Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:05 AM GMT

PDB ID	:	2PCB
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	:	2.80 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

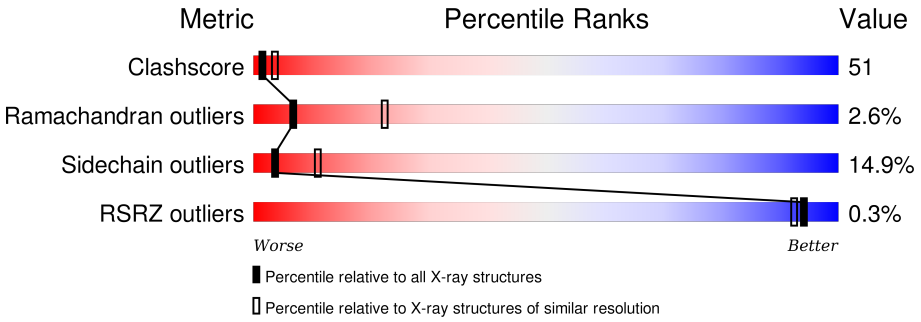
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	296	32% 45% 19%
1	C	296	30% 45% 22%
2	B	104	% 15% 50% 28% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6031 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 (CCP).

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

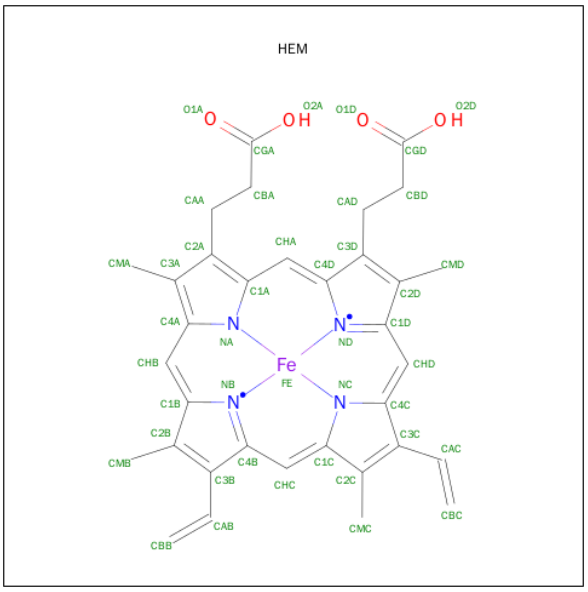
There are 4 discrepancies between the modelled and reference sequences:

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 CYTOCHROME C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	104	Total	C	N	O	S	0	0	0
			823	524	144	151	4			

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 4 is water.

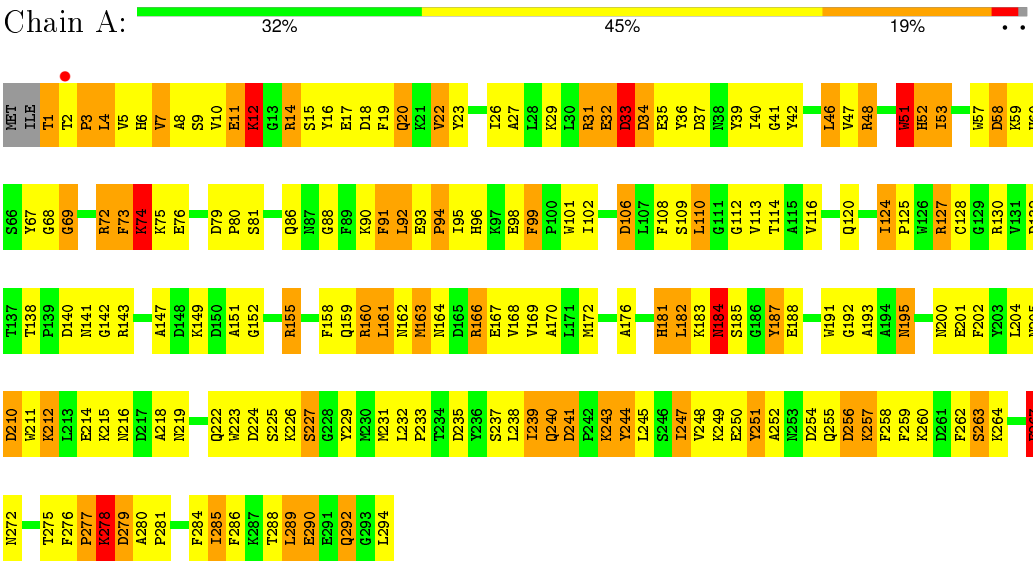
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	146	Total	O	0	0
			146	146		
4	B	41	Total	O	0	0
			41	41		
4	C	150	Total	O	0	0
			150	150		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

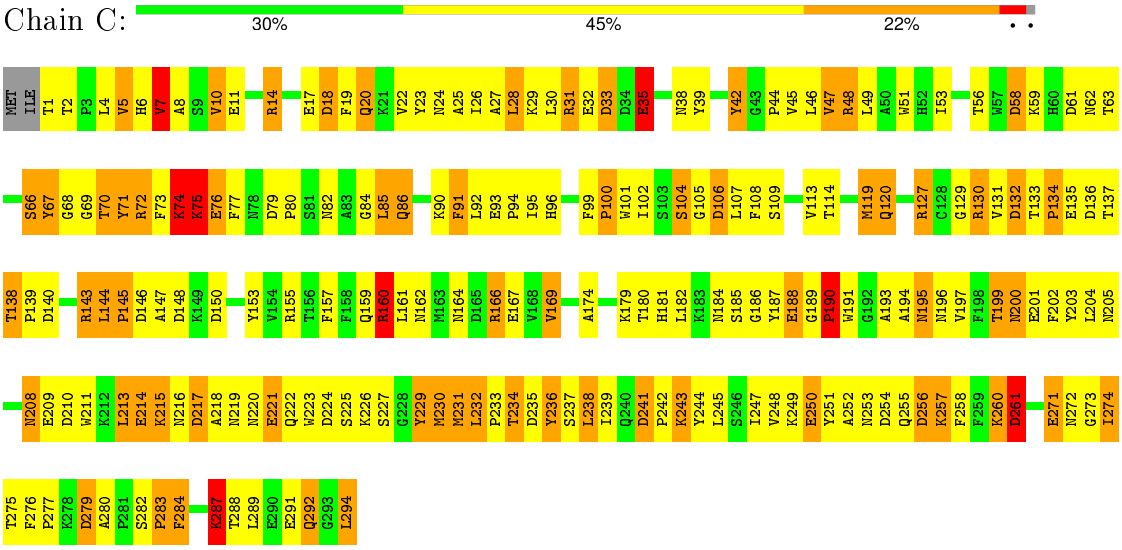
- Molecule 1: CYTOCHROME C PEROXIDASE (CCP)

Chain A:



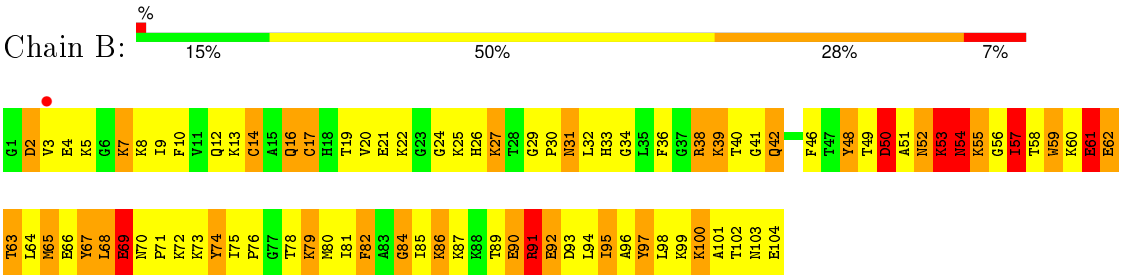
- Molecule 1: CYTOCHROME C PEROXIDASE (CCP)

Chain C:



- Molecule 2: CYTOCHROME C

Chain B:


%
15%
50%
28%
7%
G1 D2 V3 E4 K5 G6 K7 K8 I9 F10 V11 Q12 K13 C14 A15 Q16 C17 H18 T19 V20 E21 K22 G23 G24 K25 H26 K27 T28 G29 P30 N31 L32 H33 G34 L35 F36 G37 R38 K39 T40 G41 Q42 F46 T47 Y48 T49 D50 A51 N52 K53 N54 K55 G56 I57 T58 W59 K60 E61 E62
T63 L64 M65 E66 V67 L68 E69 N70 P71 K72 K73 Y74 I75 P76 G77 T78 K79 M80 I81 F82 A83 G84 I85 K86 K87 K88 T89 E90 R91 E92 D93 L94 I95 A96 Y97 L98 K99 K100 A101 T102 N103 E104

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	105.30Å 105.30Å 186.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.80 11.51 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.80) 94.2 (11.51-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.71 (at 2.82Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.178 , (Not available) 0.165 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	39.7	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 126.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 24643 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6031	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1.15	2/2438 (0.1%)	2.18	112/3302 (3.4%)
1	C	1.13	1/2438 (0.0%)	2.28	128/3302 (3.9%)
2	B	0.97	0/839	2.22	35/1118 (3.1%)
All	All	1.11	3/5715 (0.1%)	2.23	275/7722 (3.6%)

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	192	GLY	N-CA	6.73	1.56	1.46
1	C	104	SER	CB-OG	6.21	1.50	1.42
1	A	109	SER	CB-OG	5.96	1.50	1.42

