLU:HG2	1.82	0.61
1:B:449:HIS:NE2	3:B:1356:HOH:O	2.31	0.61
1:D:126[A]:ILE:CG2	2:D:754:HEM:HMD1	2.31	0.61
1:B:344:GLU:CD	1:B:344:GLU:H	2.08	0.61
1:A:386:ASN:C	1:A:386:ASN:HD22	2.09	0.61
1:D:375:LEU:N	1:D:375:LEU:HD12	2.15	0.60
1:B:29:LEU:HD13	1:C:245:LEU:HD22	1.82	0.60
1:A:126[B]:ILE:HD11	3:D:1453:HOH:O	2.01	0.60
1:C:704:PHE:O	1:C:707:THR:HG22	2.02	0.60
1:B:126[B]:ILE:CD1	2:B:754:HEM:HMD1	2.26	0.59
1:C:578:ASP:HB2	1:C:582:LEU:O	2.01	0.59
1:B:583:LYS:O	1:B:584:LYS:HB3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:754:HEM:HBC2	2:D:754:HEM:HMC2	1.85	0.58
1:A:461:GLU:HA	1:A:462:PRO:C	2.28	0.58
1:A:278:ARG:HH22	1:A:487:GLU:CD	2.12	0.57
1:A:317:PHE:O	1:A:321:GLU:HB2	2.04	0.57
1:A:121:ARG:HG2	1:D:126[B]:ILE:HD13	1.87	0.57
1:A:488:ARG:NH1	1:B:492:ASN:ND2	2.53	0.57
1:B:75:SER:HA	3:B:1368:HOH:O	2.04	0.56
1:A:488:ARG:NH1	1:B:492:ASN:HD21	2.04	0.56
1:D:726:GLY:O	1:D:730:ASP:OD1	2.24	0.56
1:A:28:SER:CB	3:A:1359:HOH:O	2.54	0.56
1:A:182:ILE:HD12	1:A:207:PHE:CE2	2.40	0.56
1:A:27:ASP:HB3	1:A:28:SER:OG	2.07	0.55
1:A:73:LYS:HE2	3:C:951:HOH:O	2.05	0.55
1:B:126[B]:ILE:CD1	1:C:118:ASP:HA	2.37	0.55
2:C:754:HEM:HBC2	2:C:754:HEM:HMC2	1.87	0.55
1:C:725:ASP:O	1:C:726:GLY:C	2.49	0.54
1:D:420:ILE:HD12	1:D:426:PRO:HA	1.89	0.54
1:B:126[B]:ILE:HD11	1:B:418:THR:OG1	2.08	0.54
1:B:330:ASP:OD2	1:B:629:HIS:HE1	1.91	0.54
1:D:39:ALA:N	1:D:48:GLN:HE21	1.96	0.54
1:B:449:HIS:CE1	3:B:1356:HOH:O	2.61	0.53
1:C:359:LEU:H	1:C:507:HIS:HD2	1.56	0.53
3:A:1474:HOH:O	1:D:126[B]:ILE:HD11	2.08	0.53
1:B:443:PHE:CZ	1:B:470:PRO:HD2	2.44	0.53
1:B:646:THR:HA	3:B:1145:HOH:O	2.08	0.53
1:D:443:PHE:CZ	1:D:470:PRO:HD2	2.44	0.53
1:A:552:LEU:HD21	1:A:571:LEU:O	2.10	0.52
1:A:583:LYS:O	1:A:584:LYS:HB3	2.08	0.52
1:C:165:ARG:HE	1:C:386:ASN:HD21	1.57	0.52
1:D:578:ASP:HB3	1:D:582:LEU:O	2.09	0.52
1:A:443:PHE:CZ	1:A:470:PRO:HD2	2.44	0.52
1:D:416:THR:HG23	3:D:1355:HOH:O	2.08	0.52
1:C:583:LYS:O	1:C:584:LYS:HB3	2.09	0.52
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.25	0.52
1:B:165:ARG:HE	1:B:386:ASN:HD21	1.57	0.52
1:A:707:THR:HG23	3:A:1402:HOH:O	2.09	0.52
1:B:155:ASP:HB3	1:B:158:LYS:HG3	1.92	0.52
1:B:38:PRO:HA	1:B:48:GLN:OE1	2.10	0.52
1:B:126[B]:ILE:HD13	1:C:118:ASP:HA	1.90	0.52
1:B:562:LEU:HA	1:C:637:MET:HB2	1.91	0.52
1:B:624:LYS:HB2	3:B:1060:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126[B]:ILE:HD12	2:B:754:HEM:CMD	2.30	0.51
1:D:144:LEU:HD11	1:D:370:VAL:HG13	1.93	0.51
1:B:438:CYS:HB2	1:B:439:PRO:HD2	1.92	0.51
1:A:28:SER:HB2	3:A:1359:HOH:O	2.08	0.51
1:D:700:ASP:O	1:D:703:LYS:HG3	2.10	0.51
1:D:359:LEU:H	1:D:507:HIS:HD2	1.58	0.51
1:A:682:ASN:HB3	1:A:707:THR:HG21	1.91	0.51
3:B:1357:HOH:O	1:D:449:HIS:CE1	2.63	0.51
1:C:416:THR:HA	3:C:1381:HOH:O	2.11	0.51
1:D:634:TYR:O	1:D:653:THR:HA	2.11	0.51
1:D:689:TYR:CE1	1:D:710:ILE:HD11	2.46	0.51
1:A:165:ARG:HE	1:A:386:ASN:HD21	1.58	0.51
1:B:637:MET:HB2	1:C:562:LEU:HA	1.93	0.51
1:C:126[B]:ILE:HD11	1:C:418:THR:OG1	2.11	0.51
1:D:725:ASP:O	1:D:726:GLY:C	2.54	0.50
1:B:118:ASP:HA	1:C:126[B]:ILE:CD1	2.42	0.50
1:A:70:ASP:OD2	3:A:1479:HOH:O	2.19	0.50
1:B:682:ASN:OD1	1:B:707:THR:HG21	2.12	0.50
1:D:165:ARG:HE	1:D:386:ASN:HD21	1.59	0.49
1:B:274:ILE:HD12	2:B:754:HEM:HMB1	1.94	0.49
1:A:120:GLU:HB2	1:D:126[A]:ILE:CD1	2.41	0.49
1:D:363:GLU:HB2	1:D:582:LEU:HD21	1.94	0.49
1:B:521:ARG:HE	1:B:745:ILE:HG21	1.78	0.49
3:B:924:HOH:O	1:D:52:PRO:HG3	2.11	0.49
1:C:732:LEU:HD13	1:C:732:LEU:C	2.37	0.49
1:A:28:SER:O	1:A:29:LEU:CG	2.55	0.49
1:A:36:HIS:CD2	1:A:36:HIS:H	2.31	0.49
1:B:413:PHE:HB2	1:D:105:LEU:HD11	1.94	0.48
1:C:359:LEU:C	1:C:359:LEU:HD12	2.39	0.48
1:D:750:LYS:HG3	1:D:750:LYS:O	2.14	0.48
1:A:411:ARG:HG2	2:A:754:HEM:C2C	2.49	0.48
1:A:745:ILE:O	1:A:748:ILE:HG12	2.14	0.48
1:B:308:GLN:OE1	1:C:313:ARG:NH1	2.43	0.48
1:B:416:THR:HA	3:B:1370:HOH:O	2.13	0.48
1:B:267:ARG:HD2	3:B:976:HOH:O	2.13	0.48
1:D:41:GLU:CD	1:D:42:PRO:HD2	2.38	0.48
1:B:583:LYS:H	1:B:583:LYS:CD	2.26	0.48
1:C:729:MET:O	1:C:733:LEU:HD13	2.14	0.48
1:D:404:ASN:O	1:D:405:ASP:C	2.56	0.48
1:A:479:ARG:HG2	1:A:479:ARG:HH11	1.79	0.47
1:B:27:ASP:O	1:B:28:SER:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:461:GLU:HA	1:D:462:PRO:C	2.38	0.47
1:D:330:ASP:OD2	1:D:629:HIS:HE1	1.97	0.47
1:D:448:MET:HE3	3:D:1457:HOH:O	2.13	0.47
1:B:710:ILE:CD1	1:B:718:ILE:HG13	2.36	0.47
1:B:29:LEU:HD13	1:C:245:LEU:HD13	1.96	0.47
1:B:126[A]:ILE:HD13	1:C:121:ARG:CZ	2.44	0.47
1:B:634:TYR:O	1:B:653:THR:HA	2.15	0.47
1:B:293:TRP:CZ3	1:B:336:LEU:HB2	2.50	0.47
1:C:211:ALA:CB	1:C:410:GLY:HA3	2.45	0.47
1:C:745:ILE:O	1:C:748:ILE:HG12	2.15	0.47
1:B:364:LEU:HD11	1:B:580:ASN:HB2	1.97	0.46
1:B:50:THR:HG21	1:C:227:TRP:CZ3	2.50	0.46
1:B:395:HIS:HE1	3:D:1445:HOH:O	1.97	0.46
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.30	0.46
1:A:51:ALA:HB1	1:A:52:PRO:CD	2.44	0.46
1:C:330:ASP:OD2	1:C:629:HIS:HE1	1.99	0.46
1:C:364:LEU:HD11	1:C:580:ASN:HB2	1.97	0.46
1:C:727:SER:O	1:C:731:GLU:HG3	2.15	0.46
1:D:251:HIS:CE1	1:D:507:HIS:HB3	2.51	0.46
1:B:535:VAL:O	1:B:537:PRO:HD3	2.15	0.46
1:B:36:HIS:CD2	1:B:37:ARG:HE	2.34	0.46
1:B:359:LEU:H	1:B:507:HIS:HD2	1.63	0.46
1:A:126[A]:ILE:HG22	2:A:754:HEM:HMD1	1.97	0.45
