



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:53 AM UTC

PDB ID : 2PCC / pdb_00002pcc
Title : CRYSTAL STRUCTURE OF A COMPLEX BETWEEN ELECTRON TRANSFER PARTNERS, CYTOCHROME C PEROXIDASE AND CYTOCHROME C
Authors : Pelletier, H.; Kraut, J.
Deposited on : 1993-04-14
Resolution : 2.30 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)
Xtrriage (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

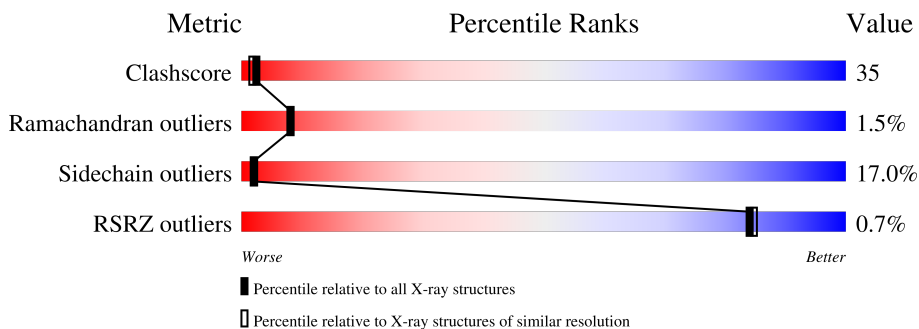
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	296	
1	C	296	
2	B	108	
2	D	108	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 7115 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 CYTOCHROME C PEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	294	2371	1514	395	456	6	0	0	0
1	C	294	2371	1514	395	456	6	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	ILE	THR	conflict	UNP P00431
A	152	GLY	ASP	conflict	UNP P00431
C	53	ILE	THR	conflict	UNP P00431
C	152	GLY	ASP	conflict	UNP P00431

- Molecule 2 is a protein called ISO-1-CYTOCHROME C.

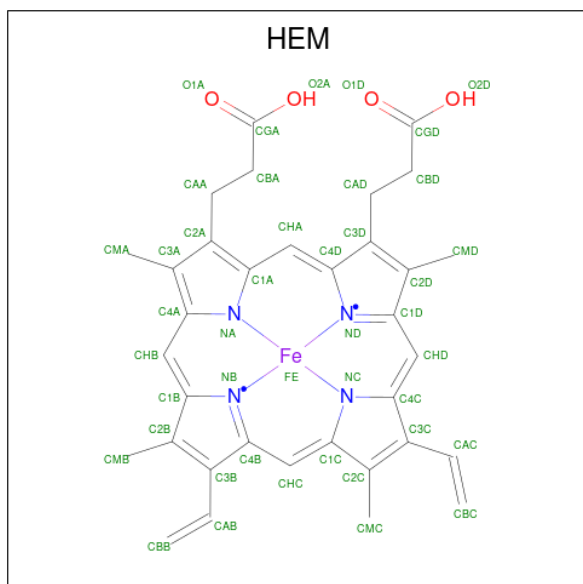
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	108	847	534	151	157	5	0	0	0
2	D	108	847	534	151	157	5	0	0	0

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			2	1	1		
3	C	1	Total	O	S	0	0
			2	1	1		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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

- Molecule 5 is water.

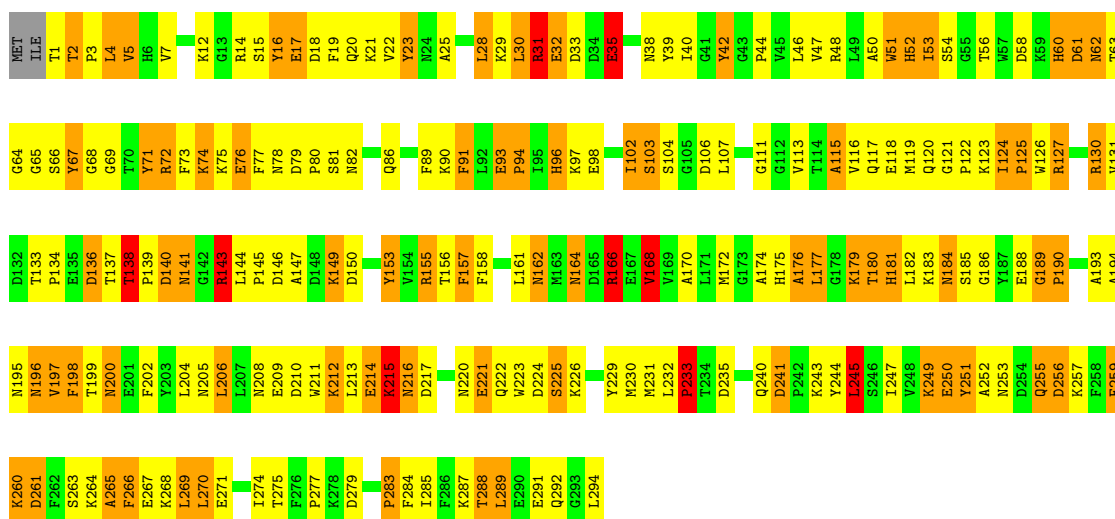
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	203	Total	O	0	0
			203	203		
5	B	46	Total	O	0	0
			46	46		
5	C	212	Total	O	0	0
			212	212		
5	D	42	Total	O	0	0
			42	42		

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.

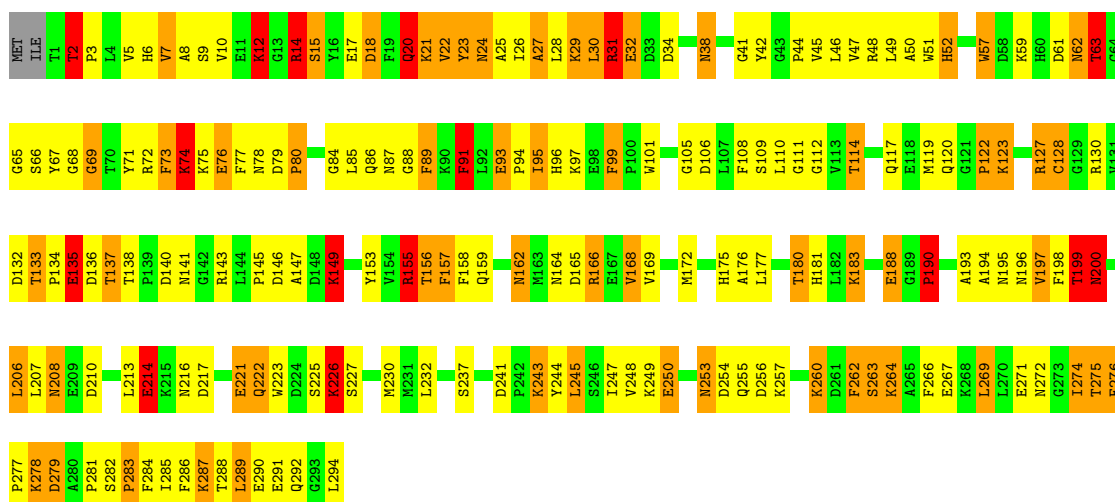
- Molecule 1: CYTOCHROME C PEROXIDASE

Chain A: 

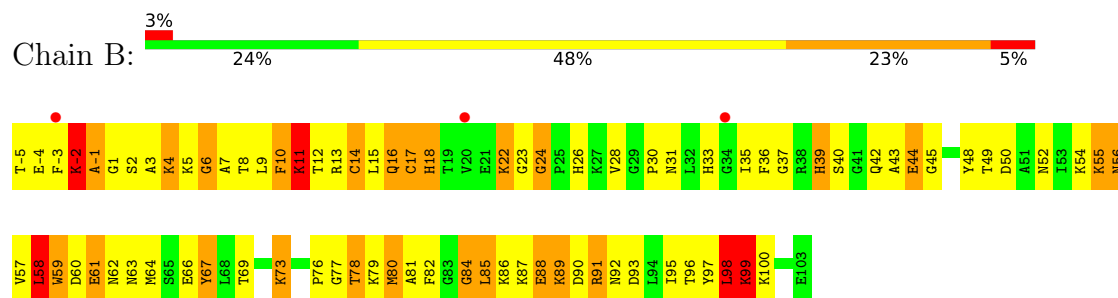


- Molecule 1: CYTOCHROME C PEROXIDASE

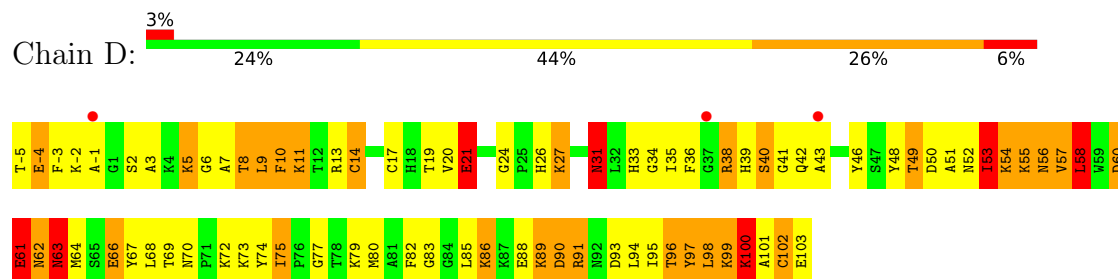
Chain C: 



- Molecule 2: ISO-1-CYTOCHROME C



- Molecule 2: ISO-1-CYTOCHROME C



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.40Å 118.60Å 45.10Å 90.00° 104.60° 90.00°	Depositor
Resolution (Å)	6.00 – 2.30 6.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.30) 91.4 (6.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.10 (at 2.24Å)	Xtrriage
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.167 , (Not available) 0.284 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtrriage
Anisotropy	0.379	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.095 for -h-1,-k,l	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7115	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.58	13/2438 (0.5%)	2.60	206/3302 (6.2%)
1	C	1.56	20/2438 (0.8%)	2.52	180/3302 (5.5%)
2	B	1.23	2/865 (0.2%)	2.32	46/1156 (4.0%)
2	D	1.22	0/865	2.34	47/1156 (4.1%)
All	All	1.49	35/6606 (0.5%)	2.50	479/8916 (5.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	C	0	3
All	All	0	7

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	181	HIS	CA-CB	9.09	1.65	1.53
1	A	265	ALA	C-N	7.04	1.42	1.33
1	C	99	PHE	N-CA	6.94	1.53	1.46
1	A	93	GLU	CA-CB	-6.44	1.44	1.53
1	C	68	GLY	C-O	6.40	1.30	1.24
1	C	52	HIS	ND1-CE1	6.38	1.39	1.32
1	A	264	LYS	N-CA	6.32	1.53	1.46
1	C	117	GLN	N-CA	6.20	1.53	1.46
1	C	112	GLY	CA-C	-6.08	1.45	1.52
1	C	177	LEU	CA-CB	5.78	1.62	1.53
1	A	65	GLY	N-CA	5.77	1.50	1.45
1	C	153	TYR	N-CA	5.73	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	175	HIS	ND1-CE1	5.71	1.38	1.32
1	A	181	HIS	CA-CB	5.68	1.61	1.53
2	B	85	LEU	CA-CB	-5.64	1.45	1.53
1	C	225	SER	N-CA	5.52	1.52	1.45
1	C	156	THR	CA-CB	5.50	1.62	1.53
1	C	243	LYS	N-CA	5.49	1.53	1.46
1	C	65	GLY	N-CA	5.48	1.50	1.45
1	A	60	HIS	CG-CD2	-5.47	1.29	1.35
1	C	106	ASP	N-CA	5.45	1.53	1.46
1	C	114	THR	CA-CB	5.40	1.61	1.53
1	C	114	THR	CA-C	-5.35	1.46	1.52
1	A	111	GLY	C-O	5.31	1.30	1.23
1	A	180	THR	N-CA	5.31	1.52	1.45
2	B	69	THR	CA-CB	5.30	1.61	1.53
1	A	266	PHE	CA-C	-5.29	1.45	1.52
1	A	125	PRO	CA-C	-5.28	1.46	1.52
1	A	124	ILE	CA-CB	5.23	1.60	1.54
1	C	232	LEU	CA-C	5.23	1.59	1.52
1	C	20	GLN	N-CA	5.21	1.52	1.46
1	A	251	TYR	C-N	-5.20	1.26	1.33
1	C	158	PHE	N-CA	5.13	1.52	1.46
1	C	2	THR	CB-OG1	5.13	1.51	1.43
1	C	175	HIS	CE1-NE2	-5.12	1.27	1.32