All (275) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	91	ARG	NE-CZ-NH1	25.01	132.80	120.30
1	C	72	ARG	NE-CZ-NH2	-18.27	111.17	120.30
1	A	155	ARG	NE-CZ-NH1	-16.91	111.84	120.30
1	C	58	ASP	CB-CG-OD2	-15.56	104.29	118.30
1	C	160	ARG	NE-CZ-NH1	15.50	128.05	120.30
1	C	127	ARG	NE-CZ-NH1	-13.62	113.49	120.30
1	C	72	ARG	NE-CZ-NH1	12.88	126.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	143	ARG	NE-CZ-NH1	12.18	126.39	120.30
1	C	106	ASP	CB-CG-OD1	11.76	128.88	118.30
1	A	31	ARG	NE-CZ-NH2	-11.59	114.51	120.30
1	C	254	ASP	CB-CG-OD1	11.47	128.62	118.30
1	C	217	ASP	CB-CG-OD2	-11.23	108.19	118.30
1	A	132	ASP	CB-CG-OD1	10.82	128.04	118.30
1	C	217	ASP	CB-CG-OD1	10.67	127.91	118.30
1	C	14	ARG	NE-CZ-NH2	-10.33	115.13	120.30
1	C	136	ASP	CB-CG-OD1	-10.32	109.01	118.30
2	B	91	ARG	NE-CZ-NH2	-10.22	115.19	120.30
1	A	33	ASP	CB-CG-OD2	10.21	127.49	118.30
1	A	159	GLN	CA-CB-CG	9.99	135.37	113.40
1	A	18	ASP	CB-CG-OD2	-9.81	109.47	118.30
1	A	279	ASP	CB-CG-OD2	-9.67	109.60	118.30
1	C	166	ARG	CD-NE-CZ	-9.40	110.44	123.60
2	B	67	TYR	CB-CG-CD2	9.09	126.45	121.00
1	A	33	ASP	CB-CG-OD1	-8.94	110.26	118.30
1	C	144	LEU	CB-CA-C	8.88	127.07	110.20
2	B	91	ARG	CD-NE-CZ	8.80	135.93	123.60
1	C	160	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	A	74	LYS	N-CA-CB	8.52	125.94	110.60
1	A	18	ASP	CB-CG-OD1	8.49	125.94	118.30
1	A	14	ARG	NE-CZ-NH2	8.35	124.47	120.30
1	A	155	ARG	NH1-CZ-NH2	8.32	128.55	119.40
1	C	31	ARG	NE-CZ-NH2	-8.22	116.19	120.30
1	A	184	ASN	N-CA-CB	8.14	125.26	110.60
1	C	30	LEU	CA-CB-CG	8.05	133.81	115.30
1	A	160	ARG	CD-NE-CZ	7.99	134.78	123.60
1	A	251	TYR	CB-CG-CD2	-7.95	116.23	121.00
1	C	221	GLU	CA-CB-CG	7.92	130.82	113.40
1	A	75	LYS	CA-CB-CG	7.88	130.74	113.40
1	A	218	ALA	C-N-CA	7.84	141.30	121.70
1	C	71	TYR	CB-CG-CD2	7.77	125.66	121.00
1	C	31	ARG	CD-NE-CZ	-7.75	112.75	123.60
1	C	32	GLU	OE1-CD-OE2	-7.73	114.03	123.30
1	C	287	LYS	CA-CB-CG	7.71	130.36	113.40
1	C	35	GLU	CA-CB-CG	7.68	130.30	113.40
2	B	93	ASP	CA-CB-CG	7.68	130.30	113.40
1	A	163	MET	CA-CB-CG	7.65	126.31	113.30
1	C	209	GLU	C-N-CA	7.62	140.74	121.70
1	C	32	GLU	CA-CB-CG	7.50	129.90	113.40
2	B	92	GLU	CA-CB-CG	7.48	129.86	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	98	GLU	OE1-CD-OE2	-7.47	114.33	123.30
1	C	48	ARG	NE-CZ-NH1	7.43	124.01	120.30
1	A	39	TYR	CA-CB-CG	-7.42	99.29	113.40
1	A	36	TYR	CB-CG-CD1	7.41	125.45	121.00
1	A	160	ARG	NE-CZ-NH1	7.37	123.99	120.30
1	C	291	GLU	OE1-CD-OE2	7.36	132.13	123.30
1	A	32	GLU	CA-CB-CG	7.33	129.53	113.40
1	A	187	TYR	CB-CG-CD1	-7.29	116.63	121.00
1	A	241	ASP	CB-CG-OD2	7.28	124.86	118.30
1	C	127	ARG	NE-CZ-NH2	7.21	123.90	120.30
1	A	224	ASP	CB-CG-OD1	7.17	124.75	118.30
2	B	38	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	A	138	THR	CA-CB-CG2	7.11	122.36	112.40
1	C	7	VAL	CB-CA-C	7.06	124.81	111.40
2	B	67	TYR	CB-CG-CD1	-7.04	116.78	121.00
1	C	32	GLU	CG-CD-OE1	7.01	132.32	118.30
1	C	132	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	A	36	TYR	CB-CG-CD2	-7.00	116.80	121.00
2	B	59	TRP	CB-CA-C	6.99	124.38	110.40
1	C	71	TYR	CG-CD1-CE1	6.98	126.89	121.30
1	A	48	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	C	260	LYS	N-CA-CB	6.89	122.99	110.60
1	C	235	ASP	CB-CG-OD2	-6.88	112.10	118.30
2	B	62	GLU	CB-CA-C	6.87	124.14	110.40
2	B	62	GLU	CB-CG-CD	6.85	132.70	114.20
1	A	279	ASP	CB-CG-OD1	6.84	124.45	118.30
2	B	82	PHE	CB-CA-C	6.82	124.03	110.40
1	C	75	LYS	CA-CB-CG	6.81	128.39	113.40
1	C	28	LEU	CA-CB-CG	6.78	130.90	115.30
1	A	120	GLN	CA-CB-CG	6.77	128.30	113.40
1	C	42	TYR	CB-CG-CD1	-6.77	116.94	121.00
2	B	91	ARG	NH1-CZ-NH2	-6.72	112.00	119.40
1	C	188	GLU	OE1-CD-OE2	-6.70	115.26	123.30
2	B	24	GLY	N-CA-C	-6.69	96.37	113.10
1	C	287	LYS	O-C-N	6.67	133.37	122.70
1	C	148	ASP	CB-CG-OD1	6.67	124.30	118.30
2	B	54	ASN	CB-CA-C	6.66	123.71	110.40
1	A	113	VAL	CA-CB-CG1	-6.64	100.93	110.90
1	C	61	ASP	N-CA-CB	-6.64	98.65	110.60
1	C	260	LYS	O-C-N	6.61	133.27	122.70
1	C	166	ARG	NE-CZ-NH2	-6.59	117.00	120.30
2	B	51	ALA	CB-CA-C	6.57	119.96	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	160	ARG	CD-NE-CZ	6.57	132.80	123.60
1	A	143	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	A	61	ASP	CB-CA-C	6.48	123.37	110.40
1	C	58	ASP	CB-CG-OD1	6.47	124.12	118.30
2	B	68	LEU	CB-CA-C	6.43	122.42	110.20
1	C	261	ASP	CB-CG-OD1	-6.43	112.52	118.30
1	A	191	TRP	C-N-CA	-6.39	108.89	122.30
1	C	5	VAL	CB-CA-C	-6.38	99.28	111.40
1	A	161	LEU	CA-CB-CG	6.38	129.96	115.30
1	A	22	VAL	CB-CA-C	6.32	123.41	111.40
1	A	31	ARG	CA-CB-CG	6.32	127.30	113.40
1	C	196	ASN	N-CA-CB	6.31	121.95	110.60
1	C	130	ARG	NE-CZ-NH1	6.29	123.45	120.30
1	C	101	TRP	CA-CB-CG	6.27	125.61	113.70
1	A	210	ASP	CB-CG-OD1	-6.25	112.67	118.30
1	A	219	ASN	CB-CA-C	6.24	122.88	110.40
1	C	211	TRP	O-C-N	6.23	132.66	122.70
1	C	74	LYS	O-C-N	6.22	132.66	122.70
1	A	286	PHE	O-C-N	6.22	132.66	122.70
1	A	240	GLN	CA-CB-CG	6.21	127.05	113.40
1	C	31	ARG	NH1-CZ-NH2	6.16	126.18	119.40
1	C	208	ASN	CB-CA-C	6.15	122.70	110.40
1	A	152	GLY	O-C-N	6.14	132.52	122.70
1	A	73	PHE	CA-CB-CG	6.13	128.62	113.90
2	B	38	ARG	CD-NE-CZ	6.13	132.18	123.60
1	A	223	TRP	CA-C-O	-6.12	107.26	120.10
1	A	229	TYR	O-C-N	6.11	132.47	122.70
1	C	174	ALA	O-C-N	6.10	132.46	122.70
1	A	142	GLY	N-CA-C	6.09	128.34	113.10
1	A	48	ARG	O-C-N	-6.08	112.96	122.70
1	A	286	PHE	CA-C-N	-6.04	103.92	117.20
2	B	62	GLU	CG-CD-OE1	6.03	130.36	118.30
1	C	190	PRO	O-C-N	-6.02	113.06	122.70
1	A	106	ASP	CB-CA-C	6.02	122.44	110.40
1	A	223	TRP	CA-CB-CG	-5.98	102.34	113.70
2	B	104	GLU	CA-CB-CG	5.98	126.55	113.40
2	B	53	LYS	CB-CA-C	-5.93	98.54	110.40
1	C	253	ASN	N-CA-CB	-5.93	99.93	110.60
1	C	271	GLU	CA-CB-CG	5.92	126.44	113.40
1	A	74	LYS	CA-C-O	-5.92	107.68	120.10
1	A	278	LYS	C-N-CA	5.92	136.49	121.70
1	C	284	PHE	O-C-N	5.90	132.15	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	42	TYR	CB-CG-CD2	5.90	124.54	121.00
1	A	184	ASN	O-C-N	5.87	132.10	122.70
1	A	20	GLN	CB-CG-CD	5.85	126.80	111.60
1	A	224	ASP	OD1-CG-OD2	-5.84	112.20	123.30
1	C	271	GLU	CB-CG-CD	5.84	129.96	114.20
1	A	48	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	A	136	ASP	CB-CG-OD1	5.83	123.54	118.30
1	A	17	GLU	CG-CD-OE1	5.82	129.94	118.30