1:B:732:LEU:C	1:B:732:LEU:HD13	2.40	0.45
1:D:629:HIS:HD2	3:D:1068:HOH:O	1.99	0.45
1:A:335:GLU:OE1	1:A:369:ARG:HG3	2.17	0.45
1:B:165:ARG:HE	1:B:386:ASN:ND2	2.14	0.45
1:B:420:ILE:HG21	1:D:119:HIS:CE1	2.51	0.45
1:D:338:PHE:HB3	1:D:340:LEU:HD13	1.98	0.45
1:B:448:MET:HG2	3:B:1358:HOH:O	2.17	0.45
1:B:521:ARG:NE	1:B:745:ILE:HG21	2.32	0.45
1:B:682:ASN:CG	1:B:707:THR:HG21	2.41	0.45
1:C:321:GLU:HG2	3:C:1201:HOH:O	2.17	0.45
1:D:747:LYS:NZ	3:D:1349:HOH:O	2.47	0.45
1:B:197:ASP:OD2	1:B:395:HIS:HD2	2.00	0.44
1:B:252:ASN:HD22	1:B:252:ASN:HA	1.61	0.44
1:A:477:PRO:HB2	1:A:478:LYS:HD2	1.99	0.44
1:C:344:GLU:O	1:C:348:LYS:NZ	2.50	0.44
1:A:404:ASN:O	1:A:405:ASP:C	2.60	0.44
1:D:583:LYS:O	1:D:584:LYS:HB3	2.17	0.44
1:D:703:LYS:HD2	3:D:1409:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ASP:HA	1:C:126[B]:ILE:HD13	1.99	0.44
1:A:725:ASP:OD1	1:A:725:ASP:C	2.60	0.44
1:D:274:ILE:HD12	2:D:754:HEM:HMB1	1.99	0.44
1:B:369:ARG:HG2	3:B:1110:HOH:O	2.18	0.44
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.33	0.44
1:A:634:TYR:HB3	1:A:650:ILE:HD13	2.00	0.44
1:A:120:GLU:HB2	1:D:126[A]:ILE:HD11	2.00	0.43
1:B:426:PRO:HB2	1:D:116:HIS:CD2	2.53	0.43
1:C:274:ILE:HD12	2:C:754:HEM:HMB1	2.00	0.43
1:A:341:ILE:HD12	1:A:353:LEU:HD21	2.00	0.43
1:B:615:ASP:O	1:B:619:ILE:HG13	2.17	0.43
1:C:443:PHE:CZ	1:C:470:PRO:HD2	2.54	0.43
1:D:252:ASN:HD22	1:D:252:ASN:HA	1.63	0.43
1:C:165:ARG:HE	1:C:386:ASN:ND2	2.16	0.43
1:D:38:PRO:HB3	1:D:49:PRO:HD2	2.00	0.43
1:D:682:ASN:HB3	1:D:707:THR:HG21	2.00	0.43
1:B:725:ASP:O	1:B:726:GLY:C	2.62	0.43
1:A:260:ARG:HD3	1:A:590:LEU:HD21	2.01	0.43
1:C:162:VAL:HG21	1:C:373:MET:SD	2.59	0.43
1:D:222:LYS:HB3	1:D:223:PRO:HD2	2.00	0.43
1:A:37:ARG:NH2	1:C:466:ASN:HA	2.34	0.43
1:B:36:HIS:HD1	1:B:36:HIS:H	1.66	0.43
1:A:76:GLU:O	1:A:77:ASN:HB2	2.19	0.42
1:A:91:ASP:OD2	1:C:461:GLU:OE2	2.36	0.42
1:B:119:HIS:CE1	1:D:420:ILE:HG21	2.54	0.42
1:C:535:VAL:O	1:C:537:PRO:HD3	2.19	0.42
1:B:251:HIS:HA	1:B:508:PRO:HG3	2.02	0.42
1:C:749:ASP:HB3	1:C:750:LYS:NZ	2.34	0.42
1:A:37:ARG:HH21	1:C:466:ASN:HA	1.84	0.42
1:A:165:ARG:HE	1:A:386:ASN:ND2	2.17	0.42
1:B:696:ALA:CB	1:B:719:VAL:HB	2.49	0.42
1:C:293:TRP:CZ3	1:C:336:LEU:HB2	2.54	0.42
1:B:65:LEU:HD21	1:B:135:HIS:CG	2.55	0.42
1:D:583:LYS:HB2	1:D:583:LYS:NZ	2.35	0.42
1:A:207:PHE:O	1:A:249:THR:HA	2.19	0.42
1:D:335:GLU:OE1	1:D:369:ARG:HG2	2.20	0.42
1:B:507:HIS:N	1:B:508:PRO:CD	2.82	0.42
1:C:51:ALA:HB1	1:C:52:PRO:HD2	2.02	0.42
1:C:125:ARG:HB2	1:C:129:ALA:HA	2.02	0.42
1:A:511:PHE:O	1:A:515:GLN:HG2	2.19	0.42
1:D:51:ALA:HB1	1:D:52:PRO:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:LEU:HD11	1:D:546:GLN:HE21	1.85	0.42
1:A:725:ASP:O	1:A:726:GLY:C	2.62	0.41
1:D:375:LEU:N	1:D:375:LEU:CD1	2.82	0.41
1:B:128:HIS:ND1	1:B:169:CYS:HA	2.34	0.41
1:C:689:TYR:CE1	1:C:710:ILE:HD11	2.55	0.41
1:A:610:GLU:OE2	1:A:643:ASP:HA	2.19	0.41
1:B:91:ASP:OD2	1:D:461:GLU:OE2	2.38	0.41
1:C:195:ILE:HD11	1:C:436:PRO:HA	2.02	0.41
1:A:478:LYS:HB3	1:A:478:LYS:HE2	1.79	0.41
1:C:449:HIS:CE1	3:C:1369:HOH:O	2.74	0.41
1:A:104:LEU:HB3	3:A:901:HOH:O	2.20	0.41
1:A:578:ASP:HB3	1:A:582:LEU:O	2.20	0.41
1:B:118:ASP:OD2	1:C:417:ASP:OD2	2.38	0.41
1:B:294:LYS:HG3	3:B:1286:HOH:O	2.20	0.41
1:A:155:ASP:CG	1:A:156:PRO:HD2	2.46	0.41
1:A:158:LYS:HB3	3:A:1097:HOH:O	2.19	0.41
1:A:631:LYS:HD3	3:A:1188:HOH:O	2.20	0.41
1:A:155:ASP:OD1	1:A:156:PRO:HD2	2.21	0.41
1:B:459:ASN:HD22	1:B:459:ASN:H	1.68	0.41
1:C:278:ARG:HH22	1:C:487:GLU:CD	2.29	0.41
1:C:709:LYS:N	1:C:709:LYS:HD2	2.36	0.41
1:D:222:LYS:HB3	1:D:223:PRO:CD	2.51	0.41
1:B:608:ASN:O	1:B:611:VAL:HG23	2.21	0.41
1:B:616:LEU:HD23	1:B:616:LEU:HA	1.93	0.41
1:C:252:ASN:HD22	1:C:252:ASN:HA	1.66	0.41
1:C:583:LYS:O	1:C:584:LYS:CB	2.68	0.41
1:D:65:LEU:HD21	1:D:135:HIS:CG	2.56	0.41
1:C:608:ASN:OD1	1:C:671:ASN:N	2.54	0.41
1:A:460:TYR:CE1	1:B:238:THR:HB	2.56	0.40
1:B:392:HIS:HB3	1:B:395:HIS:CD2	2.56	0.40
1:B:335:GLU:OE1	1:B:369:ARG:HD2	2.21	0.40
1:B:251:HIS:CE1	1:B:507:HIS:HB3	2.56	0.40
1:C:675:ILE:HG13	1:C:704:PHE:HZ	1.86	0.40
1:D:211:ALA:CB	1:D:410:GLY:HA3	2.51	0.40
1:D:574:THR:OG1	1:D:575:PRO:HD2	2.21	0.40
1:D:693:LYS:HA	1:D:694:PRO:HD3	1.97	0.40
1:B:648:LEU:HA	1:B:649:PRO:HD3	1.91	0.40
1:C:498:SER:HA	1:C:499:PRO:HD3	1.98	0.40
1:D:278:ARG:HH22	1:D:487:GLU:CD	2.30	0.40
1:A:126[A]:ILE:CG2	2:A:754:HEM:HMD1	2.51	0.40
1:A:229:ILE:HA	1:A:230:PRO:HA	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:TYR:CD1	1:B:440:TYR:C	2.99	0.40
1:C:461:GLU:HA	1:C:462:PRO:C	2.47	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:479:ARG:NH2	3:B:1105:HOH:O[2_545]	1.88	0.32
1:A:479:ARG:NH2	3:B:1315:HOH:O[2_545]	1.91	0.29
1:A:61:ARG:NH1	3:B:881:HOH:O[2_545]	2.03	0.17
1:A:479:ARG:NH1	3:B:1315:HOH:O[2_545]	2.16	0.04
1:B:146:ASP:OD1	3:C:1114:HOH:O[2_555]	2.17	0.03
1:A:479:ARG:CZ	3:B:1315:HOH:O[2_545]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	726/753 (96%)	706 (97%)	17 (2%)	3 (0%)	30	19
1	B	726/753 (96%)	707 (97%)	16 (2%)	3 (0%)	30	19
1	C	726/753 (96%)	707 (97%)	16 (2%)	3 (0%)	30	19
1	D	726/753 (96%)	707 (97%)	16 (2%)	3 (0%)	30	19
All	All	2904/3012 (96%)	2827 (97%)	65 (2%)	12 (0%)	30	19