All (479) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	ASP	CA-CB-CG	15.52	128.12	112.60
1	C	17	GLU	CB-CG-CD	13.16	134.97	112.60
2	B	18	HIS	CA-CB-CG	12.95	126.75	113.80
1	A	93	GLU	CA-CB-CG	12.23	138.56	114.10
1	C	181	HIS	CA-CB-CG	-11.98	101.82	113.80
1	A	289	LEU	N-CA-C	-11.96	98.22	111.14
1	C	91	PHE	CA-CB-CG	11.29	125.09	113.80
1	A	284	PHE	CA-CB-CG	11.20	125.00	113.80
1	A	48	ARG	CD-NE-CZ	10.99	139.78	124.40
1	A	40	ILE	N-CA-C	-10.59	100.36	111.58
1	A	136	ASP	CA-CB-CG	10.51	123.11	112.60
1	A	28	LEU	O-C-N	10.39	134.00	122.15
1	C	277	PRO	CA-C-N	10.11	135.14	120.38
1	C	277	PRO	C-N-CA	10.11	135.14	120.38
1	A	214	GLU	O-C-N	10.09	133.38	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	98	LEU	N-CA-C	10.04	121.81	111.07
1	A	98	GLU	CA-CB-CG	9.95	134.00	114.10
1	C	23	TYR	CA-C-O	9.80	131.85	121.07
1	A	241	ASP	CA-CB-CG	9.72	122.32	112.60
1	A	155	ARG	NE-CZ-NH2	9.59	127.83	119.20
1	C	99	PHE	O-C-N	9.50	127.88	121.23
1	C	99	PHE	CA-CB-CG	9.44	123.24	113.80
1	C	253	ASN	CA-CB-CG	9.42	122.02	112.60
2	D	14	CYS	N-CA-C	9.38	125.65	113.18
1	A	216	ASN	OD1-CG-ND2	9.21	131.81	122.60
1	C	31	ARG	CA-C-N	9.17	133.10	120.63
1	C	31	ARG	C-N-CA	9.17	133.10	120.63
1	A	143	ARG	CD-NE-CZ	-9.07	111.70	124.40
2	D	24	GLY	N-CA-C	-9.02	101.31	112.23
1	C	198	PHE	CA-CB-CG	8.98	122.78	113.80
2	D	31	ASN	N-CA-C	-8.97	97.22	110.23
1	A	130	ARG	NE-CZ-NH2	8.95	127.25	119.20
1	C	153	TYR	CA-C-N	8.91	131.84	120.70
1	C	153	TYR	C-N-CA	8.91	131.84	120.70
1	C	197	VAL	CA-C-O	-8.89	110.27	120.67
2	D	75	ILE	N-CA-CB	8.88	123.64	111.21
1	C	68	GLY	N-CA-C	8.80	124.36	114.67
1	A	176	ALA	CA-C-N	8.70	134.46	122.19
1	A	176	ALA	C-N-CA	8.70	134.46	122.19
1	A	214	GLU	CA-C-O	-8.70	111.97	121.28
1	C	9	SER	CA-C-O	8.69	129.76	120.46
1	A	155	ARG	NE-CZ-NH1	-8.62	112.88	121.50
1	C	141	ASN	CA-CB-CG	8.57	121.17	112.60
1	A	157	PHE	N-CA-C	-8.48	102.03	111.28
1	C	146	ASP	CB-CA-C	8.48	126.14	109.35
1	C	108	PHE	CA-CB-CG	8.47	122.27	113.80
1	A	209	GLU	CA-C-N	8.40	135.81	123.13
1	A	209	GLU	C-N-CA	8.40	135.81	123.13
1	A	53	ILE	N-CA-C	-8.34	100.74	113.16
1	A	22	VAL	CA-C-N	8.27	131.19	120.44
1	A	22	VAL	C-N-CA	8.27	131.19	120.44
1	C	222	GLN	CB-CG-CD	8.26	126.64	112.60
2	D	75	ILE	O-C-N	8.23	130.48	121.10
1	A	115	ALA	CB-CA-C	8.21	124.81	110.85
1	A	32	GLU	N-CA-C	8.17	119.96	111.14
2	B	31	ASN	N-CA-C	-8.08	97.84	109.96
2	D	20	VAL	N-CA-CB	-8.07	101.23	112.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	10	PHE	CA-CB-CG	-8.06	105.74	113.80
1	A	76	GLU	CA-C-N	8.02	131.03	120.28
1	A	76	GLU	C-N-CA	8.02	131.03	120.28
1	A	53	ILE	O-C-N	8.02	131.64	122.18
1	A	124	ILE	CB-CG1-CD1	7.99	130.58	113.80
1	C	210	ASP	O-C-N	7.85	132.39	123.05
1	C	177	LEU	N-CA-C	7.85	122.63	109.76
2	B	50	ASP	CA-CB-CG	7.82	120.42	112.60
1	C	193	ALA	CA-C-N	7.82	133.65	122.24
1	C	193	ALA	C-N-CA	7.82	133.65	122.24
1	C	119	MET	N-CA-CB	7.81	121.96	110.56
1	A	181	HIS	CA-C-O	-7.81	111.73	120.32
1	A	217	ASP	O-C-N	7.79	133.13	122.46
1	A	289	LEU	CB-CA-C	7.78	123.20	110.90
1	A	23	TYR	CA-C-O	7.77	128.98	120.82
1	C	137	THR	CA-CB-OG1	-7.75	97.97	109.60
1	A	193	ALA	CA-C-O	-7.74	110.63	120.31
1	C	132	ASP	CA-CB-CG	7.70	120.30	112.60
1	A	224	ASP	CA-C-O	-7.70	112.38	120.70
1	A	54	SER	CA-CB-OG	7.70	126.50	111.10
1	C	29	LYS	CG-CD-CE	7.68	128.97	111.30
1	A	180	THR	CA-C-O	-7.64	112.26	121.28
1	C	214	GLU	CA-CB-CG	7.62	129.33	114.10
1	A	141	ASN	CA-C-O	-7.59	113.28	121.56
1	C	2	THR	CB-CA-C	7.56	125.07	110.17
1	A	30	LEU	N-CA-C	-7.55	102.40	111.69
1	A	25	ALA	CA-C-O	7.53	128.72	120.82
1	C	146	ASP	N-CA-CB	-7.52	97.39	111.00
2	B	99	LYS	CA-C-N	7.52	130.35	120.28
2	B	99	LYS	C-N-CA	7.52	130.35	120.28
1	A	111	GLY	CA-C-N	-7.50	110.89	120.34
1	A	111	GLY	C-N-CA	-7.50	110.89	120.34
1	C	93	GLU	CA-CB-CG	7.49	129.07	114.10
1	A	73	PHE	CA-CB-CG	7.48	121.28	113.80
1	A	259	PHE	CA-CB-CG	7.45	121.25	113.80
2	D	49	THR	N-CA-CB	7.42	121.05	110.44
1	A	197	VAL	CA-C-O	-7.41	112.50	120.36
1	A	164	ASN	CA-CB-CG	7.35	119.95	112.60
2	B	4	LYS	N-CA-C	-7.28	102.33	112.45
1	C	95	ILE	CB-CG1-CD1	7.27	129.07	113.80
2	D	96	THR	N-CA-C	-7.26	103.06	110.97
1	C	2	THR	CA-CB-CG2	7.24	122.81	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	180	THR	N-CA-C	-7.21	98.56	110.17
1	A	175	HIS	CA-CB-CG	-7.17	106.63	113.80
1	A	274	ILE	O-C-N	7.15	130.69	123.18
1	C	32	GLU	CB-CG-CD	7.10	124.67	112.60
1	A	102	ILE	CA-C-O	-7.07	113.58	121.36
1	A	166	ARG	CD-NE-CZ	-7.06	114.51	124.40
1	C	276	PHE	O-C-N	7.06	127.31	121.31
1	C	262	PHE	CA-CB-CG	-7.06	106.74	113.80
2	B	98	LEU	O-C-N	7.04	129.33	122.07
1	A	71	TYR	CA-C-O	7.04	128.01	119.49
1	C	188	GLU	CB-CG-CD	7.01	124.52	112.60
2	D	9	LEU	N-CA-CB	-6.96	99.49	110.28
1	C	99	PHE	CA-C-O	-6.95	114.31	121.06
1	C	176	ALA	CA-C-O	6.95	127.97	119.97
1	A	256	ASP	CB-CA-C	6.94	121.78	110.88
1	A	35	GLU	CA-CB-CG	6.94	127.97	114.10
1	A	89	PHE	CA-C-N	6.93	129.44	120.44
1	A	89	PHE	C-N-CA	6.93	129.44	120.44
1	C	17	GLU	CA-CB-CG	6.91	127.91	114.10
1	C	88	GLY	CA-C-O	6.90	127.97	120.66
1	C	48	ARG	CD-NE-CZ	6.89	134.05	124.40
1	A	189	GLY	O-C-N	6.88	128.65	121.77
1	C	272	ASN	CA-C-O	-6.87	114.42	120.88
1	A	168	VAL	N-CA-CB	6.85	123.89	110.95
2	B	52	ASN	CA-CB-CG	6.84	119.44	112.60
2	B	17	CYS	CA-C-O	-6.84	111.52	119.05
2	D	31	ASN	CA-CB-CG	6.83	119.43	112.60
2	B	78	THR	CA-C-O	-6.82	114.07	121.44
2	D	90	ASP	CA-CB-CG	-6.81	105.79	112.60
1	C	275	THR	CA-C-N	6.81	130.73	121.20
1	C	275	THR	C-N-CA	6.81	130.73	121.20
1	A	121	GLY	O-C-N	6.80	128.57	121.77
2	D	10	PHE	CA-C-O	6.78	127.94	120.82
2	B	28	VAL	N-CA-C	-6.78	102.36	111.44
2	B	14	CYS	O-C-N	6.77	129.97	121.64
1	C	12	LYS	CA-C-O	6.77	128.11	120.80
1	A	215	LYS	CB-CA-C	-6.75	97.22	109.38
1	C	250	GLU	N-CA-CB	6.75	120.26	110.20
1	C	168	VAL	CA-C-O	-6.75	113.49	120.71
1	C	214	GLU	O-C-N	6.73	130.83	123.10
1	A	181	HIS	CA-CB-CG	-6.72	107.08	113.80
1	A	283	PRO	O-C-N	6.72	131.35	123.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	168	VAL	CA-CB-CG1	6.72	121.83	110.40
1	A	93	GLU	N-CA-CB	6.71	120.83	110.43
1	C	195	ASN	N-CA-C	6.71	120.92	112.87
1	C	225	SER	N-CA-C	-6.71	99.25	109.85
2	B	78	THR	CA-CB-OG1	-6.70	99.55	109.60
1	A	52	HIS	N-CA-C	6.70	120.55	112.38
1	A	225	SER	N-CA-C	-6.69	99.77	110.14
2	D	61	GLU	CB-CG-CD	6.69	123.98	112.60
1	A	31	ARG	O-C-N	-6.67	114.54	122.15
1	A	50	ALA	CA-C-N	6.66	129.09	120.44
1	A	50	ALA	C-N-CA	6.66	129.09	120.44
1	C	279	ASP	CA-CB-CG	6.65	119.25	112.60
1	A	153	TYR	CA-C-N	6.65	128.94	120.56
1	A	153	TYR	C-N-CA	6.65	128.94	120.56
2	D	103	GLU	CB-CG-CD	6.64	123.89	112.60
1	C	221	GLU	N-CA-CB	-6.64	99.29	111.37
1	A	14	ARG	N-CA-C	-6.60	100.18	109.69
1	C	27	ALA	N-CA-C	6.60	119.30	111.71
2	D	89	LYS	O-C-N	6.59	128.86	122.07
1	A	61	ASP	CA-CB-CG	-6.57	106.03	112.60
1	C	190	PRO	N-CA-CB	-6.52	96.40	103.25
1	C	180	THR	CA-C-N	6.51	132.17	123.05
1	C	180	THR	C-N-CA	6.51	132.17	123.05
1	A	213	LEU	CB-CA-C	6.51	120.64	109.51
1	A	224	ASP	CA-CB-CG	-6.51	106.09	112.60
2	B	12	THR	N-CA-C	6.50	118.45	111.36
1	A	261	ASP	O-C-N	6.48	129.53	122.15
1	C	283	PRO	CA-C-N	6.47	133.14	122.07
1	C	283	PRO	C-N-CA	6.47	133.14	122.07
1	C	217	ASP	CA-CB-CG	-6.46	106.14	112.60
1	C	41	GLY	CA-C-N	6.46	133.67	122.56
1	C	41	GLY	C-N-CA	6.46	133.67	122.56
1	A	179	LYS	CA-CB-CG	-6.42	101.25	114.10
1	C	207	LEU	CA-C-N	-6.42	112.06	122.26
1	C	207	LEU	C-N-CA	-6.42	112.06	122.26
2	D	100	LYS	O-C-N	6.41	128.95	122.03
2	D	33	HIS	O-C-N	6.41	130.89	122.95
1	C	27	ALA	N-CA-CB	-6.40	100.36	110.22
1	A	124	ILE	O-C-N	6.40	128.40	121.10
1	A	149	LYS	CA-CB-CG	-6.40	101.31	114.10
1	A	199	THR	CA-CB-OG1	-6.39	100.01	109.60
2	B	58	LEU	CA-C-N	-6.38	113.93	122.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	58	LEU	C-N-CA	-6.38	113.93	122.42
1	A	91	PHE	CA-C-N	-6.37	112.02	122.54
1	A	91	PHE	C-N-CA	-6.37	112.02	122.54
1	A	62	ASN	CA-CB-CG	-6.37	106.23	112.60
1	A	283	PRO	CA-C-O	-6.37	114.17	121.56
1	A	96	HIS	CA-C-N	6.36	128.81	120.28
1	A	96	HIS	C-N-CA	6.36	128.81	120.28
1	C	119	MET	CA-C-O	-6.36	112.11	119.56
1	A	65	GLY	N-CA-C	-6.36	104.64	112.33
1	C	62	ASN	CA-CB-CG	6.35	118.95	112.60
1	A	60	HIS	CA-CB-CG	-6.35	107.45	113.80
2	B	26	HIS	N-CA-CB	6.34	119.43	110.36
1	C	223	TRP	CA-C-N	6.34	132.51	122.62
1	C	223	TRP	C-N-CA	6.34	132.51	122.62
1	C	274	ILE	O-C-N	6.34	129.84	123.18
1	A	233	PRO	N-CA-CB	-6.33	96.60	103.25
1	C	23	TYR	CB-CG-CD2	6.31	130.26	120.80
1	A	157	PHE	CA-C-N	-6.31	110.72	120.31
1	A	157	PHE	C-N-CA	-6.31	110.72	120.31
1	A	125	PRO	CA-C-O	-6.30	114.37	121.43
1	A	244	TYR	N-CA-C	-6.30	103.71	111.40
1	C	69	GLY	CA-C-N	6.29	130.67	120.60
1	C	69	GLY	C-N-CA	6.29	130.67	120.60
1	A	52	HIS	CA-CB-CG	-6.29	107.51	113.80
2	D	62	ASN	CA-CB-CG	-6.29	106.31	112.60
2	D	53	ILE	CB-CA-C	6.29	120.24	111.94
1	A	185	SER	CA-C-O	-6.28	112.61	119.08
2	D	49	THR	N-CA-C	-6.27	102.44	110.53
2	B	89	LYS	N-CA-CB	6.26	119.33	109.82
2	D	33	HIS	N-CA-CB	6.25	119.26	109.69
1	A	64	GLY	CA-C-O	-6.24	113.71	122.58
1	A	215	LYS	O-C-N	6.24	131.14	123.21
1	A	216	ASN	O-C-N	6.24	129.81	121.83
1	C	96	HIS	CA-C-N	6.23	128.54	120.44
1	C	96	HIS	C-N-CA	6.23	128.54	120.44
2	D	49	THR	O-C-N	6.23	130.31	122.65
1	C	108	PHE	CA-C-O	-6.19	113.99	120.55
1	A	216	ASN	CA-C-O	-6.16	113.80	121.50
2	B	44	GLU	CA-CB-CG	6.15	126.39	114.10
1	C	290	GLU	CA-CB-CG	6.15	126.40	114.10
1	A	76	GLU	CB-CG-CD	6.13	123.03	112.60
1	A	138	THR	O-C-N	6.13	126.89	121.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	157	PHE	CA-CB-CG	-6.13	107.67	113.80
2	D	21	GLU	N-CA-CB	6.13	119.02	110.26
1	C	197	VAL	N-CA-CB	6.12	122.04	111.39
1	C	200	ASN	CA-C-N	6.12	128.76	120.38
1	C	200	ASN	C-N-CA	6.12	128.76	120.38
1	A	141	ASN	O-C-N	6.12	130.08	122.86
2	D	103	GLU	CA-CB-CG	6.12	126.34	114.10
1	C	206	LEU	CB-CA-C	6.12	120.89	110.74
1	A	270	LEU	O-C-N	6.11	130.90	122.46
1	C	123	LYS	O-C-N	6.11	130.25	123.16
2	B	92	ASN	CB-CA-C	6.11	120.42	110.95
1	A	35	GLU	CB-CG-CD	6.11	122.98	112.60
1	C	146	ASP	OD1-CG-OD2	6.10	137.54	122.90
1	A	205	ASN	CA-C-N	6.09	129.26	120.79