1	C	91	PHE	O-C-N	5.80	131.99	122.70
1	A	135	GLU	CA-CB-CG	5.80	126.17	113.40
1	A	248	VAL	CA-CB-CG2	5.80	119.60	110.90
1	C	210	ASP	O-C-N	5.80	131.97	122.70
1	A	241	ASP	CA-CB-CG	5.79	126.14	113.40
1	A	211	TRP	CA-CB-CG	-5.77	102.73	113.70
2	B	53	LYS	CA-C-N	-5.75	104.54	117.20
1	C	150	ASP	CB-CG-OD1	5.75	123.47	118.30
1	A	17	GLU	CB-CG-CD	5.74	129.70	114.20
1	A	214	GLU	OE1-CD-OE2	-5.73	116.42	123.30
2	B	38	ARG	N-CA-CB	5.73	120.91	110.60
1	A	39	TYR	O-C-N	5.72	131.85	122.70
1	C	119	MET	CA-C-O	5.72	132.11	120.10
1	C	261	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	159	GLN	CB-CA-C	5.68	121.77	110.40
1	C	279	ASP	CA-CB-CG	-5.67	100.92	113.40
1	C	134	PRO	N-CD-CG	-5.66	94.72	103.20
1	A	46	LEU	CB-CA-C	5.65	120.94	110.20
1	C	91	PHE	N-CA-CB	5.65	120.77	110.60
1	A	286	PHE	CB-CG-CD1	-5.65	116.85	120.80
2	B	93	ASP	CB-CG-OD1	5.61	123.35	118.30
1	A	106	ASP	CA-CB-CG	5.61	125.74	113.40
1	C	18	ASP	CB-CG-OD1	-5.61	113.25	118.30
1	C	201	GLU	OE1-CD-OE2	5.60	130.02	123.30
1	A	285	ILE	N-CA-C	-5.60	95.88	111.00
1	C	106	ASP	N-CA-CB	5.60	120.68	110.60
1	C	38	ASN	O-C-N	5.59	131.64	122.70
1	C	61	ASP	CB-CG-OD1	5.59	123.33	118.30
1	A	279	ASP	CA-C-N	-5.58	104.91	117.20
1	A	69	GLY	C-N-CA	5.57	135.63	121.70
1	C	201	GLU	C-N-CA	5.57	135.63	121.70
1	A	244	TYR	CB-CG-CD1	5.57	124.34	121.00
1	C	67	TYR	CB-CG-CD1	-5.56	117.66	121.00
1	A	51	TRP	CB-CA-C	5.56	121.52	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	166	ARG	CB-CA-C	5.55	121.51	110.40
1	C	254	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	A	209	GLU	CG-CD-OE2	5.54	129.38	118.30
1	A	76	GLU	OE1-CD-OE2	-5.53	116.66	123.30
1	A	3	PRO	CA-C-O	5.53	133.47	120.20
1	A	14	ARG	CA-C-O	5.52	131.69	120.10
1	A	37	ASP	C-N-CA	5.52	135.50	121.70
1	C	224	ASP	O-C-N	5.52	131.53	122.70
1	C	127	ARG	CD-NE-CZ	-5.51	115.89	123.60
1	C	127	ARG	CA-C-O	-5.50	108.55	120.10
1	A	208	ASN	CA-CB-CG	-5.50	101.30	113.40
1	C	113	VAL	CA-CB-CG2	-5.50	102.65	110.90
1	C	5	VAL	CG1-CB-CG2	5.48	119.66	110.90
1	A	40	ILE	O-C-N	5.47	132.50	123.20
1	C	271	GLU	OE1-CD-OE2	-5.46	116.75	123.30
2	B	74	TYR	CB-CG-CD1	5.46	124.27	121.00
1	A	170	ALA	CB-CA-C	5.43	118.25	110.10
1	C	31	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	C	109	SER	CB-CA-C	5.41	120.38	110.10
1	C	10	VAL	O-C-N	5.41	131.36	122.70
1	A	231	MET	CA-CB-CG	-5.40	104.12	113.30
2	B	53	LYS	CA-CB-CG	5.40	125.28	113.40
1	C	232	LEU	CB-CG-CD2	-5.40	101.82	111.00
1	A	39	TYR	CB-CG-CD2	-5.38	117.77	121.00
2	B	50	ASP	CB-CG-OD1	5.38	123.14	118.30
1	C	205	ASN	CB-CG-OD1	5.38	132.36	121.60
1	C	150	ASP	O-C-N	5.38	131.31	122.70
1	A	210	ASP	CA-CB-CG	-5.37	101.59	113.40
1	C	213	LEU	CB-CA-C	5.36	120.39	110.20
1	C	235	ASP	CB-CG-OD1	5.35	123.12	118.30
1	C	20	GLN	CB-CA-C	-5.35	99.70	110.40
1	C	273	GLY	N-CA-C	5.35	126.48	113.10
1	A	76	GLU	CA-CB-CG	5.35	125.17	113.40
1	C	215	LYS	CD-CE-NZ	-5.35	99.39	111.70
1	A	72	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	241	ASP	OD1-CG-OD2	-5.34	113.15	123.30
1	C	46	LEU	CB-CA-C	5.34	120.35	110.20
1	C	294	LEU	CB-CG-CD2	-5.34	101.93	111.00
1	A	58	ASP	CB-CG-OD2	5.33	123.09	118.30
2	B	90	GLU	OE1-CD-OE2	5.32	129.69	123.30
1	C	195	ASN	CA-CB-CG	-5.32	101.70	113.40
1	A	72	ARG	NE-CZ-NH2	-5.32	117.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	113	VAL	CG1-CB-CG2	5.31	119.40	110.90
1	C	25	ALA	N-CA-CB	-5.31	102.66	110.10
1	C	185	SER	N-CA-CB	-5.31	102.53	110.50
1	C	169	VAL	CA-C-N	5.31	128.87	117.20
1	C	214	GLU	CA-CB-CG	5.31	125.07	113.40
1	A	251	TYR	CB-CG-CD1	5.30	124.18	121.00
1	C	284	PHE	CB-CA-C	-5.29	99.81	110.40
1	A	92	LEU	CB-CG-CD1	-5.29	102.00	111.00
1	C	287	LYS	CB-CG-CD	5.29	125.36	111.60
1	C	145	PRO	O-C-N	5.29	131.16	122.70
1	C	291	GLU	CG-CD-OE1	-5.29	107.73	118.30
1	A	254	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	A	290	GLU	CG-CD-OE2	-5.27	107.76	118.30
1	C	32	GLU	CB-CG-CD	5.27	128.44	114.20
1	A	223	TRP	O-C-N	5.27	131.13	122.70
1	C	241	ASP	CB-CG-OD1	-5.27	113.56	118.30
1	A	187	TYR	CB-CG-CD2	5.26	124.16	121.00
1	C	120	GLN	CB-CG-CD	5.26	125.28	111.60
1	C	74	LYS	CA-C-N	-5.25	105.66	117.20
1	A	224	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	143	ARG	NH1-CZ-NH2	-5.20	113.68	119.40
1	A	181	HIS	CA-CB-CG	-5.19	104.78	113.60
1	C	238	LEU	CB-CA-C	5.19	120.05	110.20
1	C	231	MET	O-C-N	-5.18	114.41	122.70
1	C	159	GLN	CB-CA-C	5.18	120.77	110.40
1	C	187	TYR	N-CA-CB	5.18	119.92	110.60
1	A	53	ILE	C-N-CA	5.17	134.63	121.70
1	A	184	ASN	CA-C-O	-5.17	109.24	120.10
1	A	256	ASP	CB-CG-OD2	5.17	122.95	118.30
1	C	184	ASN	O-C-N	5.15	130.94	122.70
2	B	69	GLU	CG-CD-OE1	5.14	128.58	118.30
1	C	234	THR	CA-CB-OG1	5.14	119.79	109.00
2	B	61	GLU	N-CA-CB	5.13	119.83	110.60
1	A	163	MET	CB-CG-SD	5.12	127.76	112.40
1	C	136	ASP	OD1-CG-OD2	5.12	133.03	123.30
1	C	199	THR	N-CA-CB	5.11	120.00	110.30
1	C	190	PRO	CA-C-O	5.11	132.45	120.20
1	A	12	LYS	N-CA-CB	5.08	119.75	110.60
2	B	62	GLU	OE1-CD-OE2	-5.08	117.20	123.30
1	C	236	TYR	CB-CA-C	5.08	120.56	110.40
2	B	95	ILE	CB-CA-C	5.08	121.75	111.60
1	A	193	ALA	O-C-N	-5.07	114.59	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	17	CYS	CA-CB-SG	-5.07	104.88	114.00
2	B	62	GLU	CA-CB-CG	5.05	124.52	113.40
1	C	283	PRO	O-C-N	5.05	130.78	122.70
2	B	57	ILE	CB-CA-C	5.04	121.69	111.60
1	A	98	GLU	CG-CD-OE1	5.04	128.37	118.30
1	C	209	GLU	OE1-CD-OE2	5.04	129.34	123.30
1	A	140	ASP	CB-CG-OD2	-5.03	113.77	118.30
1	C	132	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	52	HIS	CA-C-N	5.03	128.26	117.20
1	A	99	PHE	O-C-N	5.02	130.64	121.10
1	A	267	GLU	CB-CG-CD	5.02	127.76	114.20
1	C	100	PRO	CA-C-N	-5.02	106.16	117.20
1	A	27	ALA	O-C-N	5.02	130.73	122.70
1	C	250	GLU	CA-CB-CG	5.01	124.43	113.40
1	C	155	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	A	61	ASP	N-CA-CB	-5.00	101.59	110.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	127	ARG	Sidechain
1	A	166	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	2251	176	0
1	C	2371	0	2252	199	1
2	B	823	0	849	195	0
3	A	43	0	30	5	0
3	B	43	0	30	19	0
3	C	43	0	30	1	0
4	A	146	0	0	27	2
4	B	41	0	0	15	1
4	C	150	0	0	26	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	6031	0	5442	572	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 51.