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	711	ALA
1	B	28	SER
1	C	28	SER

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Mol	Chain	Res	Type
1	D	28	SER
1	A	726	GLY
1	B	726	GLY
1	C	726	GLY
1	D	726	GLY
1	B	584	LYS
1	A	75	SER
1	C	75	SER
1	D	584	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	613/636 (96%)	589 (96%)	24 (4%)	28	16
1	B	613/636 (96%)	587 (96%)	26 (4%)	26	14
1	C	613/636 (96%)	584 (95%)	29 (5%)	23	11
1	D	613/636 (96%)	585 (95%)	28 (5%)	24	12
All	All	2452/2544 (96%)	2345 (96%)	107 (4%)	26	13

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLU
1	A	73	LYS
1	A	126[A]	ILE
1	A	126[B]	ILE
1	A	185	PHE
1	A	191	THR
1	A	198	LEU
1	A	205	ILE
1	A	252	ASN
1	A	294	LYS
1	A	375	LEU
1	A	386	ASN

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Mol	Chain	Res	Type
1	A	440	TYR
1	A	459	ASN
1	A	478	LYS
1	A	479	ARG
1	A	552	LEU
1	A	565	GLU
1	A	593	ILE
1	A	616	LEU
1	A	631	LYS
1	A	710	ILE
1	A	713	GLN
1	A	750	LYS
1	B	37	ARG
1	B	126[A]	ILE
1	B	126[B]	ILE
1	B	142	LYS
1	B	191	THR
1	B	205	ILE
1	B	213	LYS
1	B	252	ASN
1	B	265	SER
1	B	285	LYS
1	B	370	VAL
1	B	375	LEU
1	B	386	ASN
1	B	440	TYR
1	B	459	ASN
1	B	478	LYS
1	B	552	LEU
1	B	562	LEU
1	B	571	LEU
1	B	583	LYS
1	B	613	SER
1	B	633	LEU
1	B	647	VAL
1	B	708	ILE
1	B	712	ASP
1	B	722	ASP
1	C	27	ASP
1	C	29	LEU
1	C	185	PHE
1	C	195	ILE

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Mol	Chain	Res	Type
1	C	198	LEU
1	C	205	ILE
1	C	213	LYS
1	C	252	ASN
1	C	285	LYS
1	C	321	GLU
1	C	375	LEU
1	C	386	ASN
1	C	432	PRO
1	C	440	TYR
1	C	449	HIS
1	C	459	ASN
1	C	478	LYS
1	C	552	LEU
1	C	568	ASP
1	C	571	LEU
1	C	584	LYS
1	C	606	LEU
1	C	616	LEU
1	C	633	LEU
1	C	635	SER
1	C	647	VAL
1	C	648	LEU
1	C	660	LEU
1	C	733	LEU
1	D	27	ASP
1	D	41	GLU
1	D	61	ARG
1	D	73	LYS
1	D	191	THR
1	D	205	ILE
1	D	213	LYS
1	D	252	ASN
1	D	265	SER
1	D	294	LYS
1	D	340	LEU
1	D	348	LYS
1	D	352	ASP
1	D	386	ASN
1	D	440	TYR
1	D	459	ASN
1	D	478	LYS

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Mol	Chain	Res	Type
1	D	552	LEU
1	D	554	LEU
1	D	569	ASP
1	D	582	LEU
1	D	583	LYS
1	D	593	ILE
1	D	624	LYS
1	D	633	LEU
1	D	648	LEU
1	D	709	LYS
1	D	710	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	128	HIS
1	A	139	GLN
1	A	252	ASN
1	A	386	ASN
1	A	449	HIS
1	A	459	ASN
1	A	556	GLN
1	A	713	GLN
1	B	128	HIS
1	B	157	ASN
1	B	252	ASN
1	B	386	ASN
1	B	395	HIS
1	B	459	ASN
1	B	492	ASN
1	B	507	HIS
1	B	629	HIS
1	C	128	HIS
1	C	252	ASN
1	C	386	ASN
1	C	459	ASN
1	C	486	GLN
1	C	507	HIS
1	C	629	HIS
1	C	671	ASN
1	C	682	ASN

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Mol	Chain	Res	Type
1	D	48	GLN
1	D	77	ASN
1	D	212	HIS
1	D	252	ASN
1	D	386	ASN
1	D	449	HIS
1	D	459	ASN
1	D	507	HIS
1	D	546	GLN
1	D	556	GLN
1	D	629	HIS
1	D	671	ASN
1	D	682	ASN
1	D	713	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	D	754	1	50,50,50	1.54	11 (22%)	67,82,82	1.03	4 (5%)
2	HEM	A	754	1	50,50,50	1.52	13 (26%)	67,82,82	1.37	9 (13%)
2	HEM	C	754	1	50,50,50	1.39	6 (12%)	67,82,82	0.99	5 (7%)
2	HEM	B	754	1	50,50,50	1.55	10 (20%)	67,82,82	1.06	3 (4%)