1	A	205	ASN	C-N-CA	6.09	129.26	120.79
2	B	100	LYS	N-CA-C	6.06	117.88	111.28
1	C	225	SER	N-CA-CB	6.06	121.01	111.20
1	C	29	LYS	CA-CB-CG	-6.05	101.99	114.10
1	C	199	THR	CA-CB-CG2	6.05	120.79	110.50
2	D	31	ASN	CB-CA-C	6.04	119.74	109.72
2	D	66	GLU	N-CA-C	-6.03	103.46	111.24
1	C	79	ASP	CA-C-N	6.03	126.46	119.47
1	C	79	ASP	C-N-CA	6.03	126.46	119.47
1	A	33	ASP	O-C-N	-6.03	113.28	122.08
1	A	18	ASP	CA-CB-CG	6.02	118.62	112.60
1	C	155	ARG	O-C-N	-6.02	115.74	122.12
1	C	38	ASN	CA-CB-CG	-6.01	106.59	112.60
1	C	263	SER	N-CA-CB	-6.01	100.99	109.94
1	C	222	GLN	CA-C-O	-5.99	115.04	121.45
1	C	20	GLN	O-C-N	-5.98	114.61	122.39
1	A	265	ALA	CA-C-N	-5.96	112.49	120.54
1	A	265	ALA	C-N-CA	-5.96	112.49	120.54
1	A	73	PHE	CA-C-O	-5.95	114.26	121.28
2	B	88	GLU	CA-C-O	-5.93	114.56	120.90
1	A	141	ASN	CA-CB-CG	-5.93	106.67	112.60
1	C	232	LEU	N-CA-C	-5.92	102.43	110.36
1	A	73	PHE	CA-C-N	5.90	128.47	120.38
1	A	73	PHE	C-N-CA	5.90	128.47	120.38
1	A	216	ASN	N-CA-C	-5.90	100.71	109.86
2	D	86	LYS	N-CA-C	5.90	117.71	111.28
1	C	24	ASN	OD1-CG-ND2	-5.88	116.72	122.60
1	C	222	GLN	O-C-N	5.88	129.86	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	127	ARG	NE-CZ-NH2	5.88	124.49	119.20
1	A	202	PHE	CA-C-N	5.88	128.63	120.29
1	A	202	PHE	C-N-CA	5.88	128.63	120.29
2	B	89	LYS	O-C-N	5.88	128.37	122.08
1	A	98	GLU	O-C-N	-5.87	116.03	122.07
1	C	30	LEU	N-CA-C	-5.87	104.84	112.23
1	C	74	LYS	CA-C-N	5.87	128.46	120.54
1	C	74	LYS	C-N-CA	5.87	128.46	120.54
1	C	241	ASP	CA-CB-CG	5.87	118.47	112.60
2	D	85	LEU	CA-C-N	5.85	128.12	120.28
2	D	85	LEU	C-N-CA	5.85	128.12	120.28
2	D	31	ASN	OD1-CG-ND2	-5.85	116.75	122.60
1	C	31	ARG	NE-CZ-NH2	-5.85	113.93	119.20
1	A	206	LEU	CB-CA-C	5.85	120.22	110.92
1	A	31	ARG	CA-C-O	5.84	126.61	120.42
1	A	241	ASP	CA-C-O	5.84	125.86	119.32
1	C	275	THR	CB-CA-C	5.84	120.30	110.79
2	B	91	ARG	CA-C-O	5.83	126.72	120.55
1	A	155	ARG	CA-C-O	5.82	126.72	120.55
2	B	49	THR	CA-C-O	-5.82	115.38	121.55
1	A	168	VAL	CA-CB-CG1	5.81	120.28	110.40
1	C	199	THR	CA-CB-OG1	-5.80	100.89	109.60
2	D	21	GLU	O-C-N	5.80	129.54	122.75
1	C	15	SER	CA-CB-OG	-5.80	99.49	111.10
1	A	68	GLY	N-CA-C	5.80	122.50	115.31
1	A	21	LYS	O-C-N	5.79	129.76	122.23
1	A	141	ASN	OD1-CG-ND2	5.78	128.38	122.60
1	C	197	VAL	O-C-N	5.77	129.41	123.18
1	A	21	LYS	CA-C-O	-5.77	113.83	120.24
1	A	197	VAL	CB-CA-C	5.77	118.75	110.33
1	C	122	PRO	N-CA-C	-5.77	102.53	111.13
1	A	73	PHE	N-CA-C	-5.76	100.90	110.17
1	A	196	ASN	CA-C-O	-5.75	113.07	119.34
1	C	128	CYS	CA-C-N	-5.75	114.52	122.63
1	C	128	CYS	C-N-CA	-5.75	114.52	122.63
1	A	58	ASP	CA-C-O	-5.73	112.55	120.52
1	C	130	ARG	NE-CZ-NH2	5.73	124.36	119.20
2	D	14	CYS	N-CA-CB	-5.72	97.32	110.83
2	B	14	CYS	CB-CA-C	-5.71	101.79	109.16
1	A	51	TRP	CB-CA-C	5.71	119.84	110.88
1	A	177	LEU	N-CA-C	5.70	118.92	109.46
1	C	119	MET	O-C-N	5.70	129.18	122.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	63	ASN	CA-CB-CG	5.70	118.30	112.60
1	C	146	ASP	CB-CG-OD2	-5.69	105.31	118.40
1	C	168	VAL	N-CA-CB	5.69	120.07	110.56
1	A	31	ARG	CD-NE-CZ	-5.67	116.47	124.40
1	A	157	PHE	CA-C-O	5.66	126.55	120.55
1	A	266	PHE	CA-C-N	-5.66	112.26	120.29
1	A	266	PHE	C-N-CA	-5.66	112.26	120.29
1	C	254	ASP	CA-C-N	5.66	128.43	120.28
1	C	254	ASP	C-N-CA	5.66	128.43	120.28
2	D	88	GLU	CA-CB-CG	5.66	125.42	114.10
2	B	49	THR	CA-CB-OG1	-5.66	101.11	109.60
1	C	149	LYS	O-C-N	5.65	130.24	122.72
1	C	31	ARG	CA-C-O	5.65	126.41	120.42
1	C	50	ALA	CA-C-N	5.65	127.78	120.44
1	C	50	ALA	C-N-CA	5.65	127.78	120.44
2	B	67	TYR	CA-C-N	5.64	128.61	120.38
2	B	67	TYR	C-N-CA	5.64	128.61	120.38
1	C	180	THR	CA-CB-CG2	5.64	120.08	110.50
1	A	198	PHE	N-CA-C	5.63	117.92	108.23
1	C	15	SER	O-C-N	5.63	129.72	122.68
1	A	158	PHE	CA-C-O	-5.63	113.49	119.97
1	A	103	SER	CA-C-O	-5.62	115.17	121.81
2	D	10	PHE	N-CA-C	-5.62	105.05	111.07
1	C	146	ASP	CA-C-O	-5.62	114.19	120.66
1	A	14	ARG	CD-NE-CZ	-5.62	116.54	124.40
1	A	241	ASP	CB-CA-C	5.62	116.25	109.85
1	C	28	LEU	N-CA-C	-5.60	104.67	112.45
1	C	221	GLU	CA-C-O	-5.58	114.58	121.11
1	A	5	VAL	CA-C-N	5.58	131.55	123.13
1	A	5	VAL	C-N-CA	5.58	131.55	123.13
2	B	76	PRO	CB-CA-C	5.57	118.52	111.39
1	A	184	ASN	CA-C-O	5.54	126.77	120.00
1	A	224	ASP	O-C-N	5.54	130.44	123.23
1	A	77	PHE	O-C-N	5.54	127.99	122.12
1	A	179	LYS	CA-C-N	-5.54	113.23	122.64
1	A	179	LYS	C-N-CA	-5.54	113.23	122.64
1	A	48	ARG	NE-CZ-NH2	-5.53	114.22	119.20
1	C	197	VAL	CB-CA-C	5.53	118.85	110.62
1	C	210	ASP	CA-C-O	-5.52	114.80	120.54
1	A	104	SER	CA-C-N	5.51	126.10	119.98
1	A	104	SER	C-N-CA	5.51	126.10	119.98
2	B	9	LEU	N-CA-CB	-5.51	101.74	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	ARG	CG-CD-NE	-5.51	99.88	112.00
1	C	180	THR	CA-C-O	-5.51	114.78	121.28
1	C	120	GLN	O-C-N	5.49	130.15	121.91
2	D	9	LEU	CA-C-O	5.49	126.28	119.97
1	C	221	GLU	CB-CG-CD	-5.48	103.28	112.60
1	A	225	SER	CA-C-O	-5.48	114.93	121.56
1	A	118	GLU	CG-CD-OE2	5.47	130.97	118.40
1	C	269	LEU	CA-CB-CG	5.46	135.42	116.30
1	A	166	ARG	NE-CZ-NH1	-5.46	116.05	121.50
2	B	58	LEU	N-CA-C	-5.45	100.81	109.96
1	A	143	ARG	CB-CG-CD	-5.44	98.78	111.30
1	A	229	TYR	CA-C-N	5.43	131.12	122.59
1	A	229	TYR	C-N-CA	5.43	131.12	122.59
1	A	32	GLU	CG-CD-OE1	5.43	130.89	118.40
1	A	131	VAL	CA-C-N	5.43	129.18	121.42
1	A	131	VAL	C-N-CA	5.43	129.18	121.42
1	A	249	LYS	CA-C-O	5.43	126.26	120.24
1	C	57	TRP	O-C-N	5.42	129.26	122.86
1	C	194	ALA	CB-CA-C	-5.42	104.31	111.74
1	C	276	PHE	CA-CB-CG	-5.42	108.38	113.80
1	C	289	LEU	N-CA-C	-5.42	104.41	111.02
1	A	16	TYR	CB-CA-C	5.41	121.19	110.42
1	C	266	PHE	CA-CB-CG	5.41	119.20	113.80
1	A	23	TYR	N-CA-CB	-5.40	102.18	110.01
1	C	87	ASN	N-CA-C	-5.40	105.40	111.28
1	A	274	ILE	CA-C-N	-5.39	115.50	123.05
1	A	274	ILE	C-N-CA	-5.39	115.50	123.05
1	C	89	PHE	CA-CB-CG	-5.39	108.41	113.80
1	C	24	ASN	CB-CG-ND2	5.39	124.48	116.40
1	C	147	ALA	N-CA-CB	-5.38	102.00	110.46
1	C	288	THR	CB-CA-C	5.38	120.46	109.76
2	D	90	ASP	N-CA-C	-5.38	104.46	111.02
1	A	214	GLU	CB-CA-C	-5.37	101.28	110.95
1	A	245	LEU	O-C-N	-5.37	115.94	122.22
2	B	88	GLU	O-C-N	5.37	127.67	122.09
2	D	58	LEU	CB-CA-C	5.36	120.42	111.30
1	C	260	LYS	CB-CA-C	-5.36	101.89	110.79
1	A	144	LEU	O-C-N	5.36	126.03	121.20
1	A	42	TYR	CA-C-N	5.36	130.28	121.87
1	A	42	TYR	C-N-CA	5.36	130.28	121.87
1	A	64	GLY	O-C-N	5.36	128.57	123.05
1	A	288	THR	CA-C-N	5.35	127.72	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	288	THR	C-N-CA	5.35	127.72	120.44
1	C	130	ARG	NH1-CZ-NH2	-5.35	112.34	119.30
1	A	65	GLY	CA-C-N	5.34	127.87	120.29
1	A	65	GLY	C-N-CA	5.34	127.87	120.29
1	A	150	ASP	CA-C-O	-5.34	115.30	121.49
2	B	16	GLN	CB-CG-CD	-5.33	103.53	112.60
1	C	226	LYS	CA-C-N	5.33	129.14	120.60
1	C	226	LYS	C-N-CA	5.33	129.14	120.60
1	C	52	HIS	N-CA-C	5.33	117.84	111.71
1	C	284	PHE	CA-C-O	-5.33	114.96	121.36
2	B	17	CYS	O-C-N	5.33	128.91	122.35
1	C	141	ASN	N-CA-C	-5.33	103.10	110.35
1	C	159	GLN	N-CA-C	-5.33	105.88	112.38
1	C	188	GLU	CB-CA-C	-5.32	100.06	109.70
1	C	241	ASP	CB-CA-C	5.30	117.74	109.42
2	B	11	LYS	CA-C-O	-5.30	115.26	120.82
1	A	256	ASP	CA-CB-CG	-5.29	107.31	112.60
1	C	14	ARG	CA-C-N	-5.27	112.38	122.08
1	C	14	ARG	C-N-CA	-5.27	112.38	122.08
1	A	208	ASN	CA-CB-CG	5.26	117.86	112.60
2	D	97	TYR	CA-C-N	5.26	127.28	120.44
2	D	97	TYR	C-N-CA	5.26	127.28	120.44
1	A	194	ALA	CA-C-O	-5.25	114.55	122.38
1	C	41	GLY	CA-C-O	-5.25	116.48	122.78
1	C	194	ALA	N-CA-C	5.25	117.27	110.65
1	C	197	VAL	N-CA-C	-5.23	100.95	108.48
1	C	21	LYS	N-CA-C	-5.23	105.66	111.36
2	B	39	HIS	CA-CB-CG	-5.22	108.58	113.80
1	C	221	GLU	CG-CD-OE1	-5.22	106.39	118.40
1	C	106	ASP	N-CA-C	-5.22	105.67	111.36
1	A	269	LEU	N-CA-CB	-5.21	102.45	110.12
1	C	263	SER	CA-C-O	5.21	126.48	120.90
2	B	26	HIS	N-CA-C	-5.19	103.68	110.53
2	B	13	ARG	N-CA-C	5.17	120.22	113.30
1	A	255	GLN	OE1-CD-NE2	-5.16	117.44	122.60
1	A	243	LYS	CA-C-N	5.15	129.31	120.71
1	A	243	LYS	C-N-CA	5.15	129.31	120.71
2	D	50	ASP	O-C-N	5.15	128.60	122.27
1	C	52	HIS	CA-CB-CG	-5.14	108.66	113.80
1	A	130	ARG	NE-CZ-NH1	-5.14	116.36	121.50
1	C	135	GLU	CG-CD-OE1	-5.14	106.59	118.40
1	C	208	ASN	CA-C-O	-5.14	113.40	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	PHE	CB-CA-C	5.13	118.18	109.50
1	C	7	VAL	N-CA-C	5.13	115.66	108.89
1	A	221	GLU	O-C-N	5.13	129.62	123.16
1	A	162	ASN	OD1-CG-ND2	5.13	127.73	122.60
1	A	198	PHE	CA-C-O	5.13	126.52	120.98
1	A	225	SER	O-C-N	5.12	129.71	123.10
1	A	16	TYR	N-CA-CB	-5.12	101.83	110.49
2	B	10	PHE	O-C-N	5.12	128.37	122.17
1	C	34	ASP	N-CA-C	5.12	119.24	113.15
2	D	62	ASN	CB-CA-C	5.11	118.11	110.08
1	C	227	SER	CA-CB-OG	5.11	121.32	111.10
1	A	216	ASN	CA-C-N	5.10	130.64	121.66
1	A	216	ASN	C-N-CA	5.10	130.64	121.66
1	A	44	PRO	O-C-N	-5.09	116.68	122.18
1	A	197	VAL	O-C-N	5.09	128.70	123.20
1	C	34	ASP	N-CA-CB	-5.09	102.63	110.46
2	D	63	ASN	CA-C-N	5.09	127.05	120.44
2	D	63	ASN	C-N-CA	5.09	127.05	120.44
1	A	247	ILE	N-CA-C	-5.08	105.46	111.00
2	B	84	GLY	CA-C-N	-5.08	116.24	122.84
2	B	84	GLY	C-N-CA	-5.08	116.24	122.84
1	A	170	ALA	O-C-N	5.08	127.30	122.07
1	C	285	ILE	N-CA-CB	5.07	118.39	112.35
1	A	149	LYS	CA-C-O	-5.06	115.35	121.32
1	C	73	PHE	CA-C-N	5.06	128.41	120.82
1	C	73	PHE	C-N-CA	5.06	128.41	120.82
2	B	59	TRP	CB-CA-C	5.06	119.16	110.81
1	C	76	GLU	O-C-N	5.05	128.29	122.17
1	C	63	THR	CA-C-O	-5.05	115.50	121.66
1	A	250	GLU	N-CA-CB	-5.04	102.15	109.82
2	B	81	ALA	CA-C-O	5.04	128.17	122.37
1	A	98	GLU	CB-CG-CD	5.04	121.17	112.60
2	B	31	ASN	O-C-N	5.04	129.13	122.93
1	C	105	GLY	O-C-N	5.04	127.03	122.19
1	A	53	ILE	CA-CB-CG1	5.03	118.95	110.40
1	A	261	ASP	CA-CB-CG	-5.03	107.57	112.60
2	B	13	ARG	CA-C-O	-5.03	113.34	119.32
1	A	122	PRO	CA-C-N	5.02	128.60	121.42
1	A	122	PRO	C-N-CA	5.02	128.60	121.42
1	A	268	LYS	CG-CD-CE	5.02	122.85	111.30
1	C	18	ASP	CA-CB-CG	-5.01	107.59	112.60
2	D	-4	GLU	N-CA-C	-5.01	106.75	114.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	48	ARG	CB-CA-C	-5.01	102.48	110.79
1	C	285	ILE	O-C-N	5.00	127.56	122.71