All (572) 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	3:B:105:HEM:HAB	1.79	1.22
2:B:14:CYS:SG	3:B:105:HEM:CAB	2.33	1.17
1:C:147:ALA:O	1:C:233:PRO:HD2	1.51	1.06
2:B:50:ASP:HA	2:B:53:LYS:HE2	1.42	1.02
1:C:164:ASN:ND2	1:C:167:GLU:HG3	1.74	1.02
1:C:84:GLY:H	1:C:86:GLN:NE2	1.57	1.01
2:B:41:GLY:HA2	2:B:48:TYR:CE1	1.96	1.00
1:A:195:ASN:HD22	1:A:195:ASN:H	1.09	1.00
2:B:79:LYS:HG3	3:B:105:HEM:O2D	1.63	0.98
1:C:74:LYS:NZ	1:C:74:LYS:HB2	1.77	0.97
1:A:292:GLN:HB2	1:A:294:LEU:CD1	1.96	0.96
1:C:84:GLY:H	1:C:86:GLN:HE22	1.04	0.94
1:C:26:ILE:HG22	1:C:114:THR:HG21	1.48	0.92
1:C:28:LEU:HD13	1:C:289:LEU:HD13	1.50	0.91
1:C:4:LEU:HG	4:C:657:HOH:O	1.70	0.91
2:B:19:THR:HG23	2:B:27:LYS:HD3	1.53	0.91
1:A:185:SER:HB3	3:A:295:HEM:HBA1	1.52	0.91
2:B:34:GLY:O	2:B:38:ARG:HD3	1.70	0.90
1:C:74:LYS:HZ1	1:C:74:LYS:HB2	1.33	0.90
1:C:272:ASN:HA	4:C:692:HOH:O	1.72	0.90
1:C:63:THR:HA	4:C:623:HOH:O	1.72	0.90
2:B:65:MET:HE1	2:B:92:GLU:HG2	1.55	0.89
2:B:65:MET:HE1	2:B:92:GLU:CG	2.03	0.89
2:B:9:ILE:CD1	2:B:90:GLU:HG3	2.04	0.88
1:C:244:TYR:O	1:C:248:VAL:HG23	1.72	0.88
2:B:53:LYS:HB2	2:B:54:ASN:ND2	1.89	0.87
1:C:69:GLY:O	1:C:72:ARG:HG2	1.75	0.87
1:C:28:LEU:HD13	1:C:289:LEU:CD1	2.04	0.86
2:B:54:ASN:HD22	2:B:54:ASN:N	1.69	0.86
1:C:69:GLY:HA2	4:C:630:HOH:O	1.75	0.86
1:A:176:ALA:O	4:A:303:HOH:O	1.92	0.86
1:A:35:GLU:HB2	4:A:356:HOH:O	1.72	0.86
2:B:3:VAL:HG12	2:B:97:TYR:HA	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:ILE:HD13	2:B:63:THR:HG21	1.58	0.85
1:A:10:VAL:HG13	1:A:128:CYS:SG	2.16	0.85
2:B:41:GLY:HA2	2:B:48:TYR:CD1	2.12	0.84
1:A:33:ASP:OD1	1:A:33:ASP:N	2.07	0.83
1:A:216:ASN:HD22	1:A:222:GLN:NE2	1.75	0.83
1:C:20:GLN:HE22	1:C:287:LYS:H	1.22	0.83
2:B:25:LYS:HE3	2:B:27:LYS:HE2	1.61	0.83
1:C:31:ARG:HD2	4:C:608:HOH:O	1.80	0.82
1:C:215:LYS:HE3	1:C:221:GLU:OE1	1.80	0.81
1:A:292:GLN:HB2	1:A:294:LEU:HD13	1.61	0.81
1:A:1:THR:HG23	1:A:2:THR:H	1.44	0.81
1:C:20:GLN:NE2	1:C:287:LYS:H	1.79	0.81
1:C:75:LYS:HB2	4:C:619:HOH:O	1.81	0.80
1:C:161:LEU:O	1:C:162:ASN:HB3	1.82	0.80
2:B:70:ASN:OD1	2:B:72:LYS:HG3	1.81	0.80
2:B:26:HIS:CD2	2:B:31:ASN:H	2.01	0.79
2:B:41:GLY:HA2	2:B:48:TYR:CZ	2.17	0.79
2:B:9:ILE:HD11	2:B:90:GLU:HG3	1.65	0.79
2:B:39:LYS:O	2:B:42:GLN:HB2	1.83	0.78
1:C:26:ILE:CG2	1:C:114:THR:HG21	2.13	0.78
2:B:90:GLU:HB2	4:B:475:HOH:O	1.82	0.78
2:B:82:PHE:O	4:B:325:HOH:O	2.02	0.77
1:C:169:VAL:HG22	1:C:238:LEU:HD22	1.65	0.76
1:A:271:GLU:HG2	1:A:276:PHE:HE2	1.49	0.76
1:A:256:ASP:HB2	4:A:446:HOH:O	1.84	0.75
1:A:216:ASN:HD22	1:A:222:GLN:HE21	1.33	0.75
1:A:147:ALA:O	1:A:233:PRO:HD2	1.86	0.75
2:B:66:GLU:OE1	2:B:74:TYR:HE2	1.70	0.74
1:A:22:VAL:HG11	1:A:102:ILE:HD13	1.69	0.74
2:B:59:TRP:CE3	2:B:59:TRP:HA	2.22	0.74
1:C:216:ASN:HD22	1:C:222:GLN:NE2	1.85	0.74
2:B:2:ASP:HB2	2:B:5:LYS:H	1.52	0.73
1:A:32:GLU:HG3	4:A:359:HOH:O	1.88	0.72
1:A:68:GLY:HA3	1:A:133:THR:OG1	1.88	0.72
2:B:50:ASP:CA	2:B:53:LYS:HE2	2.19	0.72
1:C:223:TRP:O	1:C:230:MET:HA	1.89	0.72
2:B:3:VAL:HG12	2:B:97:TYR:CA	2.18	0.72
2:B:65:MET:CE	2:B:92:GLU:HG2	2.19	0.72
1:A:130:ARG:HG3	1:A:130:ARG:HH11	1.52	0.72
1:A:22:VAL:HG11	1:A:102:ILE:CD1	2.20	0.72
2:B:59:TRP:CZ3	2:B:64:LEU:HD23	2.25	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:ILE:HG22	1:C:71:TYR:HB2	1.71	0.71
2:B:49:THR:O	2:B:53:LYS:NZ	2.23	0.71
2:B:54:ASN:ND2	2:B:54:ASN:N	2.37	0.71
1:A:1:THR:HG23	1:A:2:THR:N	2.04	0.71
2:B:64:LEU:HB2	2:B:95:ILE:CD1	2.20	0.70
2:B:39:LYS:HA	2:B:57:ILE:O	1.91	0.70
1:A:99:PHE:O	1:A:102:ILE:HG22	1.91	0.70
1:C:225:SER:O	4:C:441:HOH:O	2.10	0.70
1:C:96:HIS:CD2	1:C:107:LEU:HD22	2.26	0.70
2:B:57:ILE:CD1	2:B:63:THR:HG21	2.22	0.70
1:A:53:ILE:HD13	1:A:108:PHE:HB2	1.73	0.70
1:A:195:ASN:ND2	1:A:195:ASN:H	1.86	0.69
2:B:82:PHE:CE2	2:B:84:GLY:HA2	2.28	0.69
1:C:200:ASN:ND2	1:C:255:GLN:OE1	2.26	0.69
1:A:240:GLN:HG2	4:A:396:HOH:O	1.91	0.69
2:B:17:CYS:SG	3:B:105:HEM:CAC	2.81	0.69
1:C:66:SER:HB2	1:C:130:ARG:HD3	1.73	0.69
1:C:67:TYR:HD2	1:C:274:ILE:HG23	1.57	0.69
1:C:7:VAL:HA	1:C:275:THR:O	1.93	0.69
1:A:47:VAL:HG22	1:A:116:VAL:HG23	1.75	0.69
1:C:146:ASP:O	1:C:234:THR:HG21	1.93	0.69
1:A:14:ARG:HG2	1:A:101:TRP:CZ3	2.27	0.69
1:A:125:PRO:HB2	1:A:267:GLU:OE1	1.92	0.68
2:B:26:HIS:CD2	2:B:31:ASN:N	2.62	0.68
1:C:93:GLU:N	1:C:94:PRO:HD2	2.08	0.68
2:B:32:LEU:O	2:B:102:THR:CG2	2.42	0.68
2:B:66:GLU:HG2	2:B:74:TYR:CD2	2.28	0.68
1:C:84:GLY:N	1:C:86:GLN:HE22	1.87	0.68
1:A:195:ASN:HD22	1:A:195:ASN:N	1.89	0.68
2:B:64:LEU:HB2	2:B:95:ILE:HD13	1.76	0.68
2:B:82:PHE:HA	4:B:357:HOH:O	1.94	0.68
1:C:71:TYR:HA	1:C:76:GLU:CG	2.24	0.68
1:C:8:ALA:HB1	1:C:129:GLY:HA3	1.76	0.67
1:A:216:ASN:ND2	1:A:222:GLN:HE21	1.91	0.67
1:A:271:GLU:HB3	4:A:447:HOH:O	1.93	0.67
1:C:84:GLY:N	1:C:86:GLN:NE2	2.39	0.67