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

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

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	754	HEM	FE-NA	3.82	2.07	1.95
2	C	754	HEM	FE-ND	3.30	2.05	1.94
2	C	754	HEM	FE-NC	3.25	2.05	1.95
2	A	754	HEM	FE-NA	3.15	2.05	1.95
2	B	754	HEM	FE-NA	3.14	2.05	1.95
2	B	754	HEM	FE-ND	3.13	2.04	1.94
2	B	754	HEM	FE-NB	3.04	2.04	1.94
2	D	754	HEM	CAB-C3B	2.96	1.55	1.47
2	C	754	HEM	FE-NB	2.93	2.03	1.94
2	C	754	HEM	CMA-C3A	2.90	1.56	1.50
2	A	754	HEM	FE-NB	2.88	2.03	1.94
2	D	754	HEM	FE-NB	2.87	2.03	1.94
2	C	754	HEM	CAB-C3B	2.83	1.54	1.47
2	A	754	HEM	CMC-C2C	2.74	1.56	1.50
2	A	754	HEM	CAC-C3C	2.72	1.54	1.47
2	D	754	HEM	CAC-C3C	2.72	1.54	1.47
2	D	754	HEM	CMA-C3A	2.71	1.56	1.50
2	B	754	HEM	CAB-C3B	2.70	1.54	1.47
2	B	754	HEM	FE-NC	2.63	2.03	1.95
2	D	754	HEM	CMC-C2C	2.56	1.56	1.50
2	D	754	HEM	FE-NC	2.56	2.03	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	754	HEM	CMD-C2D	2.55	1.56	1.50
2	B	754	HEM	CMA-C3A	2.52	1.55	1.50
2	A	754	HEM	FE-ND	2.50	2.02	1.94
2	B	754	HEM	CAC-C3C	2.41	1.53	1.47
2	D	754	HEM	FE-ND	2.38	2.02	1.94
2	A	754	HEM	C3C-C2C	-2.35	1.32	1.37
2	A	754	HEM	CBA-CGA	2.31	1.55	1.50
2	B	754	HEM	C2A-C3A	-2.31	1.32	1.38
2	A	754	HEM	CAD-C3D	2.29	1.57	1.51
2	A	754	HEM	CMD-C2D	2.29	1.55	1.50
2	B	754	HEM	C3D-C2D	-2.27	1.31	1.36
2	A	754	HEM	FE-NC	2.24	2.02	1.95
2	D	754	HEM	CAD-C3D	2.19	1.57	1.51
2	C	754	HEM	CAC-C3C	2.11	1.53	1.47
2	A	754	HEM	C3D-C2D	-2.07	1.32	1.36
2	A	754	HEM	CAA-C2A	2.06	1.56	1.51
2	D	754	HEM	C2A-C3A	-2.06	1.33	1.38
2	B	754	HEM	CAA-C2A	2.02	1.56	1.51
2	A	754	HEM	CAB-C3B	2.01	1.52	1.47

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	754	HEM	O1A-CGA-CBA	-4.12	110.02	123.09
2	A	754	HEM	O2A-CGA-O1A	3.79	133.07	123.33
2	A	754	HEM	CAA-CBA-CGA	-2.98	105.77	113.67
2	D	754	HEM	O1A-CGA-CBA	-2.96	113.70	123.09
2	A	754	HEM	CBD-CAD-C3D	-2.88	104.58	112.53
2	B	754	HEM	CAA-CBA-CGA	-2.76	106.34	113.67
2	C	754	HEM	O1A-CGA-CBA	-2.72	114.47	123.09
2	C	754	HEM	O2A-CGA-O1A	2.63	130.10	123.33
2	B	754	HEM	O1A-CGA-CBA	-2.49	115.20	123.09
2	D	754	HEM	CBD-CAD-C3D	-2.48	105.67	112.53
2	C	754	HEM	C3B-C4B-NB	2.36	111.16	109.47
2	A	754	HEM	CHD-C4C-NC	2.32	126.98	124.45
2	C	754	HEM	CAA-CBA-CGA	-2.21	107.81	113.67
2	A	754	HEM	C4C-CHD-C1D	-2.20	121.35	126.02
2	D	754	HEM	CHD-C1D-ND	2.17	126.76	124.42
2	A	754	HEM	O2D-CGD-O1D	-2.12	117.88	123.33
2	A	754	HEM	CHD-C1D-ND	2.12	126.70	124.42
2	B	754	HEM	CHA-C1A-NA	2.08	127.62	123.86
2	C	754	HEM	CAD-C3D-C4D	-2.07	121.08	124.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	754	HEM	O2A-CGA-O1A	2.06	128.62	123.33
2	A	754	HEM	C4D-C3D-C2D	2.00	109.81	106.89

There are no chirality outliers.

All (8) torsion outliers are listed below:

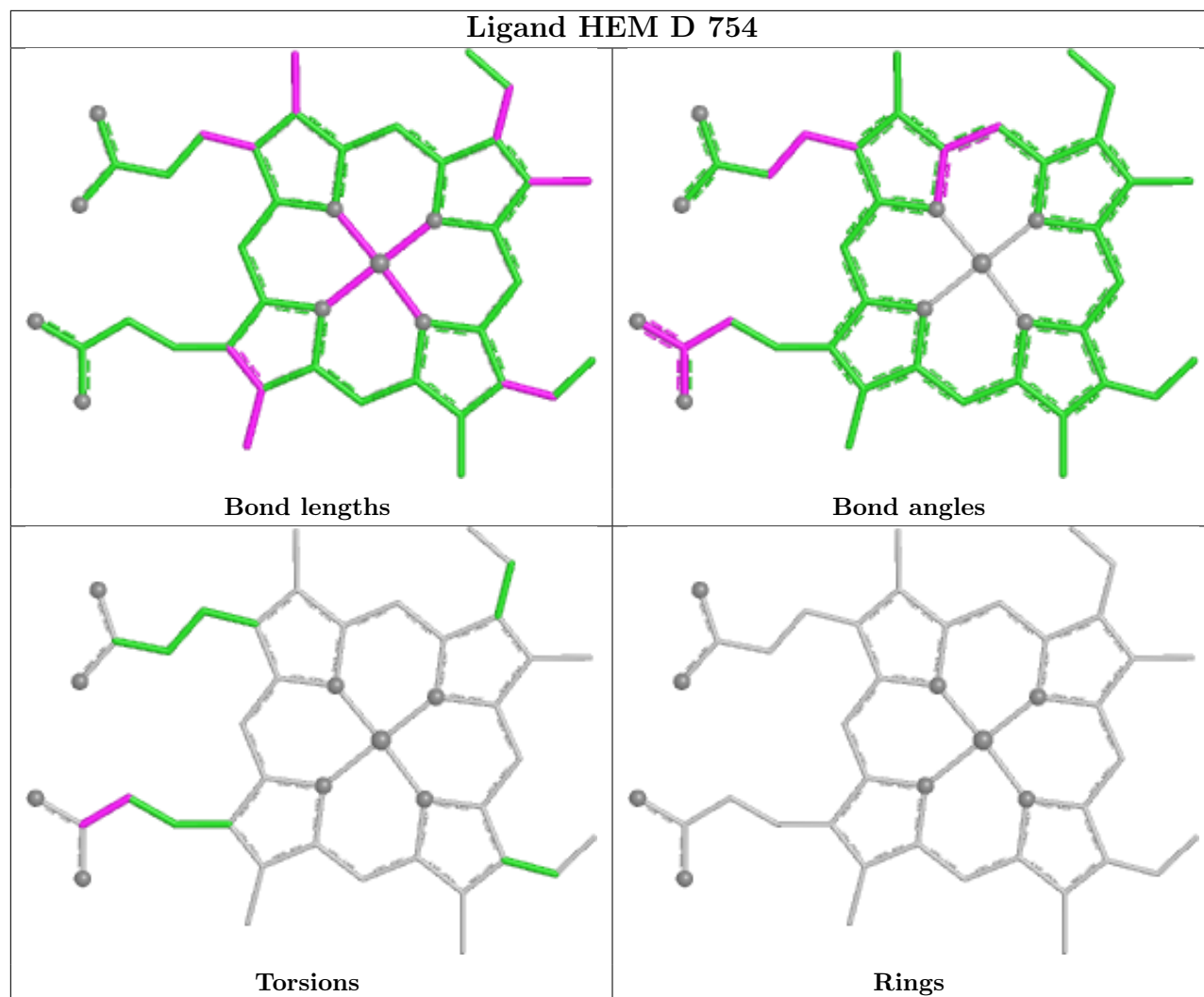
Mol	Chain	Res	Type	Atoms
2	C	754	HEM	CAA-CBA-CGA-O1A
2	B	754	HEM	CAA-CBA-CGA-O1A
2	D	754	HEM	CAA-CBA-CGA-O1A
2	A	754	HEM	CAA-CBA-CGA-O1A
2	A	754	HEM	CAA-CBA-CGA-O2A
2	C	754	HEM	CAA-CBA-CGA-O2A
2	D	754	HEM	CAA-CBA-CGA-O2A
2	B	754	HEM	CAA-CBA-CGA-O2A