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	127	ARG	Sidechain
1	A	143	ARG	Sidechain
1	A	166	ARG	Sidechain
1	A	31	ARG	Sidechain
1	C	155	ARG	Sidechain
1	C	166	ARG	Sidechain
1	C	31	ARG	Sidechain

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	2371	0	2252	118	1
1	C	2371	0	2252	145	5
2	B	847	0	851	73	1
2	D	847	0	851	111	0
3	A	2	0	0	1	0
3	C	2	0	0	1	0
4	A	43	0	30	0	0
4	B	43	0	30	14	0
4	C	43	0	30	4	0
4	D	43	0	30	19	0
5	A	203	0	0	12	4
5	B	46	0	0	5	0
5	C	212	0	0	23	1
5	D	42	0	0	11	0
All	All	7115	0	6326	452	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 35.

All (452) 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)
2:B:14:CYS:SG	4:B:104:HEM:CAB	2.29	1.20
1:C:74:LYS:HE3	1:C:78:ASN:HD21	1.14	1.13
2:B:17:CYS:SG	4:B:104:HEM:CAC	2.39	1.10
2:B:8:THR:HA	2:B:11:LYS:HD2	1.34	1.08
2:D:17:CYS:SG	4:D:104:HEM:CAC	2.43	1.06
1:C:2:THR:HG22	1:C:3:PRO:HD3	1.37	1.04
2:B:8:THR:HA	2:B:11:LYS:CD	1.91	1.00
2:B:87:LYS:HB2	2:B:90:ASP:OD2	1.61	0.99
2:D:17:CYS:HG	4:D:104:HEM:CAC	1.75	0.97
2:D:3:ALA:HB2	2:D:96:THR:HG22	1.47	0.96
1:C:63:THR:HG22	1:C:143:ARG:HH12	1.29	0.96
1:A:20:GLN:HE22	1:A:287:LYS:H	1.15	0.95
1:C:74:LYS:HE3	1:C:78:ASN:ND2	1.82	0.93
2:B:17:CYS:HG	4:B:104:HEM:CAC	1.75	0.93
1:C:213:LEU:HD11	1:C:221:GLU:HG2	1.48	0.92
1:C:63:THR:HG22	1:C:143:ARG:NH1	1.84	0.92
2:D:91:ARG:HG3	2:D:91:ARG:HH11	1.35	0.91
2:B:14:CYS:SG	4:B:104:HEM:CBB	2.59	0.91
1:C:278:LYS:HD3	1:C:278:LYS:H	1.34	0.90
2:D:14:CYS:SG	4:D:104:HEM:CBB	2.60	0.90
1:C:84:GLY:H	1:C:86:GLN:HE22	1.14	0.90
2:D:14:CYS:SG	4:D:104:HEM:C3B	2.66	0.89
2:D:98:LEU:O	2:D:102:CYS:HB2	1.73	0.88
1:C:74:LYS:HG3	1:C:78:ASN:HD22	1.37	0.87
1:C:10:VAL:HG22	1:C:128:CYS:SG	2.15	0.86
1:C:2:THR:CG2	1:C:3:PRO:HD3	2.07	0.85
2:D:14:CYS:SG	4:D:104:HEM:CAB	2.65	0.85
1:C:213:LEU:CD1	1:C:221:GLU:HG2	2.07	0.84
2:B:22:LYS:HD2	2:B:33:HIS:CD2	2.12	0.84
2:B:17:CYS:SG	4:B:104:HEM:C3C	2.71	0.83
1:A:146:ASP:HB2	5:A:439:HOH:O	1.77	0.83
1:A:2:THR:HG23	1:A:3:PRO:HD2	1.59	0.83
1:C:31:ARG:HD3	5:C:628:HOH:O	1.79	0.82
2:D:14:CYS:HB2	4:D:104:HEM:CBB	2.11	0.81
1:C:93:GLU:HB2	1:C:94:PRO:HD3	1.63	0.81
1:C:128:CYS:SG	5:C:848:HOH:O	2.38	0.81
2:D:100:LYS:HD3	2:D:101:ALA:N	1.95	0.80
1:A:147:ALA:O	1:A:233:PRO:HB2	1.82	0.80
2:D:17:CYS:SG	4:D:104:HEM:C3C	2.73	0.79
1:C:63:THR:HG21	1:C:143:ARG:HH22	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:73:LYS:HD2	5:D:774:HOH:O	1.81	0.79
1:A:31:ARG:HG3	5:A:384:HOH:O	1.82	0.79
1:C:52:HIS:NE2	3:C:300:SO4:O1	2.18	0.77
2:B:80:MET:HB2	4:B:104:HEM:C1D	2.20	0.77
1:A:200:ASN:H	1:A:200:ASN:HD22	1.33	0.77
1:A:69:GLY:O	1:A:72:ARG:HD3	1.86	0.75
1:C:3:PRO:HB2	5:C:732:HOH:O	1.86	0.75
1:C:133:THR:HG22	1:C:137:THR:OG1	1.86	0.75
1:A:17:GLU:CD	1:A:17:GLU:H	1.93	0.75
1:C:133:THR:CG2	1:C:137:THR:OG1	2.35	0.75
1:C:216:ASN:HD22	1:C:222:GLN:HE21	1.32	0.74
2:D:7:ALA:O	2:D:11:LYS:HD3	1.87	0.74
2:B:55:LYS:HD3	2:B:57:VAL:HG13	1.68	0.74
1:A:166:ARG:HH22	1:A:250:GLU:CD	1.96	0.73
1:C:84:GLY:N	1:C:86:GLN:HE22	1.83	0.73
2:B:8:THR:HG22	2:B:11:LYS:HE3	1.69	0.72
2:D:60:ASP:N	2:D:63:ASN:HD21	1.88	0.72
2:B:17:CYS:SG	4:B:104:HEM:CBC	2.78	0.71
2:B:43:ALA:HB3	2:B:48:TYR:OH	1.91	0.71
2:D:38:ARG:HH11	2:D:38:ARG:HG3	1.55	0.71
2:B:14:CYS:SG	4:B:104:HEM:HAB	2.29	0.70
1:A:119:MET:O	1:A:120:GLN:HB2	1.91	0.70
1:C:14:ARG:HG3	1:C:14:ARG:HH11	1.55	0.70
2:B:87:LYS:O	2:B:90:ASP:HB2	1.92	0.69
1:C:74:LYS:CE	1:C:78:ASN:HD21	1.99	0.69
1:C:292:GLN:C	1:C:294:LEU:H	1.99	0.69
2:D:14:CYS:CB	4:D:104:HEM:CBB	2.69	0.69
2:D:36:PHE:CD2	2:D:99:LYS:HB3	2.27	0.69
2:D:39:HIS:HB3	2:D:56:ASN:ND2	2.06	0.69
2:B:73:LYS:HD3	5:B:446:HOH:O	1.91	0.69
1:C:200:ASN:HB3	1:C:255:GLN:HG3	1.73	0.69
2:D:38:ARG:HD3	2:D:42:GLN:HB2	1.73	0.69
1:C:200:ASN:HD22	1:C:200:ASN:H	1.41	0.68
2:D:80:MET:HE1	4:D:104:HEM:NB	2.07	0.68
2:D:17:CYS:SG	4:D:104:HEM:CBC	2.81	0.68
2:D:57:VAL:HG12	2:D:63:ASN:OD1	1.93	0.68
2:B:17:CYS:HG	4:B:104:HEM:CBC	2.06	0.68
1:C:63:THR:HG21	1:C:143:ARG:NH2	2.08	0.68
2:D:41:GLY:HA2	2:D:48:TYR:CE1	2.29	0.68
2:B:22:LYS:NZ	2:B:33:HIS:HD2	1.92	0.67
1:C:93:GLU:HB2	1:C:94:PRO:CD	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:94:LEU:O	2:D:97:TYR:HB3	1.95	0.67
1:A:16:TYR:O	1:A:19:PHE:N	2.28	0.67
1:C:74:LYS:HG3	1:C:78:ASN:ND2	2.10	0.67
2:D:74:TYR:HB2	5:D:744:HOH:O	1.94	0.67
1:A:23:TYR:CD1	1:A:23:TYR:C	2.73	0.66
1:C:133:THR:HG23	1:C:137:THR:HG21	1.78	0.66
4:C:296:HEM:HMC2	4:C:296:HEM:HBC2	1.75	0.66
1:C:216:ASN:HD22	1:C:222:GLN:NE2	1.93	0.66
1:C:29:LYS:O	1:C:29:LYS:HG3	1.95	0.65
1:C:80:PRO:O	5:C:664:HOH:O	2.15	0.65
1:C:278:LYS:HD3	1:C:278:LYS:N	2.10	0.65
1:C:145:PRO:HD3	1:C:157:PHE:CZ	2.32	0.65
1:C:264:LYS:HB3	5:C:802:HOH:O	1.96	0.65
1:C:267:GLU:OE2	1:C:271:GLU:OE2	2.15	0.64
1:C:278:LYS:H	1:C:278:LYS:CD	1.96	0.64
1:A:245:LEU:O	1:A:245:LEU:HD22	1.97	0.64
1:C:7:VAL:HG22	5:C:623:HOH:O	1.97	0.63
1:C:59:LYS:NZ	5:C:757:HOH:O	2.31	0.63
2:B:8:THR:CG2	2:B:11:LYS:HE3	2.28	0.63
2:D:67:TYR:HA	5:D:744:HOH:O	1.99	0.63
2:B:1:GLY:O	2:B:96:THR:HG21	1.98	0.63
1:A:125:PRO:HG3	1:A:285:ILE:HD11	1.79	0.63
2:D:60:ASP:H	2:D:63:ASN:HD21	1.46	0.63
1:A:4:LEU:HD12	1:A:62:ASN:O	1.99	0.62
1:A:267:GLU:OE2	1:A:271:GLU:OE2	2.16	0.62
1:A:287:LYS:HA	1:A:291:GLU:OE1	1.99	0.62
1:A:127:ARG:HG2	1:A:283:PRO:HA	1.82	0.62
1:A:288:THR:OG1	1:A:291:GLU:HG3	2.00	0.62
1:A:166:ARG:NH2	1:A:250:GLU:CD	2.57	0.62
1:C:200:ASN:HD22	1:C:200:ASN:N	1.95	0.62
1:A:2:THR:HG23	1:A:3:PRO:CD	2.30	0.62
1:A:292:GLN:O	1:A:294:LEU:HD12	2.00	0.61
2:D:53:ILE:HG13	5:D:782:HOH:O	2.00	0.61
1:C:29:LYS:HG2	1:C:91:PHE:CE2	2.36	0.61
1:C:287:LYS:HA	1:C:291:GLU:OE1	2.01	0.61
2:D:11:LYS:HD2	2:D:11:LYS:N	2.16	0.61
2:D:14:CYS:HG	4:D:104:HEM:CAB	2.11	0.61
2:D:19:THR:HA	5:D:641:HOH:O	2.00	0.61
1:A:186:GLY:O	1:A:216:ASN:ND2	2.34	0.60
2:B:22:LYS:C	2:B:24:GLY:H	2.09	0.60
1:C:20:GLN:HE22	1:C:287:LYS:H	1.50	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:TYR:O	1:C:46:LEU:HG	2.01	0.60
1:C:286:PHE:C	1:C:287:LYS:HE2	2.26	0.60
1:C:166:ARG:HH22	1:C:250:GLU:CD	2.09	0.60
2:B:91:ARG:O	2:B:95:ILE:HG12	2.00	0.60
2:D:17:CYS:HG	4:D:104:HEM:CBC	2.14	0.60
2:D:36:PHE:CE1	2:D:64:MET:HE3	2.37	0.60
1:A:76:GLU:HB2	1:A:138:THR:CG2	2.30	0.60
2:B:6:GLY:HA3	2:B:93:ASP:O	2.01	0.60
2:D:91:ARG:HB3	5:D:779:HOH:O	2.00	0.60
2:D:9:LEU:O	2:D:13:ARG:HB2	2.01	0.59
1:A:86:GLN:O	1:A:90:LYS:HG2	2.02	0.59
2:B:8:THR:CB	2:B:11:LYS:HE3	2.31	0.59
1:C:71:TYR:O	1:C:77:PHE:HB2	2.01	0.59
2:D:51:ALA:HB1	2:D:75:ILE:CG2	2.32	0.59
1:A:113:VAL:O	1:A:117:GLN:HG3	2.02	0.59
2:B:44:GLU:HA	5:B:444:HOH:O	2.01	0.59
2:D:64:MET:HG2	2:D:95:ILE:CD1	2.33	0.59
2:D:54:LYS:HA	2:D:54:LYS:HE3	1.83	0.59
1:C:123:LYS:HE2	1:C:287:LYS:NZ	2.18	0.58
4:D:104:HEM:HMB2	4:D:104:HEM:HBB2	1.83	0.58
1:C:133:THR:HG23	1:C:137:THR:CG2	2.33	0.58
2:D:34:GLY:HA2	2:D:102:CYS:O	2.03	0.58
1:A:267:GLU:O	1:A:271:GLU:HG3	2.04	0.58
2:D:46:TYR:C	2:D:46:TYR:CD1	2.80	0.58
2:B:58:LEU:O	2:B:63:ASN:ND2	2.31	0.58
1:C:38:ASN:N	1:C:38:ASN:HD22	2.01	0.58
2:B:37:GLY:O	2:B:58:LEU:HD11	2.04	0.58
1:C:12:LYS:HE3	5:C:696:HOH:O	2.02	0.58
1:A:123:LYS:HE2	5:A:542:HOH:O	2.03	0.58
1:C:183:LYS:HD3	1:C:183:LYS:N	2.19	0.58
2:D:14:CYS:SG	4:D:104:HEM:HBB2	2.43	0.58
1:A:29:LYS:O	1:A:29:LYS:HG2	2.04	0.58
2:D:41:GLY:HA2	2:D:48:TYR:CZ	2.39	0.58
2:D:60:ASP:O	2:D:62:ASN:N	2.37	0.58
1:C:183:LYS:HB2	5:C:716:HOH:O	2.03	0.57
1:C:190:PRO:O	1:C:190:PRO:HG2	2.03	0.57
1:A:156:THR:HG22	5:A:513:HOH:O	2.02	0.57
2:D:38:ARG:HH11	2:D:38:ARG:CG	2.17	0.57
1:A:103:SER:OG	1:A:106:ASP:HB2	2.05	0.57
2:B:87:LYS:CB	2:B:90:ASP:OD2	2.46	0.57
1:C:10:VAL:O	1:C:12:LYS:HE3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:THR:CG2	1:C:143:ARG:HH22	2.16	0.57
1:C:26:ILE:HG22	1:C:114:THR:HG21	1.86	0.57
1:A:52:HIS:NE2	3:A:299:SO4:O1	2.38	0.57
2:B:8:THR:O	2:B:11:LYS:HD3	2.05	0.57
2:B:16:GLN:OE1	2:B:16:GLN:N	2.35	0.57
2:D:5:LYS:HA	2:D:8:THR:HG23	1.87	0.57
2:B:5:LYS:O	2:B:6:GLY:C	2.48	0.56
2:B:8:THR:HB	2:B:11:LYS:HE3	1.88	0.56
2:D:69:THR:O	2:D:86:LYS:HE2	2.05	0.56
2:B:22:LYS:HZ3	2:B:33:HIS:HD2	1.51	0.56
1:C:29:LYS:O	1:C:29:LYS:CG	2.53	0.56
1:A:255:GLN:NE2	1:A:259:PHE:CZ	2.73	0.56
1:C:51:TRP:CD1	1:C:52:HIS:HD2	2.24	0.56
1:C:110:LEU:O	1:C:111:GLY:C	2.46	0.56
2:D:3:ALA:HB1	2:D:97:TYR:HA	1.87	0.56
1:A:79:ASP:O	1:A:82:ASN:HB2	2.06	0.55
1:A:42:TYR:O	1:A:46:LEU:HG	2.05	0.55
1:A:96:HIS:CD2	1:A:107:LEU:HD22	2.41	0.55
1:C:256:ASP:O	1:C:260:LYS:HG2	2.05	0.55
2:B:5:LYS:O	2:B:7:ALA:N	2.40	0.55
2:B:89:LYS:HB3	2:B:93:ASP:OD2	2.05	0.55
4:C:296:HEM:HBC2	4:C:296:HEM:CMC	2.36	0.55
2:B:39:HIS:CD2	2:B:56:ASN:OD1	2.60	0.55
1:C:140:ASP:HB3	5:C:731:HOH:O	2.07	0.55
1:A:251:TYR:OH	1:A:261:ASP:OD2	2.20	0.55
1:C:7:VAL:O	1:C:7:VAL:HG23	2.06	0.55
2:B:82:PHE:CE2	2:B:84:GLY:HA2	2.42	0.54
1:C:226:LYS:HE2	5:C:702:HOH:O	2.07	0.54
2:D:83:GLY:HA3	5:D:640:HOH:O	2.06	0.54
1:A:75:LYS:HE3	1:A:140:ASP:HA	1.89	0.54
2:B:55:LYS:HD3	2:B:57:VAL:CG1	2.36	0.54
1:A:155:ARG:NH1	1:A:241:ASP:OD2	2.33	0.54
1:C:49:LEU:HB2	1:C:85:LEU:HD22	1.90	0.54
1:C:136:ASP:HB3	5:C:749:HOH:O	2.07	0.54
2:D:60:ASP:H	2:D:63:ASN:ND2	2.04	0.54
1:A:166:ARG:NH2	1:A:250:GLU:OE2	2.41	0.54
1:A:145:PRO:HD3	1:A:157:PHE:CZ	2.44	0.53
1:A:60:HIS:HE1	5:A:341:HOH:O	1.91	0.53
1:C:133:THR:HG22	1:C:137:THR:HG1	1.72	0.53
1:C:61:ASP:N	1:C:61:ASP:OD1	2.30	0.53
2:D:39:HIS:CE1	2:D:58:LEU:HB2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:22:LYS:HD2	2:B:33:HIS:NE2	2.23	0.53
1:C:20:GLN:HG3	1:C:20:GLN:O	2.07	0.53
1:C:133:THR:CG2	1:C:137:THR:HG21	2.39	0.53
1:A:93:GLU:N	1:A:94:PRO:CD	2.71	0.53
2:B:55:LYS:O	2:B:56:ASN:C	2.52	0.53
1:C:292:GLN:C	1:C:294:LEU:N	2.66	0.53
2:D:39:HIS:HB3	2:D:56:ASN:CG	2.33	0.53
1:C:63:THR:CG2	1:C:143:ARG:NH2	2.72	0.52
1:A:164:ASN:O	1:A:168:VAL:HG13	2.09	0.52
1:A:216:ASN:HB2	5:A:420:HOH:O	2.10	0.52
2:B:42:GLN:O	2:B:43:ALA:C	2.50	0.52
2:D:2:SER:O	2:D:93:ASP:HB3	2.10	0.52
1:A:115:ALA:O	1:A:119:MET:HG3	2.09	0.52
2:B:7:ALA:HB2	2:B:97:TYR:CD2	2.44	0.52
2:B:8:THR:CA	2:B:11:LYS:CD	2.77	0.52
1:A:2:THR:CG2	1:A:3:PRO:HD2	2.36	0.52
2:D:7:ALA:HB2	2:D:97:TYR:CD1	2.44	0.52