3:B:105:HEM:HHD	3:B:105:HEM:HBC2	1.77	0.67
1:A:128:CYS:SG	4:A:492:HOH:O	2.52	0.67
1:A:47:VAL:HG22	1:A:116:VAL:CG2	2.24	0.67
2:B:16:GLN:OE1	2:B:16:GLN:N	2.28	0.67
2:B:36:PHE:HA	2:B:59:TRP:O	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:LYS:HB2	2:B:54:ASN:HD22	1.61	0.66
1:A:11:GLU:O	1:A:14:ARG:HB2	1.96	0.66
1:C:143:ARG:CG	4:C:672:HOH:O	2.42	0.66
1:C:58:ASP:HB2	1:C:143:ARG:NH1	2.10	0.66
1:A:62:ASN:HB2	4:A:382:HOH:O	1.96	0.66
2:B:26:HIS:HD2	2:B:31:ASN:N	1.93	0.66
1:C:29:LYS:HG2	1:C:91:PHE:CZ	2.31	0.66
2:B:39:LYS:C	2:B:42:GLN:NE2	2.50	0.65
2:B:9:ILE:HD13	2:B:90:GLU:CG	2.26	0.65
1:C:119:MET:O	1:C:120:GLN:HB2	1.95	0.65
1:A:155:ARG:NH2	1:A:243:LYS:HE3	2.11	0.65
2:B:9:ILE:CD1	2:B:90:GLU:CG	2.74	0.65
1:C:292:GLN:HB3	1:C:294:LEU:HD12	1.79	0.65
2:B:3:VAL:HA	2:B:97:TYR:HB2	1.79	0.64
1:A:53:ILE:HD13	1:A:108:PHE:CB	2.28	0.64
1:A:59:LYS:HD2	1:A:162:ASN:HD21	1.62	0.64
2:B:39:LYS:HB3	2:B:42:GLN:NE2	2.12	0.64
1:A:106:ASP:OD1	1:A:130:ARG:NH1	2.31	0.64
1:C:75:LYS:HE3	1:C:140:ASP:HA	1.80	0.64
1:C:279:ASP:N	1:C:279:ASP:OD1	2.29	0.64
1:A:278:LYS:HG2	1:A:279:ASP:N	2.11	0.64
1:A:31:ARG:CZ	1:A:289:LEU:HD23	2.28	0.64
2:B:31:ASN:OD1	2:B:32:LEU:N	2.31	0.64
2:B:9:ILE:HG22	2:B:94:LEU:HD22	1.79	0.63
2:B:14:CYS:HB3	3:B:105:HEM:C3B	2.33	0.63
1:C:76:GLU:HB3	1:C:138:THR:CG2	2.29	0.63
2:B:3:VAL:HG12	2:B:97:TYR:N	2.13	0.63
1:C:104:SER:HB3	1:C:108:PHE:CE2	2.33	0.63
1:C:26:ILE:HA	1:C:95:ILE:HD11	1.81	0.62
2:B:66:GLU:OE1	2:B:74:TYR:CE2	2.52	0.62
1:A:281:PRO:HD3	4:A:338:HOH:O	1.98	0.62
1:C:134:PRO:HD2	1:C:137:THR:CG2	2.29	0.62
1:C:67:TYR:CD2	1:C:274:ILE:HG23	2.35	0.62
2:B:38:ARG:O	2:B:59:TRP:N	2.33	0.62
1:A:200:ASN:HA	4:A:423:HOH:O	1.98	0.62
2:B:66:GLU:HG2	2:B:74:TYR:HD2	1.64	0.62
1:A:155:ARG:HA	1:A:244:TYR:OH	1.99	0.62
1:A:163:MET:HE2	1:A:167:GLU:HB3	1.80	0.62
2:B:17:CYS:SG	3:B:105:HEM:CBC	2.88	0.61
2:B:30:PRO:HG3	2:B:46:PHE:CD2	2.34	0.61
1:C:282:SER:HB3	1:C:283:PRO:HD2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:TYR:HD1	1:C:24:ASN:HD22	1.48	0.61
1:A:72:ARG:NH2	1:A:73:PHE:CZ	2.68	0.61
2:B:59:TRP:HA	2:B:59:TRP:HE3	1.65	0.61
1:A:294:LEU:O	4:A:361:HOH:O	2.16	0.61
1:A:172:MET:SD	3:A:295:HEM:CBB	2.89	0.61
2:B:14:CYS:CB	3:B:105:HEM:CAB	2.79	0.61
1:C:26:ILE:HA	1:C:95:ILE:CD1	2.30	0.61
1:C:10:VAL:HG12	1:C:11:GLU:O	1.99	0.61
1:A:281:PRO:CD	4:A:338:HOH:O	2.49	0.61
1:C:135:GLU:HG3	1:C:135:GLU:O	1.99	0.60
1:C:248:VAL:O	1:C:252:ALA:HB2	2.02	0.60
2:B:80:MET:HB2	3:B:105:HEM:C1D	2.37	0.60
1:A:96:HIS:HE1	1:A:102:ILE:O	1.83	0.60
1:C:7:VAL:HG22	4:C:728:HOH:O	2.01	0.60
1:A:271:GLU:HG2	1:A:276:PHE:CE2	2.33	0.60
1:C:213:LEU:HD13	1:C:223:TRP:CE2	2.37	0.60
1:C:195:ASN:OD1	1:C:195:ASN:N	2.29	0.60
1:A:225:SER:OG	1:A:227:SER:HB2	2.03	0.59
1:C:261:ASP:OD1	1:C:261:ASP:N	2.35	0.59
2:B:40:THR:HG21	2:B:55:LYS:HB3	1.85	0.59
1:A:4:LEU:HD12	1:A:6:HIS:CE1	2.38	0.59
2:B:64:LEU:O	2:B:66:GLU:N	2.36	0.59
2:B:70:ASN:HB3	2:B:73:LYS:HB3	1.84	0.59
1:C:143:ARG:O	1:C:157:PHE:CE1	2.55	0.59
1:A:255:GLN:NE2	1:A:259:PHE:CZ	2.68	0.59
2:B:49:THR:C	2:B:53:LYS:NZ	2.56	0.59
1:C:134:PRO:HD2	1:C:137:THR:HG21	1.85	0.58
1:A:166:ARG:HH21	1:A:257:LYS:HE3	1.67	0.58
1:A:169:VAL:HG12	1:A:251:TYR:CE2	2.38	0.58
1:C:99:PHE:N	1:C:100:PRO:HD3	2.17	0.58
1:C:99:PHE:O	1:C:102:ILE:HG22	2.02	0.58
2:B:55:LYS:HD3	2:B:55:LYS:O	2.03	0.58
2:B:25:LYS:HE3	2:B:27:LYS:CE	2.33	0.58
1:A:216:ASN:ND2	1:A:222:GLN:NE2	2.47	0.58
2:B:79:LYS:HZ2	3:B:105:HEM:CGD	2.16	0.58
1:A:93:GLU:HB3	1:A:94:PRO:HD3	1.84	0.58
2:B:2:ASP:N	2:B:2:ASP:OD1	2.36	0.58
1:C:70:THR:HB	1:C:138:THR:HG23	1.86	0.58
1:C:250:GLU:OE2	1:C:257:LYS:HE3	2.04	0.58
2:B:14:CYS:HB3	3:B:105:HEM:CAB	2.33	0.58
1:A:124:ILE:HD13	1:A:263:SER:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:MET:HE3	1:C:231:MET:CA	2.33	0.58
1:C:143:ARG:O	1:C:157:PHE:HE1	1.86	0.57
2:B:14:CYS:SG	3:B:105:HEM:CBB	2.91	0.57
2:B:53:LYS:C	2:B:54:ASN:HD22	2.07	0.57
2:B:3:VAL:CG1	2:B:97:TYR:HA	2.31	0.57
2:B:82:PHE:HE2	2:B:84:GLY:HA2	1.68	0.57
1:C:282:SER:HB3	1:C:283:PRO:CD	2.34	0.57
2:B:9:ILE:HD13	2:B:90:GLU:HG2	1.86	0.57
1:C:22:VAL:O	1:C:23:TYR:C	2.42	0.57
2:B:7:LYS:CD	4:B:415:HOH:O	2.52	0.57
1:C:130:ARG:HG3	1:C:130:ARG:HH11	1.69	0.57
2:B:55:LYS:O	2:B:57:ILE:HG23	2.04	0.57
1:C:26:ILE:HG13	1:C:95:ILE:HD13	1.87	0.57
1:C:130:ARG:NH1	1:C:130:ARG:HG3	2.20	0.57
1:C:28:LEU:HD13	1:C:289:LEU:HD11	1.87	0.57
2:B:14:CYS:HB3	3:B:105:HEM:C4B	2.40	0.56
3:B:105:HEM:HBB2	3:B:105:HEM:HHC	1.86	0.56
2:B:9:ILE:CG2	2:B:94:LEU:HD22	2.34	0.56
2:B:61:GLU:OE2	2:B:99:LYS:HE3	2.05	0.56
1:C:20:GLN:HE22	1:C:287:LYS:N	1.96	0.56
2:B:48:TYR:HA	2:B:79:LYS:HZ1	1.69	0.56
1:A:80:PRO:HD3	1:A:141:ASN:ND2	2.20	0.56
2:B:16:GLN:CD	2:B:16:GLN:H	2.09	0.56