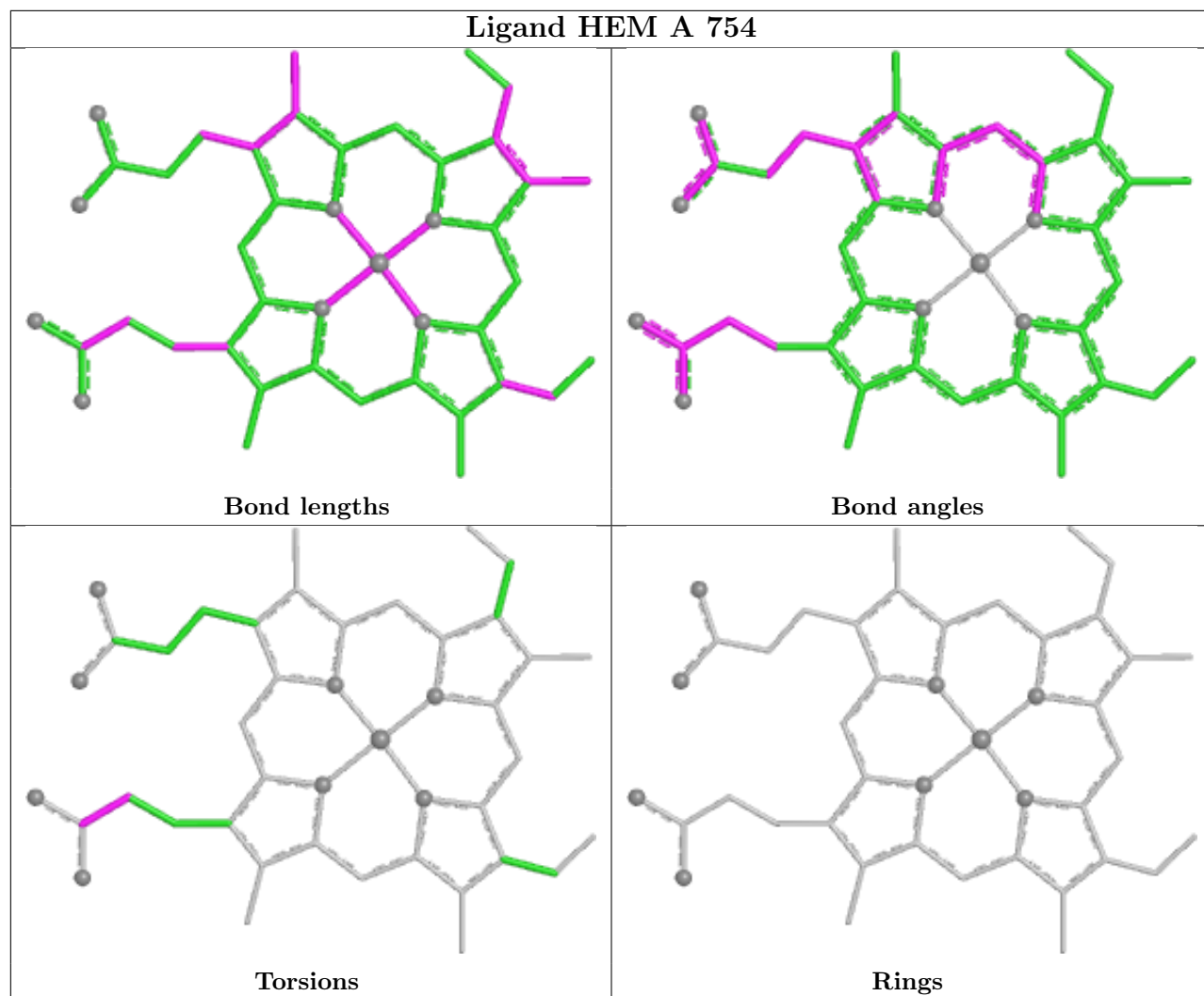
There are no ring outliers.

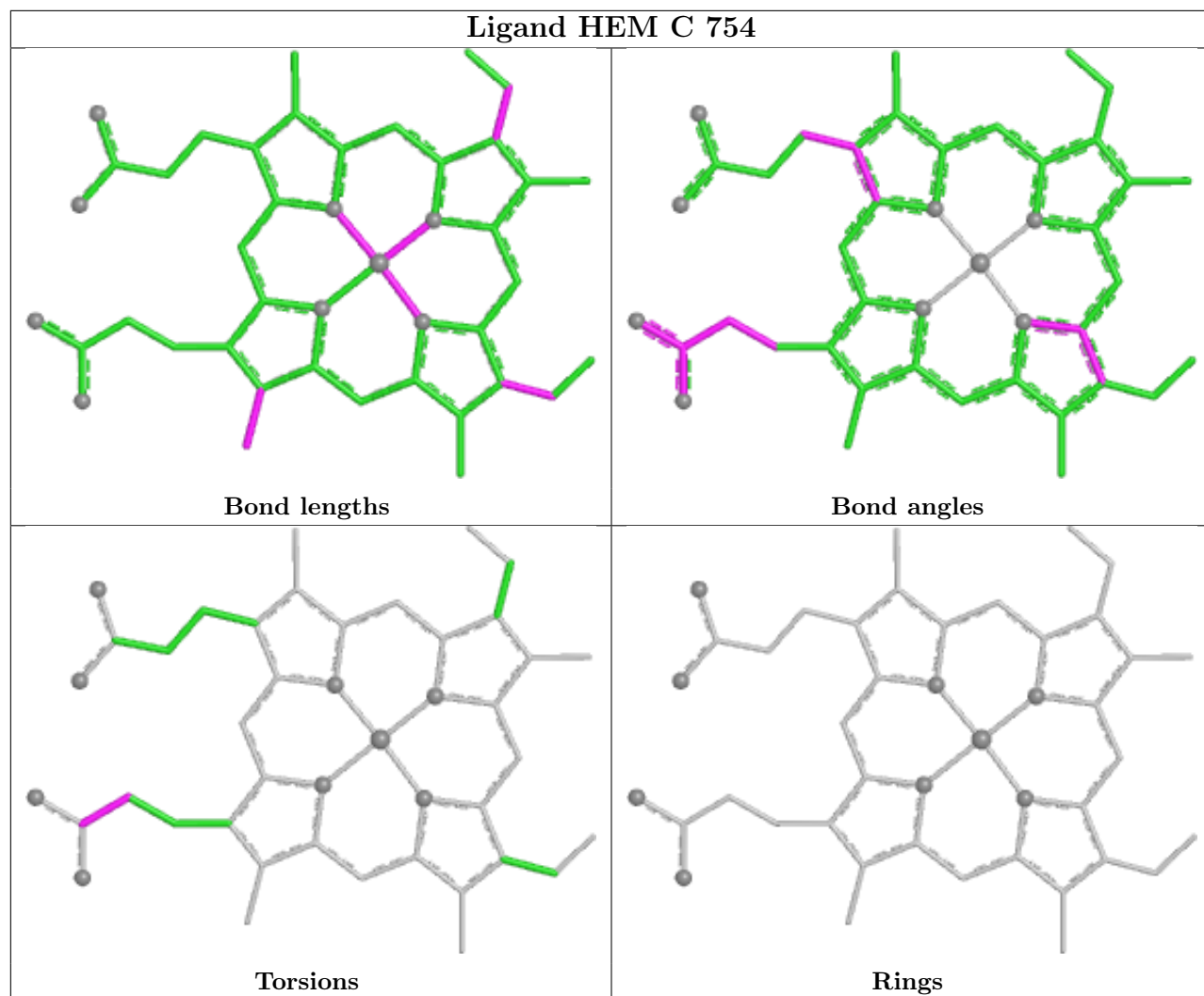
4 monomers are involved in 14 short contacts:

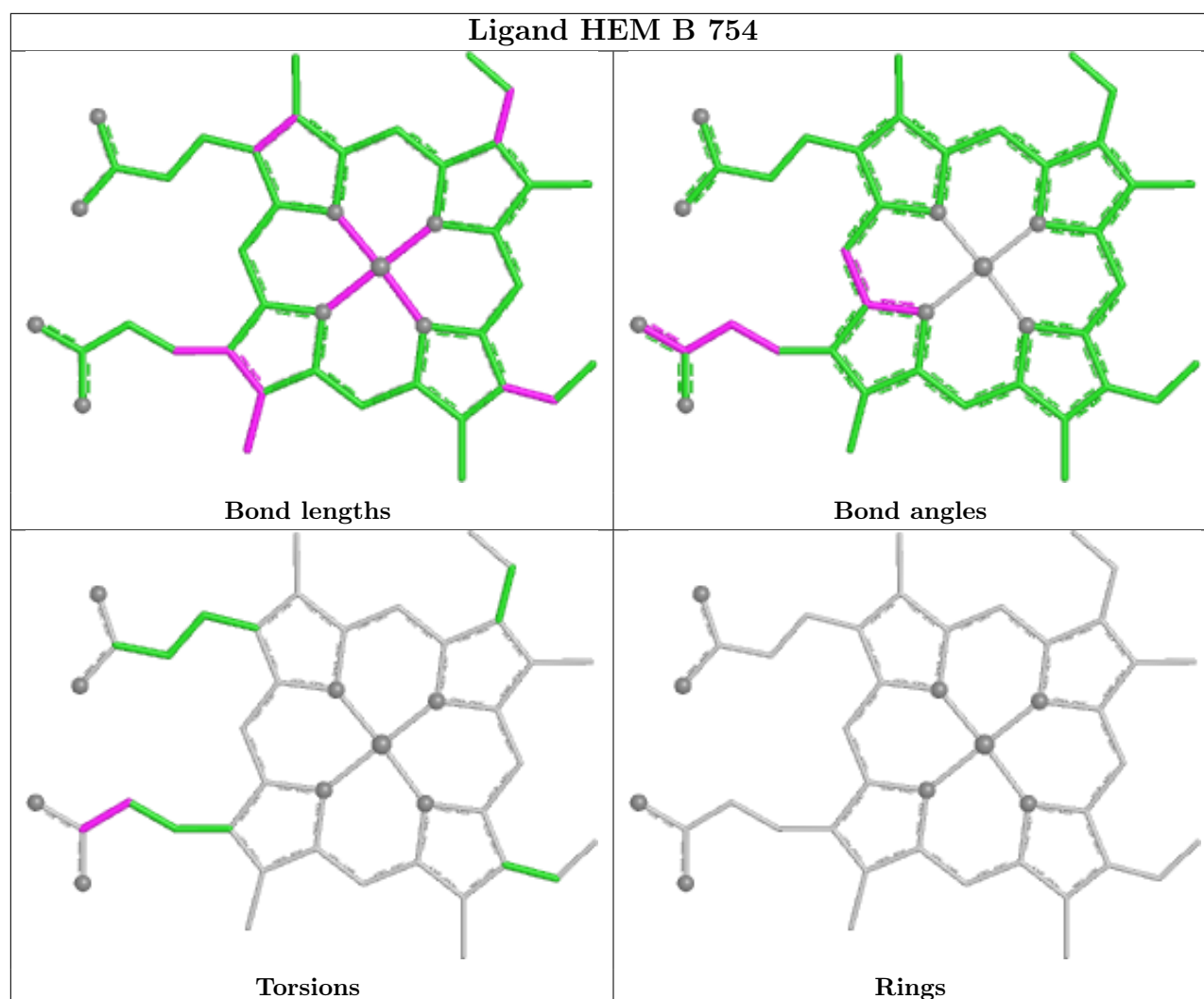
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	754	HEM	4	0
2	A	754	HEM	3	0
2	C	754	HEM	3	0
2	B	754	HEM	4	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	727/753 (96%)	0.14	81 (11%) 10 8	7, 16, 52, 85	1 (0%)
1	B	727/753 (96%)	0.15	64 (8%) 15 13	7, 17, 52, 85	1 (0%)
1	C	727/753 (96%)	0.12	65 (8%) 15 13	7, 17, 52, 85	1 (0%)
1	D	727/753 (96%)	0.10	62 (8%) 16 14	7, 16, 51, 85	1 (0%)
All	All	2908/3012 (96%)	0.13	272 (9%) 14 12	7, 17, 52, 85	4 (0%)