1:A:86:GLN:OE1	1:A:86:GLN:N	2.34	0.52
1:C:183:LYS:H	1:C:183:LYS:CE	2.23	0.52
2:D:70:ASN:ND2	5:D:774:HOH:O	2.42	0.52
1:C:15:SER:O	1:C:18:ASP:HB2	2.10	0.51
1:A:161:LEU:O	1:A:162:ASN:HB3	2.10	0.51
1:A:188:GLU:H	1:A:222:GLN:HE22	1.58	0.51
1:C:281:PRO:HG2	5:C:848:HOH:O	2.09	0.51
1:A:141:ASN:N	1:A:141:ASN:HD22	2.07	0.51
1:A:200:ASN:H	1:A:200:ASN:ND2	2.05	0.51
1:A:30:LEU:HD12	1:A:42:TYR:HB2	1.92	0.51
1:A:81:SER:HB3	5:A:367:HOH:O	2.11	0.51
1:C:183:LYS:H	1:C:183:LYS:CD	2.23	0.51
2:B:18:HIS:CE1	2:B:30:PRO:HD2	2.45	0.51
2:D:10:PHE:O	2:D:14:CYS:HB3	2.11	0.51
2:B:8:THR:HA	2:B:11:LYS:HD3	1.87	0.51
2:D:19:THR:OG1	2:D:31:ASN:HB2	2.11	0.51
2:D:38:ARG:HD2	2:D:39:HIS:N	2.27	0.50
1:A:52:HIS:ND1	1:A:82:ASN:OD1	2.31	0.50
2:B:23:GLY:O	2:B:24:GLY:C	2.55	0.50
1:C:133:THR:CG2	1:C:137:THR:CB	2.89	0.50
2:D:60:ASP:C	2:D:60:ASP:OD1	2.54	0.50
1:A:23:TYR:C	1:A:23:TYR:HD1	2.18	0.50
2:D:49:THR:HG21	2:D:77:GLY:O	2.12	0.50
1:A:149:LYS:HD2	1:A:153:TYR:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:TRP:C	1:A:127:ARG:HG3	2.37	0.50
1:A:206:LEU:HD13	1:A:231:MET:SD	2.51	0.50
1:C:292:GLN:O	1:C:294:LEU:N	2.44	0.50
2:D:56:ASN:O	2:D:57:VAL:C	2.55	0.50
2:D:60:ASP:C	2:D:62:ASN:H	2.19	0.50
2:B:-2:LYS:O	2:B:-1:ALA:HB2	2.12	0.49
2:B:23:GLY:O	2:B:24:GLY:O	2.30	0.49
1:C:63:THR:HG22	1:C:143:ARG:CZ	2.42	0.49
2:B:15:LEU:O	2:B:16:GLN:C	2.54	0.49
2:D:55:LYS:HG3	2:D:57:VAL:HG22	1.95	0.49
1:A:180:THR:N	1:A:189:GLY:O	2.29	0.49
1:C:21:LYS:HB2	1:C:99:PHE:CE2	2.47	0.49
2:B:45:GLY:N	5:B:444:HOH:O	2.44	0.49
2:D:91:ARG:HG3	2:D:91:ARG:NH1	2.09	0.49
1:A:86:GLN:H	1:A:86:GLN:CD	2.18	0.49
1:A:177:LEU:HD11	1:A:198:PHE:HD2	1.78	0.49
2:D:35:ILE:HG22	2:D:102:CYS:SG	2.53	0.49
1:A:60:HIS:CE1	5:A:341:HOH:O	2.65	0.49
1:A:183:LYS:HG2	5:A:375:HOH:O	2.12	0.49
1:C:45:VAL:HG22	1:C:45:VAL:O	2.12	0.48
1:A:38:ASN:O	1:A:39:TYR:HB2	2.13	0.48
1:A:166:ARG:HH12	1:A:257:LYS:HE2	1.78	0.48
1:A:204:LEU:HD21	1:A:252:ALA:O	2.12	0.48
1:C:162:ASN:CG	5:C:723:HOH:O	2.56	0.48
2:D:93:ASP:O	2:D:94:LEU:C	2.56	0.48
1:A:250:GLU:O	1:A:253:ASN:HB2	2.13	0.48
2:B:3:ALA:HB2	2:B:96:THR:HG22	1.95	0.48
2:D:11:LYS:NZ	5:D:621:HOH:O	2.46	0.48
2:B:18:HIS:HE1	2:B:30:PRO:HD2	1.78	0.48
2:D:42:GLN:C	2:D:43:ALA:O	2.56	0.48
2:B:14:CYS:SG	4:B:104:HEM:C3B	3.02	0.48
4:B:104:HEM:HBC2	4:B:104:HEM:HMC2	1.95	0.48
1:C:183:LYS:N	1:C:183:LYS:CD	2.77	0.48
1:C:190:PRO:O	1:C:190:PRO:CG	2.60	0.48
2:D:48:TYR:CE1	4:D:104:HEM:O2A	2.66	0.48
1:A:52:HIS:HE1	1:A:81:SER:O	1.97	0.47
1:A:265:ALA:O	1:A:266:PHE:C	2.56	0.47
1:A:156:THR:CG2	5:A:513:HOH:O	2.60	0.47
1:C:8:ALA:HB2	1:C:274:ILE:HG22	1.96	0.47
2:D:63:ASN:HD22	2:D:63:ASN:H	1.61	0.47
2:D:86:LYS:HA	2:D:86:LYS:HD3	1.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:46:TYR:C	2:D:46:TYR:HD1	2.21	0.47
1:C:38:ASN:N	1:C:38:ASN:ND2	2.63	0.47
2:D:34:GLY:N	2:D:102:CYS:O	2.46	0.47
1:C:8:ALA:HB3	1:C:276:PHE:HA	1.97	0.47
1:C:287:LYS:HA	1:C:287:LYS:NZ	2.30	0.47
1:C:72:ARG:NH2	1:C:133:THR:O	2.47	0.47
1:C:245:LEU:O	1:C:249:LYS:HG3	2.14	0.47
2:D:96:THR:O	2:D:97:TYR:C	2.57	0.47
2:B:57:VAL:HA	5:B:474:HOH:O	2.13	0.47
2:B:98:LEU:O	2:B:99:LYS:C	2.57	0.47
1:C:155:ARG:HB2	1:C:244:TYR:OH	2.13	0.47
1:A:134:PRO:C	1:A:136:ASP:N	2.73	0.47
1:C:6:HIS:CD2	5:C:627:HOH:O	2.68	0.47
1:C:208:ASN:ND2	5:C:819:HOH:O	2.47	0.46
2:B:77:GLY:O	2:B:78:THR:C	2.58	0.46
2:D:39:HIS:O	2:D:40:SER:C	2.58	0.46
2:D:11:LYS:N	2:D:11:LYS:CD	2.77	0.46
2:D:34:GLY:CA	2:D:102:CYS:O	2.64	0.46
2:D:67:TYR:CD2	2:D:68:LEU:HD23	2.50	0.46
2:D:64:MET:O	2:D:68:LEU:HG	2.15	0.46
1:A:174:ALA:C	1:A:176:ALA:H	2.24	0.46
1:C:89:PHE:CD1	1:C:89:PHE:C	2.93	0.46
1:C:133:THR:CG2	1:C:137:THR:CG2	2.94	0.46
2:D:-3:PHE:HB3	2:D:62:ASN:OD1	2.15	0.46
2:D:21:GLU:H	2:D:21:GLU:CD	2.23	0.46
2:D:52:ASN:OD1	2:D:52:ASN:O	2.33	0.46
1:C:127:ARG:HA	5:C:674:HOH:O	2.16	0.46
2:B:55:LYS:O	2:B:56:ASN:O	2.34	0.46
1:C:93:GLU:N	1:C:94:PRO:HD2	2.31	0.46
2:D:60:ASP:C	2:D:62:ASN:N	2.74	0.46
1:C:26:ILE:CG2	1:C:114:THR:HG21	2.46	0.46
1:C:183:LYS:HD3	1:C:183:LYS:H	1.80	0.46
2:D:5:LYS:O	2:D:9:LEU:HB2	2.17	0.46
1:A:4:LEU:CD1	1:A:62:ASN:O	2.63	0.45
2:B:86:LYS:N	5:B:507:HOH:O	2.50	0.45
2:B:97:TYR:CD1	2:B:97:TYR:C	2.94	0.45
2:D:42:GLN:O	2:D:43:ALA:C	2.59	0.45
1:A:141:ASN:N	1:A:141:ASN:ND2	2.65	0.45
2:B:18:HIS:CD2	4:B:104:HEM:NB	2.85	0.45
1:C:226:LYS:HD3	1:C:226:LYS:HA	1.65	0.45
1:A:130:ARG:NH1	1:A:130:ARG:HG3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:GLY:HA2	5:C:778:HOH:O	2.16	0.45
1:C:247:ILE:O	1:C:248:VAL:C	2.58	0.45
1:A:29:LYS:HD3	1:A:91:PHE:CE2	2.52	0.45
1:A:119:MET:O	1:A:120:GLN:CB	2.61	0.45
1:A:232:LEU:O	1:A:235:ASP:N	2.47	0.45
2:D:93:ASP:N	2:D:93:ASP:OD1	2.44	0.45
1:A:7:VAL:HA	1:A:275:THR:O	2.17	0.45
2:D:5:LYS:C	2:D:7:ALA:H	2.24	0.45
1:A:211:TRP:CZ3	1:A:225:SER:HB3	2.52	0.45
1:A:294:LEU:HD11	1:C:294:LEU:CD1	2.47	0.45
1:A:137:THR:O	1:A:139:PRO:HD3	2.17	0.44
1:C:164:ASN:C	1:C:164:ASN:OD1	2.60	0.44
2:D:14:CYS:HB2	4:D:104:HEM:HBB1	1.96	0.44
1:C:135:GLU:HG3	5:C:749:HOH:O	2.17	0.44
1:A:256:ASP:O	1:A:260:LYS:HD3	2.17	0.44
1:C:282:SER:O	1:C:283:PRO:C	2.59	0.44
1:A:172:MET:HE2	1:A:172:MET:HB2	1.61	0.44
2:B:89:LYS:C	2:B:93:ASP:OD2	2.60	0.44
2:D:6:GLY:CA	2:D:94:LEU:HA	2.48	0.44
1:C:26:ILE:HA	1:C:95:ILE:HD13	1.99	0.44
1:A:155:ARG:HH11	1:A:155:ARG:HD2	1.33	0.44
1:C:264:LYS:HB2	1:C:264:LYS:HE3	1.45	0.44
2:D:100:LYS:HD3	2:D:101:ALA:CA	2.47	0.44
2:B:15:LEU:HD12	2:B:15:LEU:HA	1.82	0.44
1:C:200:ASN:H	1:C:200:ASN:ND2	2.11	0.44
2:D:70:ASN:OD1	2:D:70:ASN:C	2.61	0.44
2:B:40:SER:HA	2:B:59:TRP:HE1	1.83	0.44
1:C:30:LEU:HD23	1:C:42:TYR:HB2	1.99	0.44
1:C:84:GLY:CA	1:C:86:GLN:NE2	2.80	0.44
2:D:13:ARG:NH1	2:D:82:PHE:CE1	2.85	0.44
2:D:19:THR:O	2:D:31:ASN:HA	2.18	0.44
2:D:60:ASP:O	2:D:63:ASN:ND2	2.51	0.44
2:D:100:LYS:CD	2:D:100:LYS:C	2.90	0.43
1:A:93:GLU:N	1:A:94:PRO:HD2	2.32	0.43
1:A:155:ARG:HH22	1:A:241:ASP:CG	2.26	0.43
2:B:43:ALA:CB	2:B:48:TYR:OH	2.62	0.43
2:D:5:LYS:C	2:D:7:ALA:N	2.76	0.43
1:A:15:SER:O	1:A:16:TYR:C	2.61	0.43
1:A:123:LYS:C	1:A:124:ILE:HG13	2.42	0.43
1:C:206:LEU:HD12	1:C:206:LEU:HA	1.88	0.43
2:D:36:PHE:CE1	2:D:64:MET:CE	3.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LEU:HD12	1:A:294:LEU:N	2.34	0.43
1:C:76:GLU:HB2	1:C:138:THR:CG2	2.48	0.43
1:C:133:THR:HA	1:C:134:PRO:HD3	1.81	0.43
1:A:28:LEU:O	1:A:31:ARG:HB3	2.17	0.43
1:A:66:SER:O	1:A:67:TYR:C	2.61	0.43
1:A:116:VAL:HG11	1:A:124:ILE:HD12	2.00	0.43
1:A:214:GLU:O	1:A:221:GLU:HA	2.19	0.43
2:B:79:LYS:HE3	4:B:104:HEM:HMD1	2.01	0.43
2:D:26:HIS:C	2:D:27:LYS:HG3	2.43	0.43
1:C:74:LYS:CE	1:C:78:ASN:ND2	2.68	0.43
1:A:215:LYS:CB	1:A:215:LYS:NZ	2.82	0.43
1:A:215:LYS:HA	1:A:220:ASN:O	2.18	0.43
1:C:8:ALA:HB2	1:C:274:ILE:CG2	2.49	0.43
1:C:14:ARG:HG2	1:C:101:TRP:CZ3	2.53	0.43
1:C:38:ASN:HD22	1:C:38:ASN:H	1.67	0.43
1:C:199:THR:HG23	5:C:652:HOH:O	2.18	0.43
4:C:296:HEM:HMB1	4:C:296:HEM:HBB2	2.00	0.43
2:D:-2:LYS:O	2:D:-1:ALA:C	2.62	0.43
1:A:214:GLU:N	1:A:222:GLN:O	2.50	0.42
1:C:15:SER:HB2	5:C:738:HOH:O	2.19	0.42
1:C:127:ARG:HH11	1:C:127:ARG:HD2	1.68	0.42
1:C:165:ASP:O	1:C:169:VAL:HG23	2.19	0.42
1:C:180:THR:HG21	1:C:230:MET:HE1	2.00	0.42
1:A:181:HIS:HB2	1:A:184:ASN:HB2	2.01	0.42
2:B:35:ILE:HG23	2:B:36:PHE:N	2.34	0.42
1:C:66:SER:O	1:C:67:TYR:C	2.60	0.42
2:D:48:TYR:HE1	4:D:104:HEM:O2A	2.02	0.42
1:C:6:HIS:HD2	5:C:627:HOH:O	2.02	0.42
1:C:256:ASP:O	1:C:257:LYS:C	2.62	0.42
1:A:17:GLU:CD	1:A:17:GLU:N	2.72	0.42
4:B:104:HEM:HBC2	4:B:104:HEM:CMC	2.49	0.42
1:C:172:MET:HB2	1:C:172:MET:HE2	1.85	0.42
2:D:67:TYR:CA	5:D:744:HOH:O	2.65	0.42
1:A:133:THR:HA	1:A:134:PRO:HD3	1.90	0.42
1:A:35:GLU:HG3	5:A:552:HOH:O	2.20	0.42
1:A:190:PRO:HG2	1:A:190:PRO:O	2.20	0.42
1:C:22:VAL:O	1:C:23:TYR:C	2.63	0.42
2:D:38:ARG:CD	2:D:42:GLN:HB2	2.44	0.42
2:B:10:PHE:CD1	2:B:10:PHE:C	2.98	0.42
1:C:262:PHE:CD1	1:C:262:PHE:C	2.97	0.42
5:C:838:HOH:O	2:D:13:ARG:CD	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:39:HIS:ND1	2:D:58:LEU:HB2	2.35	0.42
1:A:200:ASN:ND2	1:A:200:ASN:N	2.67	0.42
2:D:67:TYR:HB2	2:D:74:TYR:CD2	2.55	0.42
1:A:53:ILE:HG22	1:A:71:TYR:HB2	2.01	0.41
2:B:89:LYS:O	2:B:93:ASP:OD2	2.37	0.41
1:C:57:TRP:HE1	1:C:62:ASN:HD22	1.68	0.41
1:C:75:LYS:HE2	1:C:140:ASP:HA	2.02	0.41
1:A:56:THR:O	1:A:143:ARG:HD2	2.21	0.41
1:C:243:LYS:HZ2	1:C:243:LYS:HG2	1.77	0.41
4:C:296:HEM:HBB2	4:C:296:HEM:CMB	2.50	0.41
2:D:79:LYS:HG2	4:D:104:HEM:HBD2	2.01	0.41
2:D:90:ASP:O	2:D:91:ARG:C	2.60	0.41
2:B:60:ASP:O	2:B:62:ASN:N	2.54	0.41
1:A:91:PHE:CD1	1:A:91:PHE:C	2.99	0.41
1:C:24:ASN:O	1:C:25:ALA:C	2.59	0.41
1:C:149:LYS:HA	1:C:149:LYS:HD2	1.78	0.41
1:A:212:LYS:O	1:A:223:TRP:HA	2.21	0.41
1:A:249:LYS:O	1:A:250:GLU:C	2.62	0.41
1:A:7:VAL:HG13	1:A:277:PRO:HD3	2.03	0.41
1:A:61:ASP:CG	1:A:63:THR:HG23	2.46	0.41
2:B:5:LYS:O	2:B:8:THR:N	2.53	0.41
1:A:79:ASP:OD1	1:A:80:PRO:HD2	2.20	0.41
1:A:230:MET:HE2	1:A:230:MET:HB2	1.87	0.41
1:C:74:LYS:O	1:C:78:ASN:N	2.50	0.41
1:C:133:THR:CG2	1:C:137:THR:HG1	2.26	0.41
1:C:162:ASN:HD22	1:C:162:ASN:HA	1.65	0.41
2:D:26:HIS:C	2:D:27:LYS:CG	2.94	0.41
1:C:214:GLU:O	1:C:221:GLU:HA	2.20	0.41
1:A:174:ALA:C	1:A:176:ALA:N	2.79	0.40
2:B:64:MET:O	2:B:67:TYR:HB3	2.21	0.40
1:C:44:PRO:O	1:C:45:VAL:C	2.62	0.40
2:D:80:MET:HE1	4:D:104:HEM:C1B	2.55	0.40
1:A:35:GLU:CG	5:A:552:HOH:O	2.70	0.40
1:A:266:PHE:O	1:A:270:LEU:HG	2.21	0.40
1:A:294:LEU:HD21	1:C:294:LEU:HD22	2.04	0.40
1:C:27:ALA:HB2	1:C:114:THR:CG2	2.52	0.40
1:C:73:PHE:CE2	1:C:135:GLU:HA	2.55	0.40
2:D:6:GLY:HA3	2:D:93:ASP:C	2.47	0.40
2:D:55:LYS:C	2:D:57:VAL:N	2.79	0.40
1:A:74:LYS:C	1:A:78:ASN:HD22	2.29	0.40
2:B:8:THR:CA	2:B:11:LYS:HD3	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:PHE:O	1:C:263:SER:C	2.60	0.40
2:D:51:ALA:HA	5:D:649:HOH:O	2.20	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:C:221:GLU:OE2	5:A:549:HOH:O[1_656]	1.11	1.09
1:C:221:GLU:CD	5:A:549:HOH:O[1_656]	1.12	1.08
1:C:221:GLU:CG	5:A:549:HOH:O[1_656]	1.91	0.29
1:A:240:GLN:NE2	5:C:635:HOH:O[1_455]	2.15	0.05
2:B:54:LYS:CE	1:C:253:ASN:ND2[2_646]	2.15	0.05
1:C:221:GLU:OE1	5:A:549:HOH:O[1_656]	2.17	0.03