1:A:128:CYS:HB2	4:A:492:HOH:O	2.04	0.56
2:B:14:CYS:HB3	3:B:105:HEM:CHC	2.36	0.56
1:C:216:ASN:HD22	1:C:222:GLN:HE21	1.54	0.56
1:C:24:ASN:O	1:C:28:LEU:HD22	2.05	0.56
2:B:64:LEU:CB	2:B:95:ILE:HD11	2.35	0.56
2:B:20:VAL:O	2:B:33:HIS:HB2	2.06	0.55
1:A:163:MET:CE	1:A:167:GLU:HB3	2.36	0.55
1:C:236:TYR:CE2	1:C:239:ILE:HD11	2.40	0.55
2:B:74:TYR:O	2:B:75:ILE:HG12	2.07	0.55
1:C:93:GLU:N	1:C:94:PRO:CD	2.70	0.55
2:B:42:GLN:HB3	4:B:468:HOH:O	2.06	0.55
1:C:204:LEU:O	1:C:208:ASN:HB2	2.07	0.55
1:A:169:VAL:HG12	1:A:251:TYR:HE2	1.68	0.55
1:A:16:TYR:CG	1:A:16:TYR:O	2.60	0.55
1:A:292:GLN:C	1:A:294:LEU:HD12	2.27	0.55
2:B:8:LYS:HG3	4:B:415:HOH:O	2.07	0.55
1:A:134:PRO:O	1:A:136:ASP:N	2.40	0.55
1:A:212:LYS:HE2	4:A:445:HOH:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:ASN:HD21	1:C:167:GLU:HG3	1.68	0.55
2:B:94:LEU:O	2:B:98:LEU:HG	2.07	0.54
2:B:59:TRP:CE3	2:B:64:LEU:HD23	2.42	0.54
1:A:158:PHE:HB3	1:A:163:MET:HB2	1.88	0.54
1:C:48:ARG:O	1:C:49:LEU:C	2.46	0.54
1:C:72:ARG:NH2	1:C:133:THR:O	2.41	0.54
1:A:128:CYS:CB	4:A:492:HOH:O	2.56	0.54
2:B:82:PHE:CE2	2:B:84:GLY:CA	2.91	0.54
1:C:271:GLU:O	1:C:274:ILE:HG13	2.08	0.54
1:C:292:GLN:CB	1:C:294:LEU:HD12	2.38	0.54
1:A:277:PRO:HG2	4:A:487:HOH:O	2.07	0.54
1:A:1:THR:CG2	1:A:2:THR:N	2.70	0.54
1:C:92:LEU:C	1:C:94:PRO:HD2	2.28	0.54
1:A:172:MET:SD	3:A:295:HEM:HBB2	2.47	0.54
1:C:82:ASN:O	1:C:85:LEU:HB2	2.07	0.54
2:B:32:LEU:O	2:B:102:THR:HG22	2.08	0.54
1:C:166:ARG:HB2	1:C:247:ILE:HD13	1.90	0.54
1:A:201:GLU:O	1:A:202:PHE:C	2.46	0.54
1:A:15:SER:O	1:A:19:PHE:HD2	1.91	0.54
2:B:81:ILE:HG12	4:B:456:HOH:O	2.08	0.54
2:B:65:MET:N	2:B:95:ILE:CD1	2.71	0.54
1:A:147:ALA:HB1	1:A:232:LEU:HD13	1.90	0.54
1:A:59:LYS:HD2	1:A:162:ASN:ND2	2.23	0.54
1:A:241:ASP:O	1:A:245:LEU:HB2	2.08	0.53
1:C:48:ARG:HD3	1:C:85:LEU:HD21	1.88	0.53
3:B:105:HEM:HHC	3:B:105:HEM:CBB	2.38	0.53
2:B:59:TRP:CE3	2:B:64:LEU:CD2	2.91	0.53
1:C:26:ILE:HG22	1:C:114:THR:CG2	2.31	0.53
1:C:230:MET:HE2	1:C:230:MET:O	2.08	0.53
2:B:62:GLU:HB2	4:B:352:HOH:O	2.09	0.53
1:C:203:TYR:HD1	1:C:248:VAL:HG13	1.74	0.53
2:B:30:PRO:HG3	2:B:46:PHE:CG	2.44	0.53
1:A:34:ASP:HA	4:A:411:HOH:O	2.08	0.52
1:C:105:GLY:O	1:C:130:ARG:HD2	2.09	0.52
2:B:21:GLU:CD	2:B:21:GLU:H	2.12	0.52
2:B:65:MET:N	2:B:95:ILE:HD11	2.24	0.52
1:C:133:THR:HB	1:C:134:PRO:CD	2.38	0.52
1:A:73:PHE:CE2	1:A:135:GLU:HA	2.45	0.52
1:C:33:ASP:N	1:C:33:ASP:OD1	2.43	0.52
1:A:182:LEU:N	1:A:187:TYR:O	2.43	0.52
2:B:80:MET:HB2	3:B:105:HEM:C4D	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ARG:HG3	1:A:130:ARG:NH1	2.23	0.52
1:C:257:LYS:O	1:C:261:ASP:OD1	2.27	0.52
1:C:73:PHE:O	1:C:77:PHE:N	2.41	0.52
1:A:16:TYR:HD1	1:A:284:PHE:CD1	2.28	0.52
1:C:166:ARG:CA	1:C:247:ILE:HD13	2.40	0.52
1:A:202:PHE:HZ	1:A:235:ASP:HB3	1.74	0.52
2:B:41:GLY:HA2	2:B:48:TYR:CG	2.45	0.52
1:A:280:ALA:HA	4:A:338:HOH:O	2.10	0.52
2:B:25:LYS:CE	2:B:27:LYS:HE2	2.34	0.51
2:B:70:ASN:OD1	2:B:72:LYS:CG	2.54	0.51
1:C:73:PHE:O	1:C:77:PHE:HB2	2.11	0.51
2:B:69:GLU:HA	2:B:85:ILE:O	2.11	0.51
1:A:3:PRO:HB3	1:A:61:ASP:O	2.09	0.51
1:C:71:TYR:CE2	1:C:77:PHE:CE1	2.98	0.51
2:B:56:GLY:O	2:B:57:ILE:HG22	2.10	0.51
1:C:133:THR:HB	1:C:137:THR:HG21	1.92	0.51
1:C:182:LEU:HD11	1:C:218:ALA:HB2	1.93	0.51
2:B:41:GLY:HA2	2:B:48:TYR:CE2	2.46	0.51
1:C:238:LEU:HD23	1:C:244:TYR:CD2	2.45	0.51
1:C:179:LYS:HE3	1:C:180:THR:O	2.10	0.51
1:C:58:ASP:HB2	1:C:143:ARG:HH12	1.74	0.51
1:C:145:PRO:HA	1:C:153:TYR:OH	2.10	0.51
1:C:4:LEU:CG	4:C:657:HOH:O	2.45	0.51
1:A:125:PRO:HG3	1:A:285:ILE:HD11	1.93	0.51
2:B:50:ASP:O	2:B:54:ASN:HB2	2.11	0.51
2:B:7:LYS:HD3	4:B:415:HOH:O	2.09	0.51
1:C:230:MET:HE3	1:C:231:MET:C	2.31	0.51
1:C:39:TYR:HD2	4:C:429:HOH:O	1.93	0.51
2:B:94:LEU:O	2:B:94:LEU:HD12	2.11	0.50
1:A:275:THR:O	1:A:277:PRO:HD3	2.12	0.50
1:C:204:LEU:O	1:C:208:ASN:N	2.38	0.50
1:C:249:LYS:O	1:C:252:ALA:HB3	2.12	0.50
2:B:78:THR:OG1	2:B:79:LYS:N	2.45	0.50
1:A:46:LEU:O	1:A:47:VAL:C	2.50	0.50
2:B:32:LEU:O	2:B:102:THR:HB	2.11	0.50
2:B:12:GLN:NE2	4:B:413:HOH:O	2.33	0.50
1:C:139:PRO:HB3	1:C:143:ARG:HH21	1.76	0.50
2:B:68:LEU:C	2:B:91:ARG:HD2	2.31	0.50
1:A:26:ILE:HB	1:A:114:THR:HG21	1.93	0.49
1:A:26:ILE:CG2	1:A:114:THR:HG21	2.42	0.49
2:B:40:THR:HB	2:B:52:ASN:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:ASP:HB3	4:C:680:HOH:O	2.13	0.49
1:C:26:ILE:CG1	1:C:95:ILE:HD13	2.42	0.49
1:C:120:GLN:HB2	1:C:197:VAL:HG23	1.95	0.49
1:A:257:LYS:O	1:A:258:PHE:C	2.50	0.49
2:B:26:HIS:HB3	4:B:354:HOH:O	2.13	0.49
2:B:48:TYR:HA	2:B:79:LYS:NZ	2.28	0.49
2:B:66:GLU:CD	2:B:74:TYR:CE2	2.86	0.49
1:C:105:GLY:HA2	4:C:630:HOH:O	2.13	0.49
1:A:15:SER:O	1:A:19:PHE:CD2	2.65	0.49
1:C:144:LEU:CD1	4:C:612:HOH:O	2.60	0.49
2:B:87:LYS:HB3	2:B:87:LYS:HE2	1.66	0.49
1:A:51:TRP:O	1:A:52:HIS:C	2.46	0.49