All (272) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	27	ASP	7.4
1	D	726	GLY	7.2
1	A	711	ALA	7.2
1	A	645	GLY	6.8
1	B	29	LEU	6.5
1	D	710	ILE	6.2
1	A	28	SER	6.2
1	C	726	GLY	5.9
1	A	646	THR	5.8
1	A	611	VAL	5.6
1	D	29	LEU	5.6
1	A	642	ALA	5.6
1	A	30	ALA	5.6
1	B	701	ALA	5.6
1	B	614	ALA	5.4
1	B	642	ALA	5.4
1	C	30	ALA	5.3
1	C	725	ASP	5.1
1	D	35	SER	5.1
1	A	29	LEU	5.0
1	A	673	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	712	ASP	4.9
1	C	34	GLY	4.9
1	A	710	ILE	4.8
1	C	701	ALA	4.7
1	A	676	ALA	4.7
1	D	711	ALA	4.7
1	A	699	GLY	4.7
1	A	613	SER	4.6
1	B	608	ASN	4.6
1	D	676	ALA	4.5
1	C	31	PRO	4.5
1	A	35	SER	4.5
1	B	30	ALA	4.5
1	B	710	ILE	4.5
1	C	710	ILE	4.3
1	B	726	GLY	4.3
1	A	726	GLY	4.3
1	B	617	LEU	4.3
1	C	642	ALA	4.3
1	D	34	GLY	4.2
1	C	29	LEU	4.2
1	C	711	ALA	4.2
1	B	611	VAL	4.2
1	D	714	GLY	4.1
1	A	614	ALA	4.1
1	A	749	ASP	4.1
1	A	751	ILE	4.1
1	C	751	ILE	4.1
1	C	676	ALA	4.1
1	A	714	GLY	4.1
1	D	724	ALA	4.0
1	B	641	THR	4.0
1	D	28	SER	4.0
1	C	615	ASP	4.0
1	A	644	ASP	4.0
1	A	34	GLY	3.9
1	A	753	ALA	3.9
1	C	677	ASP	3.9
1	C	678	ASN	3.8
1	A	641	THR	3.8
1	A	669	CYS	3.8
1	C	699	GLY	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	721	ALA	3.8
1	A	31	PRO	3.7
1	D	725	ASP	3.7
1	C	645	GLY	3.7
1	D	30	ALA	3.7
1	A	701	ALA	3.6
1	B	670	GLY	3.6
1	A	670	GLY	3.6
1	C	670	GLY	3.6
1	A	725	ASP	3.6
1	C	33	ASP	3.6
1	C	614	ALA	3.6
1	B	36	HIS	3.6
1	C	28	SER	3.6
1	D	727	SER	3.6
1	A	612	ARG	3.6
1	D	750	LYS	3.6
1	B	706	ALA	3.5
1	C	669	CYS	3.5
1	B	27	ASP	3.5
1	A	724	ALA	3.5
1	B	638	GLY	3.5
1	D	707	THR	3.5
1	A	643	ASP	3.5
1	A	640	VAL	3.5
1	A	647	VAL	3.4
1	A	27	ASP	3.4
1	A	707	THR	3.4
1	D	749	ASP	3.4
1	A	706	ALA	3.4
1	D	595	ASP	3.3
1	B	672	ILE	3.3
1	B	640	VAL	3.3
1	B	698	ALA	3.3
1	D	701	ALA	3.3
1	D	753	ALA	3.3
1	B	31	PRO	3.3
1	B	634	TYR	3.2
1	D	36	HIS	3.2
1	B	595	ASP	3.2
1	B	676	ALA	3.2
1	D	31	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	616	LEU	3.2
1	A	648	LEU	3.2
1	B	677	ASP	3.2
1	C	35	SER	3.2
1	B	650	ILE	3.1
1	D	677	ASP	3.1
1	A	698	ALA	3.1
1	B	28	SER	3.1
1	B	34	GLY	3.1
1	D	611	VAL	3.1
1	B	749	ASP	3.1
1	A	696	ALA	3.1
1	C	724	ALA	3.1
1	D	642	ALA	3.1
1	A	672	ILE	3.1
1	B	647	VAL	3.1
1	A	713	GLN	3.1
1	A	610	GLU	3.1
1	C	27	ASP	3.0
1	C	750	LYS	3.0
1	D	617	LEU	3.0
1	B	568	ASP	3.0
1	C	679	GLY	3.0
1	A	652	ALA	3.0
1	C	753	ALA	3.0
1	D	39	ALA	3.0
1	D	708	ILE	3.0
1	A	750	LYS	2.9
1	C	612	ARG	2.9
1	C	647	VAL	2.9
1	A	38	PRO	2.9
1	D	594	PRO	2.9
1	C	673	ALA	2.9
1	B	673	ALA	2.8
1	D	698	ALA	2.8
1	D	751	ILE	2.8
1	B	714	GLY	2.8
1	D	32	GLU	2.8
1	B	669	CYS	2.8
1	D	748	ILE	2.8
1	C	568	ASP	2.8
1	C	712	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	616	LEU	2.7
1	D	521	ARG	2.7
1	D	618	ALA	2.7
1	B	37	ARG	2.7
1	A	32	GLU	2.7
1	B	646	THR	2.7
1	C	713	GLN	2.7
1	A	617	LEU	2.7
1	A	708	ILE	2.7
1	A	748	ILE	2.7
1	A	36	HIS	2.7
1	D	614	ALA	2.6
1	A	615	ASP	2.6
1	B	753	ALA	2.6
1	C	700	ASP	2.6
1	A	552	LEU	2.6
1	A	716	GLU	2.6
1	A	39	ALA	2.6
1	C	36	HIS	2.6
1	A	717	GLY	2.6
1	B	750	LYS	2.6
1	A	721	ALA	2.6
1	D	706	ALA	2.6
1	C	727	SER	2.6
1	C	37	ARG	2.5
1	A	609	ASP	2.5
1	B	615	ASP	2.5
1	D	700	ASP	2.5
1	C	672	ILE	2.5
1	C	675	ILE	2.5
1	C	706	ALA	2.5
1	C	721	ALA	2.5
1	D	673	ALA	2.5
1	B	727	SER	2.5
1	D	640	VAL	2.5
1	A	59	ASP	2.5
1	B	59	ASP	2.5
1	B	671	ASN	2.5
1	A	369	ARG	2.5
1	C	635	SER	2.5
1	C	640	VAL	2.5
1	C	641	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	649	PRO	2.5
1	B	712	ASP	2.5
1	B	645	GLY	2.4
1	D	699	GLY	2.4
1	D	678	ASN	2.4
1	C	654	PHE	2.4
1	A	595	ASP	2.4
1	A	677	ASP	2.4
1	D	38	PRO	2.4
1	A	596	GLY	2.4
1	A	675	ILE	2.4
1	C	698	ALA	2.4
1	B	678	ASN	2.4
1	C	608	ASN	2.4
1	C	613	SER	2.4
1	B	655	ALA	2.4
1	B	711	ALA	2.4
1	B	724	ALA	2.4
1	A	709	LYS	2.4
1	A	569	ASP	2.3
1	A	674	ASP	2.3
1	C	595	ASP	2.3
1	D	680	ASP	2.3
1	B	38	PRO	2.3
1	C	594	PRO	2.3
1	D	424	GLY	2.3
1	D	596	GLY	2.3
1	D	569	ASP	2.3
1	B	618	ALA	2.3
1	A	679	GLY	2.3
1	B	707	THR	2.3
1	C	39	ALA	2.3
1	C	655	ALA	2.3
1	D	752	PRO	2.3
1	A	656	GLY	2.3
1	B	596	GLY	2.3
1	B	613	SER	2.3
1	B	713	GLN	2.3
1	A	479	ARG	2.2
1	A	33	ASP	2.2
1	B	610	GLU	2.2
1	B	633	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	38	PRO	2.2
1	D	713	GLN	2.2
1	D	33	ASP	2.2
1	D	722	ASP	2.2
1	C	671	ASN	2.2
1	C	730	ASP	2.2
1	A	727	SER	2.2
1	B	679	GLY	2.2
1	C	714	GLY	2.2
1	D	582	LEU	2.2
1	C	696	ALA	2.2
1	A	703	LYS	2.2
1	D	612	ARG	2.2
1	D	709	LYS	2.2
1	B	654	PHE	2.1
1	A	700	ASP	2.1
1	B	284	GLY	2.1
1	D	645	GLY	2.1
1	C	648	LEU	2.1
1	C	40	ALA	2.1
1	D	716	GLU	2.1
1	A	651	ALA	2.1
1	C	622	ALA	2.1
1	B	700	ASP	2.1
1	C	643	ASP	2.1
1	A	715	GLU	2.1
1	D	574	THR	2.1
1	B	699	GLY	2.1
1	A	752	PRO	2.1
1	B	652	ALA	2.1
1	C	651	ALA	2.1
1	B	33	ASP	2.1
1	C	597	ASP	2.1
1	C	609	ASP	2.1
1	D	449	HIS	2.0
1	A	678	ASN	2.0
1	D	712	ASP	2.0
1	A	650	ILE	2.0
1	D	672	ILE	2.0
1	D	717	GLY	2.0
1	B	719	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

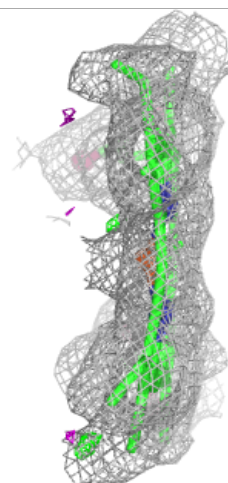
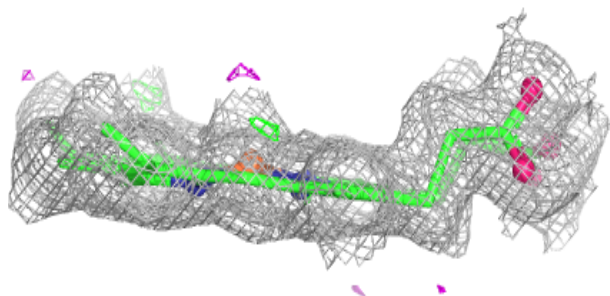
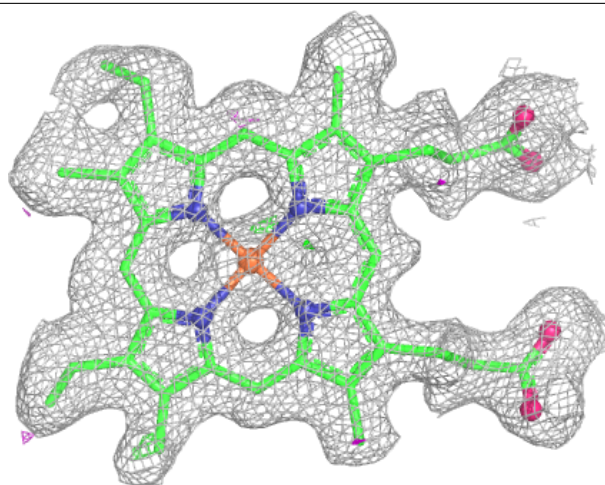
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	A	754	43/43	0.98	0.05	7,12,16,22	0
2	HEM	B	754	43/43	0.98	0.05	8,12,16,22	0
2	HEM	C	754	43/43	0.98	0.05	8,12,16,22	0
2	HEM	D	754	43/43	0.98	0.05	7,12,16,22	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.