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	292/296 (99%)	264 (90%)	27 (9%)	1 (0%)	36	46
1	C	292/296 (99%)	272 (93%)	19 (6%)	1 (0%)	36	46
2	B	106/108 (98%)	91 (86%)	9 (8%)	6 (6%)	1	0
2	D	106/108 (98%)	89 (84%)	13 (12%)	4 (4%)	2	1
All	All	796/808 (98%)	716 (90%)	68 (8%)	12 (2%)	8	8

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	-2	LYS
2	B	-1	ALA
2	B	56	ASN

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Mol	Chain	Res	Type
1	C	2	THR
2	D	61	GLU
2	B	6	GLY
2	B	24	GLY
2	B	61	GLU
2	D	56	ASN
1	A	67	TYR
2	D	40	SER
2	D	27	LYS

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	252/254 (99%)	216 (86%)	36 (14%)	3	3
1	C	252/254 (99%)	213 (84%)	39 (16%)	2	3
2	B	89/89 (100%)	71 (80%)	18 (20%)	1	1
2	D	89/89 (100%)	66 (74%)	23 (26%)	0	0
All	All	682/686 (99%)	566 (83%)	116 (17%)	2	2

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	THR
1	A	2	THR
1	A	4	LEU
1	A	5	VAL
1	A	12	LYS
1	A	17	GLU
1	A	32	GLU
1	A	35	GLU
1	A	47	VAL
1	A	51	TRP
1	A	72	ARG
1	A	74	LYS

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Mol	Chain	Res	Type
1	A	94	PRO
1	A	97	LYS
1	A	102	ILE
1	A	138	THR
1	A	140	ASP
1	A	168	VAL
1	A	179	LYS
1	A	182	LEU
1	A	190	PRO
1	A	195	ASN
1	A	196	ASN
1	A	197	VAL
1	A	200	ASN
1	A	210	ASP
1	A	212	LYS
1	A	215	LYS
1	A	226	LYS
1	A	233	PRO
1	A	245	LEU
1	A	260	LYS
1	A	263	SER
1	A	269	LEU
1	A	279	ASP
1	A	289	LEU
2	B	-5	THR
2	B	-4	GLU
2	B	-3	PHE
2	B	-2	LYS
2	B	2	SER
2	B	4	LYS
2	B	11	LYS
2	B	22	LYS
2	B	55	LYS
2	B	58	LEU
2	B	61	GLU
2	B	66	GLU
2	B	73	LYS
2	B	80	MET
2	B	85	LEU
2	B	88	GLU
2	B	98	LEU
2	B	99	LYS

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Mol	Chain	Res	Type
1	C	2	THR
1	C	5	VAL
1	C	12	LYS
1	C	14	ARG
1	C	20	GLN
1	C	22	VAL
1	C	32	GLU
1	C	47	VAL
1	C	63	THR
1	C	74	LYS
1	C	80	PRO
1	C	91	PHE
1	C	97	LYS
1	C	109	SER
1	C	122	PRO
1	C	133	THR
1	C	135	GLU
1	C	149	LYS
1	C	156	THR
1	C	162	ASN
1	C	168	VAL
1	C	183	LYS
1	C	188	GLU
1	C	190	PRO
1	C	196	ASN
1	C	197	VAL
1	C	199	THR
1	C	200	ASN
1	C	214	GLU
1	C	226	LYS
1	C	237	SER
1	C	245	LEU
1	C	264	LYS
1	C	269	LEU
1	C	275	THR
1	C	278	LYS
1	C	279	ASP
1	C	287	LYS
1	C	289	LEU
2	D	-5	THR
2	D	-4	GLU
2	D	5	LYS

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Mol	Chain	Res	Type
2	D	8	THR
2	D	11	LYS
2	D	21	GLU
2	D	31	ASN
2	D	38	ARG
2	D	53	ILE
2	D	54	LYS
2	D	55	LYS
2	D	57	VAL
2	D	58	LEU
2	D	60	ASP
2	D	61	GLU
2	D	63	ASN
2	D	66	GLU
2	D	72	LYS
2	D	89	LYS
2	D	91	ARG
2	D	99	LYS
2	D	100	LYS
2	D	102	CYS

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	20	GLN
1	A	24	ASN
1	A	60	HIS
1	A	78	ASN
1	A	96	HIS
1	A	120	GLN
1	A	141	ASN
1	A	159	GLN
1	A	200	ASN
1	A	208	ASN
1	A	222	GLN
1	A	255	GLN
1	A	292	GLN
2	B	33	HIS
2	B	39	HIS
1	C	20	GLN
1	C	24	ASN
1	C	38	ASN

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Mol	Chain	Res	Type
1	C	60	HIS
1	C	62	ASN
1	C	78	ASN
1	C	86	GLN
1	C	162	ASN
1	C	196	ASN
1	C	200	ASN
1	C	222	GLN
1	C	292	GLN
2	D	26	HIS
2	D	33	HIS
2	D	63	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
4	HEM	B	104	2	50,50,50	1.39	8 (16%)	67,82,82	1.24	6 (8%)
3	SO4	C	300	4	0,1,4	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	299	4	0,1,4	-	-	-	-	-
4	HEM	A	296	1,3	50,50,50	1.73	12 (24%)	67,82,82	1.31	9 (13%)
4	HEM	C	296	1,3	50,50,50	1.31	6 (12%)	67,82,82	1.28	8 (11%)
4	HEM	D	104	2	50,50,50	1.20	3 (6%)	67,82,82	1.02	4 (5%)

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
4	HEM	A	296	1,3	-	3/14/54/54	-
4	HEM	C	296	1,3	-	2/14/54/54	-
4	HEM	B	104	2	-	1/14/54/54	-
4	HEM	D	104	2	-	0/14/54/54	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	296	HEM	FE-NB	5.16	2.10	1.94
4	A	296	HEM	FE-ND	3.90	2.06	1.94
4	C	296	HEM	FE-ND	3.63	2.06	1.94
4	B	104	HEM	CAC-C3C	3.38	1.56	1.47
4	A	296	HEM	C3B-C2B	-3.35	1.30	1.37
4	D	104	HEM	CAC-C3C	3.32	1.56	1.47
4	C	296	HEM	FE-NB	3.19	2.04	1.94
4	A	296	HEM	CAB-C3B	3.14	1.55	1.47
4	B	104	HEM	CMC-C2C	3.11	1.57	1.50
4	A	296	HEM	CMA-C3A	3.08	1.57	1.50
4	B	104	HEM	FE-NC	3.03	2.05	1.95
4	A	296	HEM	CMB-C2B	2.97	1.56	1.50
4	D	104	HEM	CAB-C3B	2.89	1.55	1.47
4	A	296	HEM	C2A-C3A	-2.74	1.31	1.38
4	C	296	HEM	CMA-C3A	2.65	1.56	1.50
4	C	296	HEM	CAB-C3B	2.64	1.54	1.47
4	C	296	HEM	C3B-C2B	-2.49	1.32	1.37
4	B	104	HEM	C3C-C2C	-2.49	1.32	1.37
4	B	104	HEM	CMA-C3A	2.47	1.55	1.50
4	A	296	HEM	C3D-C2D	-2.34	1.31	1.36
4	D	104	HEM	CMD-C2D	2.31	1.55	1.50
4	C	296	HEM	CMB-C2B	2.28	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	296	HEM	C1B-NB	-2.27	1.36	1.40
4	A	296	HEM	CAA-C2A	2.25	1.57	1.51
4	B	104	HEM	CAA-C2A	2.22	1.57	1.51
4	A	296	HEM	CMD-C2D	2.13	1.55	1.50
4	A	296	HEM	C4D-ND	-2.10	1.36	1.40
4	B	104	HEM	CMD-C2D	2.10	1.55	1.50
4	B	104	HEM	FE-ND	2.07	2.01	1.94