1:C:179:LYS:HB3	1:C:190:PRO:HB3	1.94	0.49
1:A:47:VAL:CG2	1:A:116:VAL:CG2	2.91	0.49
1:C:119:MET:O	1:C:120:GLN:CB	2.60	0.49
1:A:79:ASP:OD2	4:A:432:HOH:O	2.20	0.49
1:A:164:ASN:O	1:A:168:VAL:HG13	2.12	0.49
2:B:16:GLN:CD	2:B:16:GLN:N	2.65	0.49
1:A:184:ASN:ND2	3:A:295:HEM:O2A	2.46	0.49
1:A:58:ASP:OD1	1:A:60:HIS:ND1	2.46	0.49
2:B:33:HIS:HA	2:B:102:THR:O	2.13	0.48
1:C:166:ARG:HA	1:C:247:ILE:HD13	1.94	0.48
2:B:64:LEU:CB	2:B:95:ILE:CD1	2.89	0.48
1:C:272:ASN:CA	4:C:692:HOH:O	2.45	0.48
1:A:212:LYS:HD3	4:A:445:HOH:O	2.12	0.48
2:B:57:ILE:CD1	2:B:58:THR:O	2.61	0.48
1:C:93:GLU:HB3	1:C:94:PRO:HD3	1.95	0.48
1:C:23:TYR:OH	1:C:288:THR:HG22	2.13	0.48
2:B:3:VAL:O	2:B:7:LYS:HB2	2.13	0.48
2:B:60:LYS:HB3	2:B:63:THR:OG1	2.14	0.48
1:A:271:GLU:O	1:A:272:ASN:C	2.52	0.48
1:A:166:ARG:NH2	1:A:250:GLU:OE2	2.46	0.48
1:C:143:ARG:HG3	4:C:672:HOH:O	2.13	0.48
2:B:14:CYS:C	2:B:16:GLN:N	2.64	0.48
1:C:27:ALA:HB1	1:C:289:LEU:HG	1.96	0.48
1:C:214:GLU:O	1:C:221:GLU:HA	2.13	0.48
1:A:181:HIS:C	1:A:187:TYR:O	2.53	0.48
2:B:7:LYS:HD2	4:B:415:HOH:O	2.10	0.47
1:C:44:PRO:HD2	4:C:712:HOH:O	2.13	0.47
1:C:42:TYR:CG	1:C:91:PHE:CD2	3.02	0.47
1:A:73:PHE:CE1	1:A:135:GLU:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:THR:O	2:B:52:ASN:N	2.38	0.47
1:C:186:GLY:O	1:C:220:ASN:ND2	2.41	0.47
2:B:98:LEU:O	2:B:99:LYS:C	2.53	0.47
1:A:155:ARG:NH2	1:A:241:ASP:OD1	2.42	0.47
1:A:202:PHE:CZ	1:A:235:ASP:HB3	2.49	0.47
1:A:68:GLY:CA	1:A:133:THR:OG1	2.62	0.47
1:C:213:LEU:HD13	1:C:223:TRP:NE1	2.29	0.47
1:C:48:ARG:NH1	1:C:85:LEU:HG	2.29	0.47
2:B:26:HIS:CB	4:B:354:HOH:O	2.62	0.47
2:B:80:MET:HB2	3:B:105:HEM:ND	2.29	0.47
1:C:134:PRO:HD2	1:C:137:THR:HG23	1.96	0.47
1:C:42:TYR:O	1:C:45:VAL:HG12	2.15	0.47
1:A:182:LEU:HB2	1:A:188:GLU:HB2	1.95	0.47
2:B:69:GLU:HB2	2:B:91:ARG:NH2	2.29	0.47
1:A:29:LYS:HE3	4:A:437:HOH:O	2.15	0.47
2:B:3:VAL:HG11	2:B:100:LYS:CD	2.44	0.47
2:B:70:ASN:HD22	2:B:73:LYS:NZ	2.12	0.47
1:C:133:THR:HB	1:C:134:PRO:HD3	1.95	0.47
1:A:290:GLU:O	1:A:290:GLU:HG3	2.14	0.47
1:A:20:GLN:O	1:A:23:TYR:HB3	2.15	0.47
1:A:34:ASP:N	1:A:34:ASP:OD1	2.48	0.46
2:B:22:LYS:HA	2:B:31:ASN:HD21	1.80	0.46
2:B:3:VAL:O	2:B:7:LYS:N	2.47	0.46
1:A:69:GLY:O	1:A:72:ARG:HD3	2.15	0.46
1:C:144:LEU:HD11	4:C:612:HOH:O	2.13	0.46
1:C:182:LEU:HB2	1:C:188:GLU:HG2	1.97	0.46
1:C:79:ASP:HA	1:C:80:PRO:HD3	1.82	0.46
2:B:48:TYR:CA	2:B:79:LYS:HZ1	2.28	0.46
1:C:6:HIS:HB3	1:C:67:TYR:CE2	2.51	0.46
1:A:155:ARG:HH22	1:A:241:ASP:CG	2.19	0.46
1:A:243:LYS:HB2	1:A:243:LYS:HE3	1.51	0.46
1:C:236:TYR:O	1:C:239:ILE:HG13	2.15	0.46
2:B:62:GLU:O	2:B:63:THR:C	2.52	0.46
2:B:36:PHE:HE1	2:B:98:LEU:HB3	1.80	0.46
1:A:1:THR:O	1:A:3:PRO:HD3	2.15	0.46
1:A:166:ARG:NH2	1:A:257:LYS:HE3	2.28	0.46
1:C:276:PHE:HA	1:C:277:PRO:HD2	1.64	0.46
1:A:167:GLU:CD	1:A:268:LYS:HZ2	2.19	0.46
2:B:13:LYS:NZ	4:B:383:HOH:O	2.49	0.46
2:B:26:HIS:CD2	2:B:30:PRO:HA	2.50	0.46
2:B:54:ASN:C	2:B:56:GLY:N	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:LEU:CB	4:C:657:HOH:O	2.63	0.46
2:B:39:LYS:C	2:B:42:GLN:HE21	2.18	0.46
2:B:40:THR:HG23	2:B:57:ILE:H	1.79	0.46
2:B:3:VAL:HG11	2:B:100:LYS:HG3	1.97	0.46
1:A:59:LYS:CD	1:A:162:ASN:ND2	2.79	0.46
1:A:34:ASP:OD2	2:B:90:GLU:OE1	2.33	0.46
2:B:31:ASN:C	2:B:31:ASN:OD1	2.54	0.46
2:B:57:ILE:C	2:B:57:ILE:HD12	2.36	0.46
1:C:241:ASP:HA	1:C:242:PRO:HD3	1.74	0.46
1:A:10:VAL:HA	4:A:492:HOH:O	2.16	0.46
1:A:112:GLY:O	1:A:116:VAL:HG23	2.16	0.46
1:C:215:LYS:HD3	1:C:219:ASN:O	2.15	0.46
1:C:200:ASN:H	1:C:200:ASN:HD22	1.63	0.46
1:A:46:LEU:C	1:A:48:ARG:N	2.69	0.46
1:A:4:LEU:O	1:A:62:ASN:ND2	2.48	0.46
1:A:7:VAL:HG23	1:A:8:ALA:O	2.15	0.46
2:B:56:GLY:O	2:B:57:ILE:CG2	2.64	0.45
1:A:232:LEU:HB2	1:A:235:ASP:OD2	2.15	0.45
1:C:138:THR:HA	1:C:139:PRO:HD3	1.83	0.45
1:C:71:TYR:HA	1:C:76:GLU:HG2	1.94	0.45
1:C:19:PHE:CD2	1:C:284:PHE:HE2	2.33	0.45
2:B:27:LYS:N	2:B:27:LYS:HD2	2.32	0.45
1:C:71:TYR:CE2	1:C:77:PHE:HE1	2.35	0.45
1:A:243:LYS:O	1:A:247:ILE:HG13	2.16	0.45
1:C:191:TRP:HD1	1:C:231:MET:CE	2.29	0.45
2:B:31:ASN:ND2	4:B:349:HOH:O	2.23	0.45
1:A:2:THR:HG23	1:A:2:THR:O	2.17	0.45
1:A:42:TYR:CD2	1:A:91:PHE:CD2	3.04	0.45
2:B:38:ARG:O	2:B:58:THR:HA	2.16	0.45
2:B:65:MET:HE1	2:B:92:GLU:HG3	1.96	0.45
1:C:289:LEU:HD23	1:C:289:LEU:HA	1.69	0.45
1:C:68:GLY:O	1:C:72:ARG:NH1	2.50	0.45
1:C:216:ASN:OD1	1:C:218:ALA:HB3	2.17	0.45
1:A:204:LEU:O	1:A:205:ASN:C	2.55	0.45
2:B:89:THR:O	2:B:92:GLU:HB2	2.17	0.45
2:B:64:LEU:O	2:B:65:MET:C	2.55	0.45
1:A:288:THR:O	1:A:292:GLN:HG3	2.17	0.45
1:A:47:VAL:CG2	1:A:116:VAL:HG22	2.47	0.45
2:B:75:ILE:HA	2:B:76:PRO:HD2	1.74	0.45
1:A:11:GLU:OE2	1:A:106:ASP:OD2	2.35	0.45
1:C:127:ARG:CD	1:C:271:GLU:OE2	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:ASN:O	1:C:28:LEU:CD2	2.65	0.45