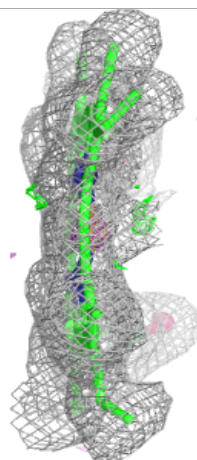
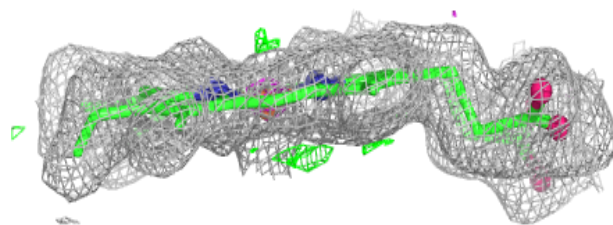
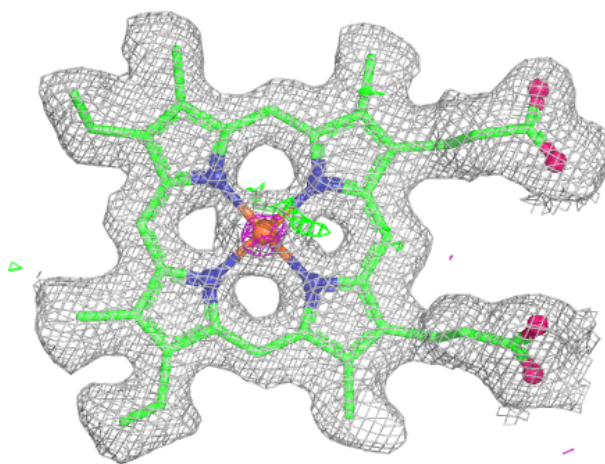
Electron density around HEM A 754:

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



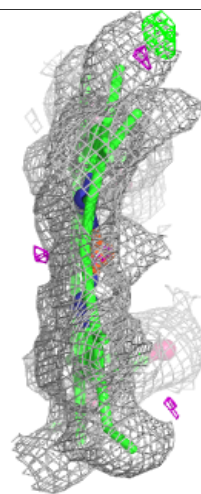
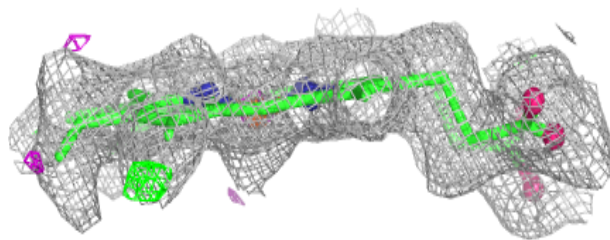
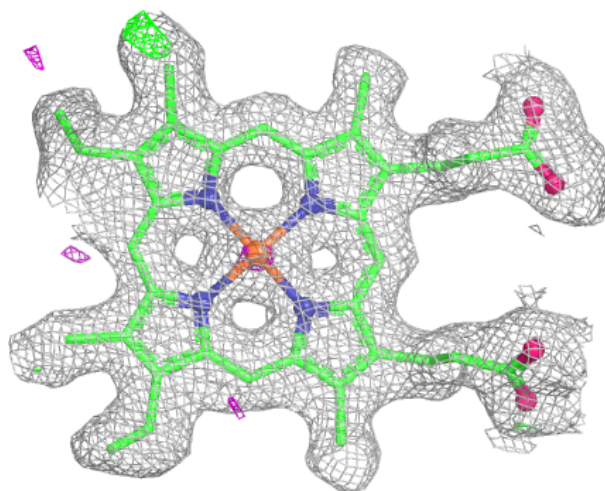
Electron density around HEM B 754:

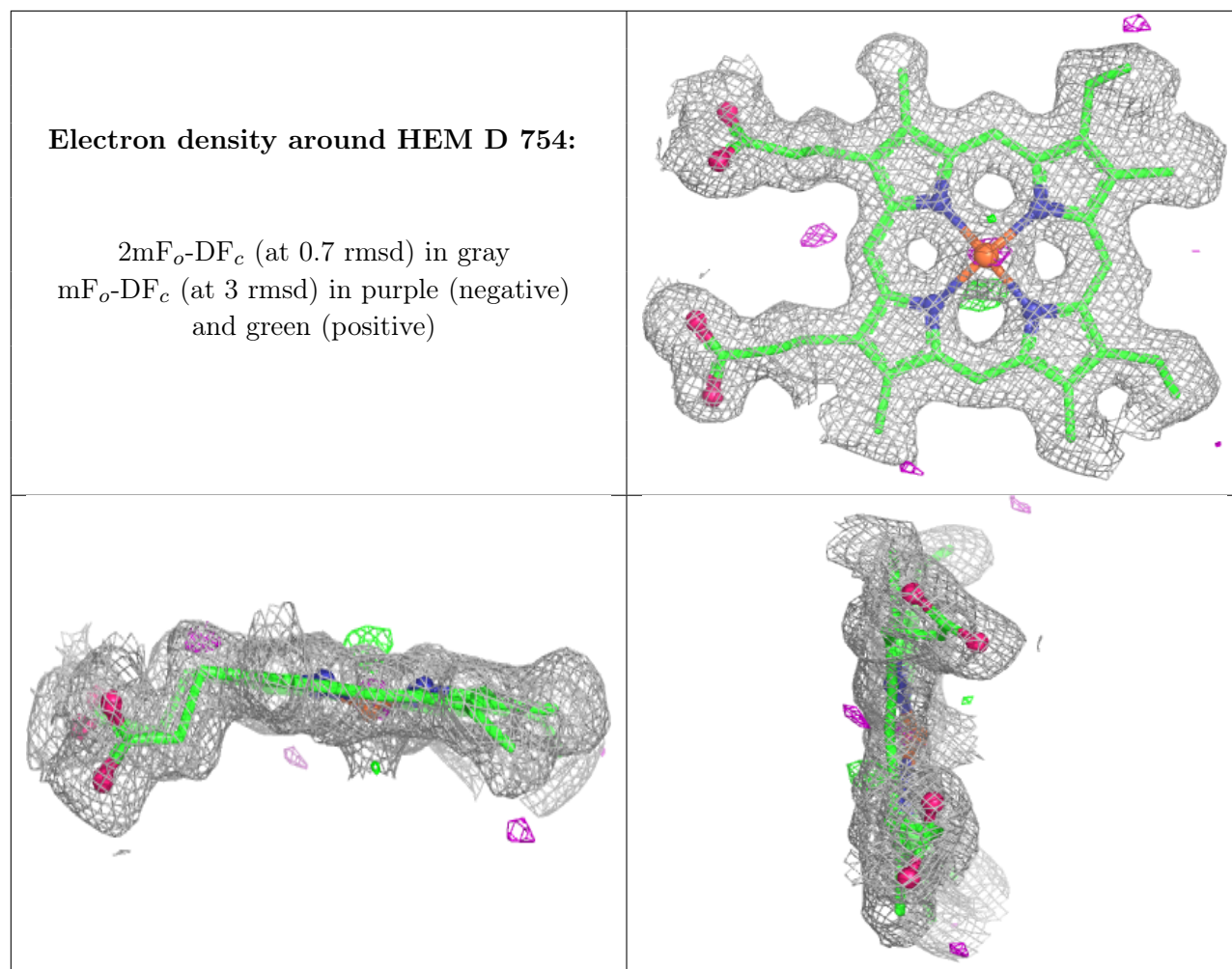
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers ⓘ

There are no such residues in this entry.