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	296	HEM	CBC-CAC-C3C	4.09	147.95	127.53
4	B	104	HEM	O2D-CGD-O1D	3.72	132.91	123.33
4	C	296	HEM	CHB-C1B-NB	-3.06	120.58	124.37
4	A	296	HEM	CAA-C2A-C1A	-2.92	119.24	124.94
4	C	296	HEM	O1D-CGD-CBD	-2.67	114.62	123.09
4	D	104	HEM	O1D-CGD-CBD	-2.49	115.21	123.09
4	C	296	HEM	C4A-CHB-C1B	2.48	132.08	126.25
4	C	296	HEM	C4C-C3C-C2C	2.43	108.92	106.81
4	A	296	HEM	CHA-C1A-NA	2.39	128.19	123.86
4	A	296	HEM	CMB-C2B-C1B	-2.37	121.33	125.03
4	A	296	HEM	CMA-C3A-C2A	2.35	130.61	125.62
4	B	104	HEM	O2A-CGA-O1A	2.34	129.35	123.33
4	A	296	HEM	CMD-C2D-C1D	-2.32	121.41	125.03
4	A	296	HEM	O1D-CGD-CBD	-2.28	115.85	123.09
4	D	104	HEM	CAC-C3C-C4C	-2.27	119.41	124.82
4	B	104	HEM	CBD-CAD-C3D	-2.26	106.28	112.53
4	C	296	HEM	CMA-C3A-C4A	-2.26	121.98	125.42
4	B	104	HEM	CHA-C4D-ND	2.21	127.10	124.37
4	C	296	HEM	CMC-C2C-C1C	2.18	128.56	124.73
4	C	296	HEM	CBA-CAA-C2A	2.18	118.55	112.53
4	D	104	HEM	O2D-CGD-O1D	2.12	128.79	123.33
4	A	296	HEM	CMD-C2D-C3D	2.11	131.85	126.15
4	A	296	HEM	CMA-C3A-C4A	-2.08	122.25	125.42
4	B	104	HEM	O1D-CGD-CBD	-2.08	116.50	123.09
4	D	104	HEM	CHA-C4D-ND	2.03	126.88	124.37
4	B	104	HEM	O1A-CGA-CBA	-2.02	116.67	123.09
4	C	296	HEM	C3B-C2B-C1B	2.01	107.92	106.41

There are no chirality outliers.

All (6) torsion outliers are listed below:

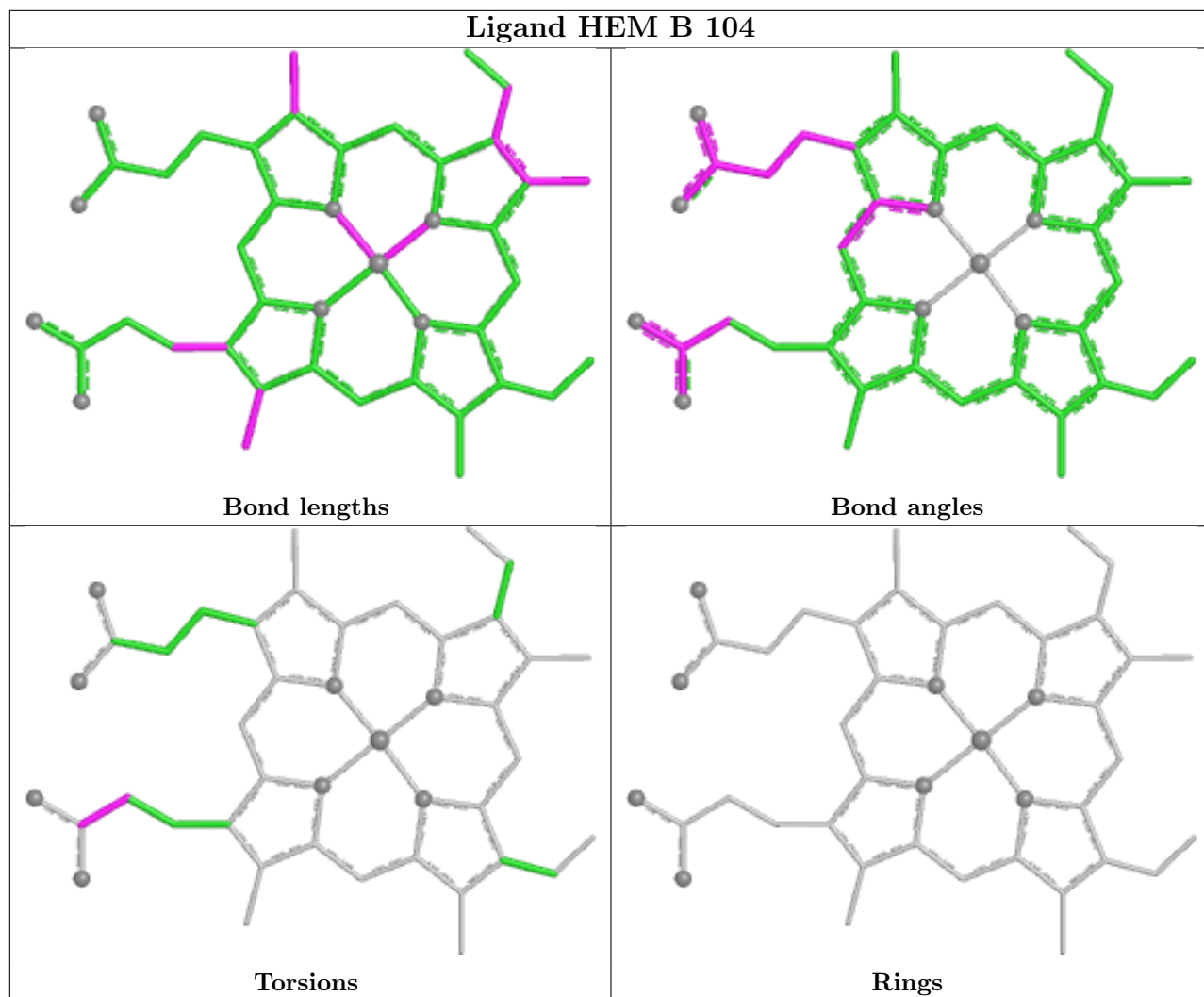
Mol	Chain	Res	Type	Atoms
4	A	296	HEM	CAA-CBA-CGA-O2A
4	C	296	HEM	CAA-CBA-CGA-O2A
4	A	296	HEM	CAA-CBA-CGA-O1A
4	B	104	HEM	CAA-CBA-CGA-O1A
4	C	296	HEM	CAA-CBA-CGA-O1A
4	A	296	HEM	CAD-CBD-CGD-O2D

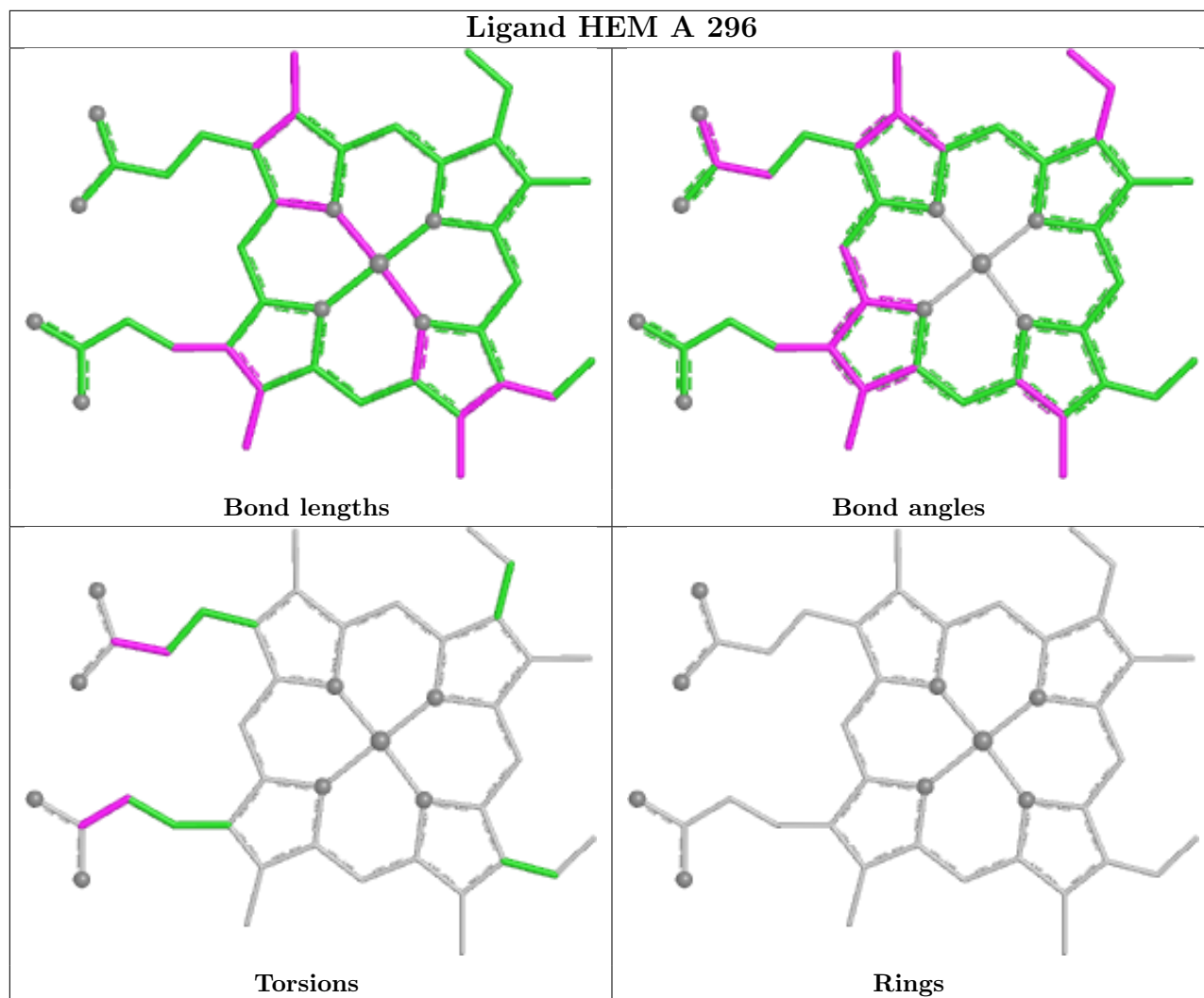
There are no ring outliers.

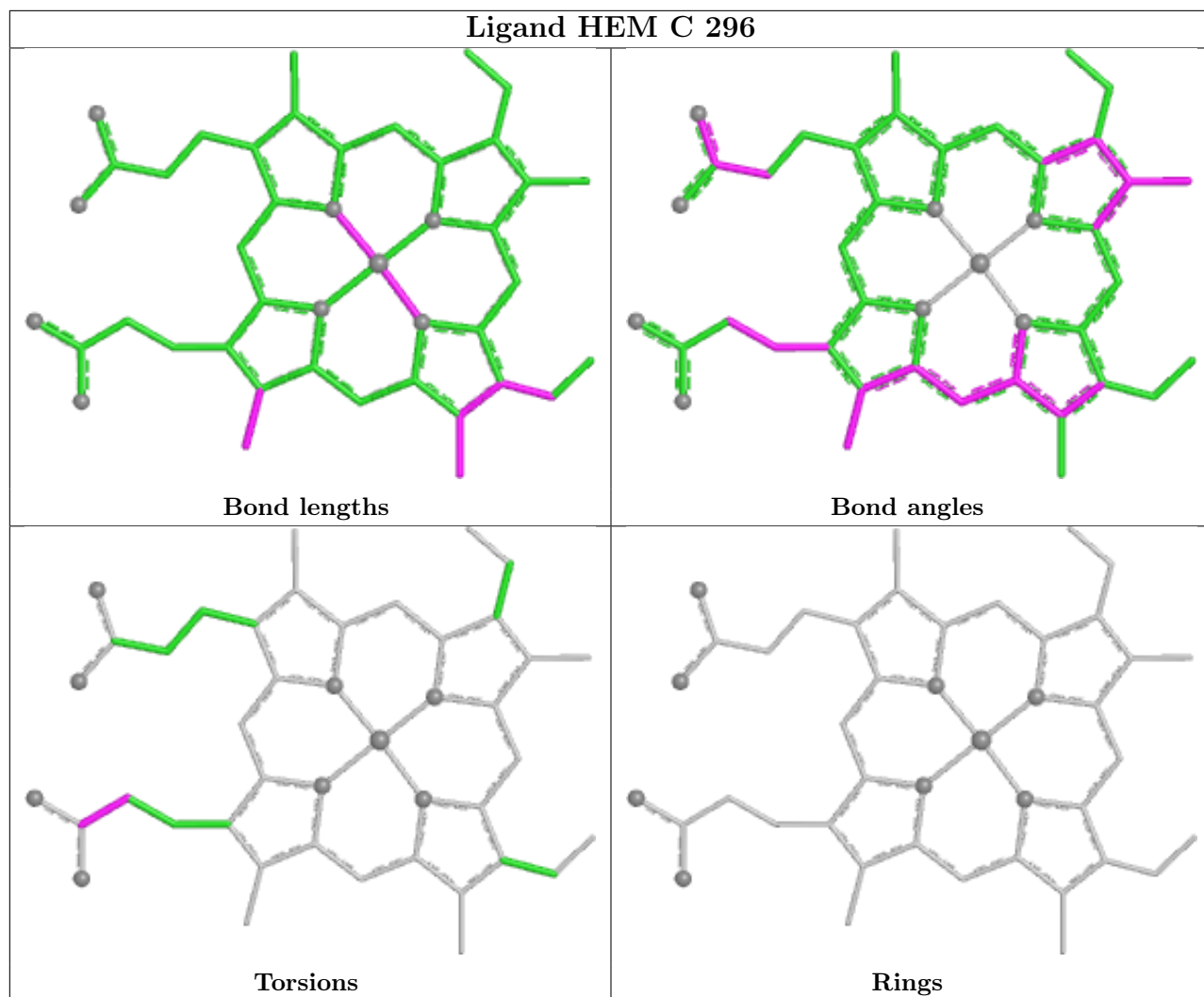
5 monomers are involved in 39 short contacts:

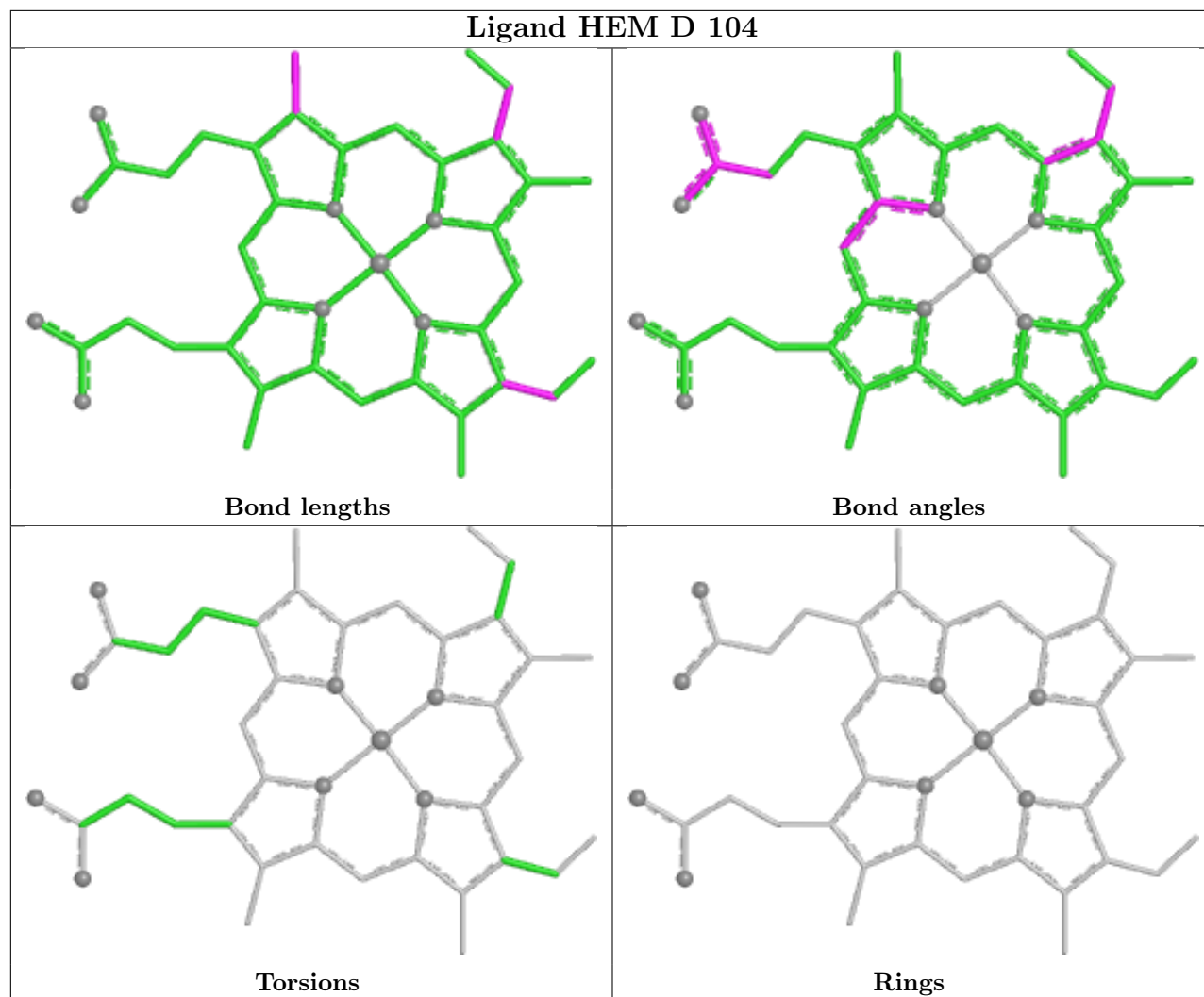
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	104	HEM	14	0
3	C	300	SO4	1	0
3	A	299	SO4	1	0
4	C	296	HEM	4	0
4	D	104	HEM	19	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	294/296 (99%)	-0.65	0 100 100	10, 24, 48, 90	0
1	C	294/296 (99%)	-0.51	0 100 100	8, 24, 42, 72	0
2	B	108/108 (100%)	0.02	3 (2%) 55 57	16, 43, 73, 118	0
2	D	108/108 (100%)	0.11	3 (2%) 55 57	22, 54, 83, 119	0
All	All	804/808 (99%)	-0.40	6 (0%) 84 85	8, 29, 67, 119	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	37	GLY	3.7
2	B	34	GLY	3.5
2	D	-1	ALA	3.5
2	B	-3	PHE	2.8
2	B	20	VAL	2.4
2	D	43	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.

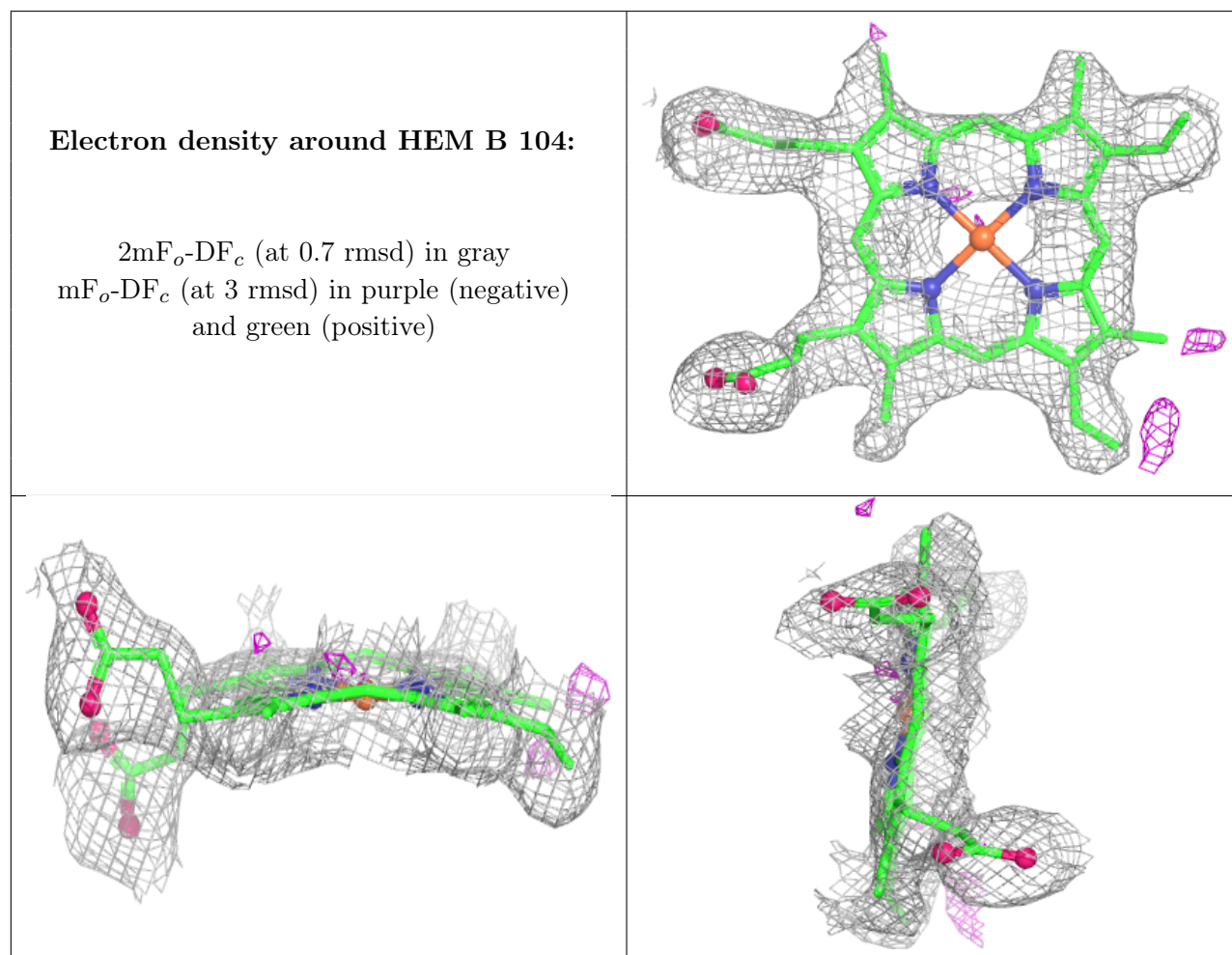
6.4 Ligands [i](#)

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

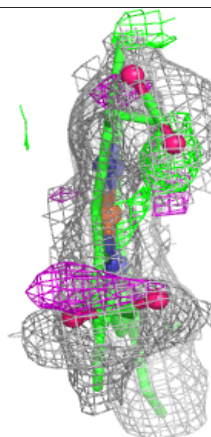
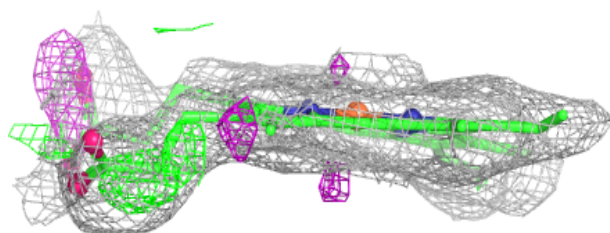
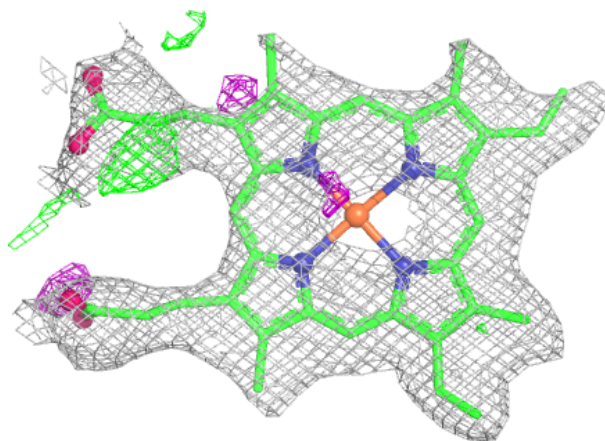
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	C	300	2/5	0.97	0.07	22,22,22,25	0
4	HEM	B	104	43/43	0.98	0.07	24,30,33,35	0
4	HEM	C	296	43/43	0.98	0.06	7,16,20,24	0
3	SO4	A	299	2/5	0.99	0.09	28,28,28,29	0
4	HEM	A	296	43/43	0.99	0.05	9,18,20,24	0
4	HEM	D	104	43/43	0.99	0.06	26,32,42,48	0

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.



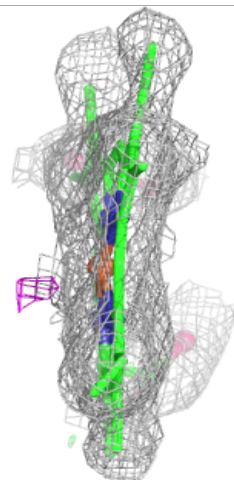
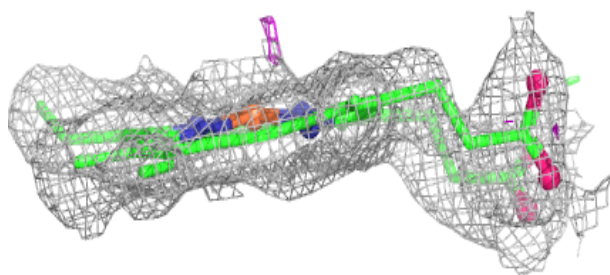
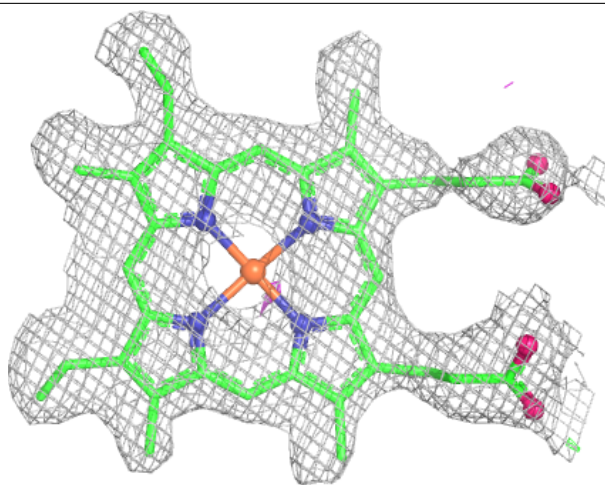
Electron density around HEM C 296:

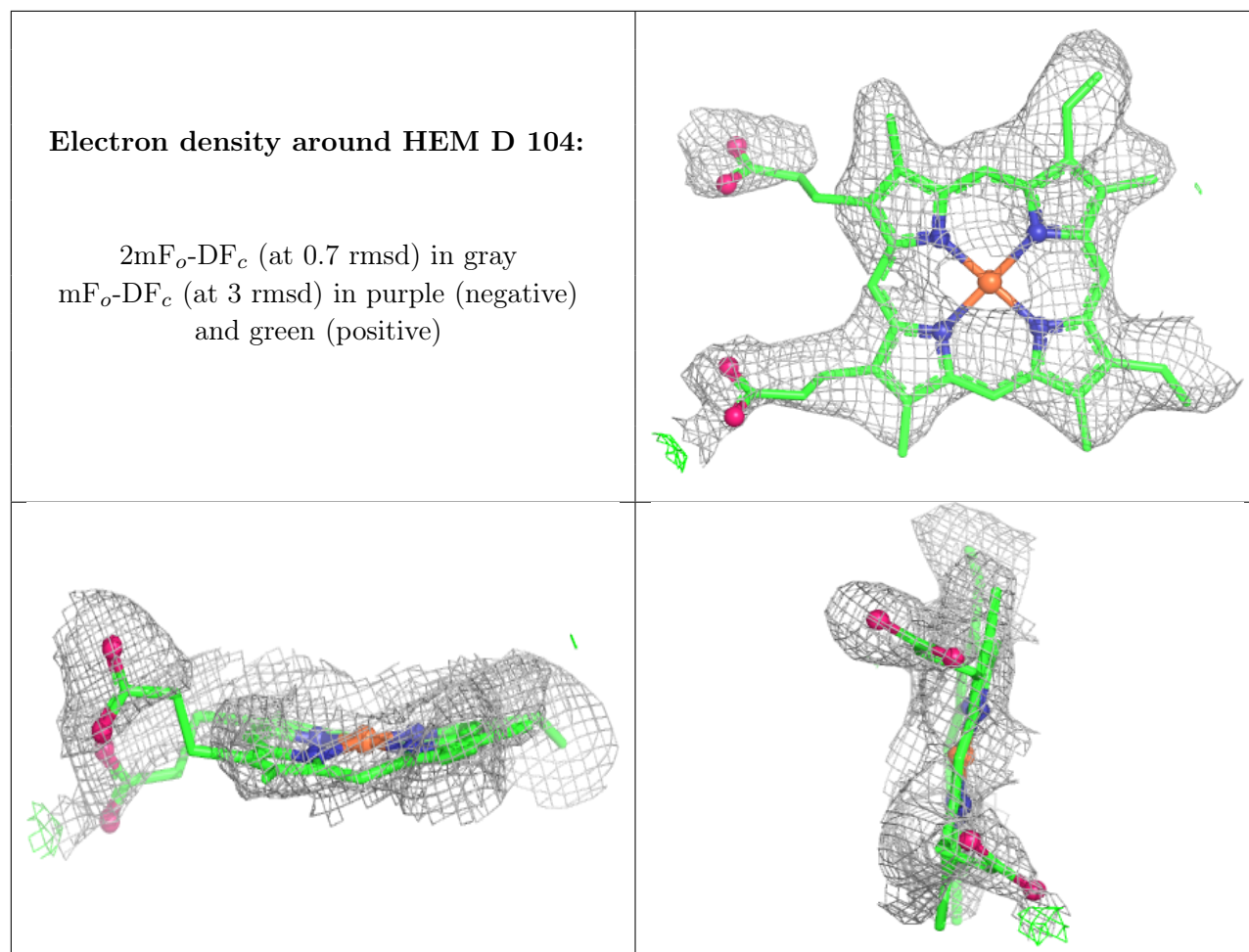
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM A 296:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.