2:B:4:GLU:HA	2:B:4:GLU:OE1	2.17	0.45
2:B:79:LYS:NZ	3:B:105:HEM:CGD	2.80	0.44
2:B:33:HIS:CD2	2:B:103:ASN:HA	2.52	0.44
2:B:39:LYS:HB3	2:B:42:GLN:HE22	1.80	0.44
1:C:143:ARG:HG2	4:C:672:HOH:O	2.13	0.44
1:A:53:ILE:CD1	1:A:108:PHE:HB2	2.44	0.44
1:C:127:ARG:HG3	1:C:271:GLU:OE2	2.16	0.44
1:A:110:LEU:HD23	1:A:110:LEU:O	2.16	0.44
1:C:6:HIS:HB3	1:C:67:TYR:CD2	2.53	0.44
1:A:207:LEU:HD12	1:A:252:ALA:CB	2.46	0.44
1:A:58:ASP:CG	1:A:160:ARG:HD2	2.38	0.44
1:C:280:ALA:HA	4:C:622:HOH:O	2.16	0.44
2:B:54:ASN:O	2:B:55:LYS:C	2.54	0.44
1:C:216:ASN:ND2	1:C:222:GLN:NE2	2.61	0.44
2:B:48:TYR:HB3	2:B:53:LYS:HZ1	1.82	0.44
1:C:232:LEU:O	1:C:233:PRO:C	2.55	0.44
3:A:295:HEM:HBC2	3:A:295:HEM:HMC1	2.00	0.44
1:A:151:ALA:CA	1:A:237:SER:HB3	2.47	0.44
2:B:57:ILE:HD12	2:B:58:THR:O	2.18	0.44
2:B:66:GLU:CG	2:B:74:TYR:CD2	3.00	0.44
1:C:14:ARG:HB3	1:C:18:ASP:HB2	1.99	0.44
1:A:147:ALA:O	1:A:233:PRO:HB2	2.18	0.44
2:B:85:ILE:C	2:B:86:LYS:HD3	2.38	0.44
1:A:210:ASP:HB3	4:A:439:HOH:O	2.16	0.44
2:B:66:GLU:CD	2:B:74:TYR:HE2	2.19	0.44
1:C:130:ARG:NH2	4:C:664:HOH:O	2.51	0.44
1:A:4:LEU:HD12	1:A:6:HIS:HE1	1.83	0.44
1:A:237:SER:O	1:A:238:LEU:C	2.55	0.44
1:C:193:ALA:HB2	1:C:229:TYR:OH	2.18	0.44
2:B:50:ASP:HA	2:B:53:LYS:CE	2.30	0.43
1:C:24:ASN:N	1:C:24:ASN:HD22	2.15	0.43
1:A:53:ILE:O	1:A:65:GLY:O	2.36	0.43
1:A:206:LEU:HG	1:A:239:ILE:CG2	2.48	0.43
1:A:127:ARG:O	1:A:130:ARG:NH1	2.47	0.43
1:A:155:ARG:HH11	1:A:155:ARG:HD2	1.37	0.43
2:B:22:LYS:HB2	2:B:33:HIS:ND1	2.34	0.43
1:C:56:THR:HA	1:C:143:ARG:HB2	2.00	0.43
1:A:3:PRO:HG3	1:A:61:ASP:HA	2.00	0.43
1:C:8:ALA:HB3	1:C:276:PHE:CD1	2.53	0.43
1:A:15:SER:OG	1:A:16:TYR:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:TRP:HB3	1:A:161:LEU:HD22	1.99	0.43
2:B:56:GLY:C	2:B:57:ILE:CG2	2.87	0.43
1:C:143:ARG:HB3	1:C:160:ARG:NH2	2.34	0.43
1:A:67:TYR:HA	1:A:130:ARG:HB3	2.01	0.43
1:C:243:LYS:HG3	4:C:639:HOH:O	2.18	0.43
1:C:19:PHE:CD2	1:C:284:PHE:CE2	3.07	0.43
1:C:74:LYS:HB3	1:C:75:LYS:H	1.25	0.43
1:A:48:ARG:NH1	4:A:364:HOH:O	2.49	0.43
1:A:2:THR:HA	1:A:3:PRO:HD3	1.80	0.43
1:A:130:ARG:CG	1:A:130:ARG:NH1	2.80	0.43
1:A:280:ALA:HA	1:A:281:PRO:HD3	1.53	0.42
1:A:74:LYS:HE3	1:A:74:LYS:HB2	1.82	0.42
1:C:62:ASN:O	1:C:62:ASN:CG	2.57	0.42
2:B:10:PHE:HA	2:B:14:CYS:SG	2.60	0.42
2:B:63:THR:HG22	2:B:74:TYR:OH	2.20	0.42
1:C:42:TYR:CD2	1:C:91:PHE:CD2	3.08	0.42
1:A:79:ASP:HA	1:A:141:ASN:ND2	2.34	0.42
2:B:10:PHE:CD1	2:B:10:PHE:C	2.92	0.42
1:C:166:ARG:O	1:C:167:GLU:C	2.56	0.42
1:A:11:GLU:O	1:A:12:LYS:C	2.57	0.42
1:C:144:LEU:HA	1:C:145:PRO:HD3	1.81	0.42
1:A:204:LEU:HD21	1:A:252:ALA:O	2.19	0.42
2:B:74:TYR:O	2:B:75:ILE:CG1	2.67	0.42
2:B:62:GLU:HA	2:B:65:MET:HB2	2.02	0.42
2:B:74:TYR:C	2:B:75:ILE:CG1	2.88	0.42
1:C:31:ARG:NE	4:C:740:HOH:O	2.48	0.42
1:A:241:ASP:O	1:A:245:LEU:CB	2.68	0.42
2:B:68:LEU:HB2	2:B:91:ARG:CG	2.50	0.42
2:B:59:TRP:CE3	2:B:64:LEU:HD21	2.55	0.42
1:C:238:LEU:HA	1:C:238:LEU:HD23	1.81	0.42
1:C:106:ASP:OD1	1:C:130:ARG:NH1	2.49	0.42
1:A:271:GLU:C	4:A:447:HOH:O	2.58	0.42
1:C:53:ILE:HG22	1:C:71:TYR:CB	2.44	0.42
2:B:65:MET:H	2:B:95:ILE:CD1	2.32	0.41
1:C:4:LEU:CA	4:C:657:HOH:O	2.68	0.41
1:C:241:ASP:HB3	1:C:244:TYR:HB2	2.00	0.41
1:C:131:VAL:O	1:C:132:ASP:C	2.58	0.41
1:C:127:ARG:HD2	1:C:127:ARG:HH11	1.53	0.41
1:C:42:TYR:CD2	1:C:91:PHE:HD2	2.39	0.41
1:C:230:MET:CE	1:C:230:MET:O	2.67	0.41
1:C:164:ASN:HD22	1:C:167:GLU:HG3	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:LYS:HE3	2:B:27:LYS:HB3	2.01	0.41
1:C:71:TYR:O	1:C:77:PHE:HD1	2.03	0.41
1:A:41:GLY:HA3	4:A:398:HOH:O	2.20	0.41
1:C:251:TYR:HB3	1:C:258:PHE:HB2	2.03	0.41
2:B:53:LYS:NZ	2:B:53:LYS:H	2.18	0.41
1:A:147:ALA:CB	1:A:232:LEU:HD13	2.50	0.41
1:A:14:ARG:HG2	1:A:101:TRP:CE3	2.56	0.41
1:A:278:LYS:C	1:A:280:ALA:H	2.24	0.41
1:A:79:ASP:HA	1:A:80:PRO:HD3	1.82	0.41
2:B:68:LEU:CB	2:B:91:ARG:HD2	2.50	0.41
2:B:67:TYR:O	2:B:71:PRO:HD3	2.19	0.41
2:B:46:PHE:HE2	2:B:79:LYS:HZ3	1.68	0.41
2:B:49:THR:C	2:B:53:LYS:HZ3	2.21	0.41
2:B:53:LYS:HG3	2:B:53:LYS:HZ2	1.41	0.41
1:C:68:GLY:O	1:C:132:ASP:HA	2.21	0.41
1:C:189:GLY:HA2	1:C:190:PRO:HD3	1.87	0.41
1:C:199:THR:HB	1:C:200:ASN:H	1.68	0.41
1:A:72:ARG:NH2	1:A:73:PHE:HZ	2.14	0.41
1:A:262:PHE:O	1:A:263:SER:C	2.58	0.41
1:A:151:ALA:N	1:A:237:SER:HB3	2.36	0.41
2:B:29:GLY:HA2	2:B:30:PRO:HD3	1.84	0.41
2:B:19:THR:CG2	2:B:25:LYS:O	2.69	0.41
2:B:72:LYS:HB3	2:B:72:LYS:HE3	1.89	0.41
1:C:179:LYS:HA	1:C:191:TRP:CZ3	2.56	0.41
2:B:49:THR:C	2:B:53:LYS:HZ1	2.23	0.41
2:B:62:GLU:O	2:B:65:MET:N	2.54	0.41
2:B:14:CYS:C	2:B:16:GLN:H	2.23	0.41
1:A:12:LYS:NZ	1:A:12:LYS:HB2	2.36	0.41
1:C:127:ARG:HG2	1:C:283:PRO:HB3	2.02	0.41
1:C:194:ALA:HB1	1:C:197:VAL:HG12	2.02	0.41
1:A:245:LEU:HD12	1:A:245:LEU:O	2.21	0.41
1:C:202:PHE:HB3	4:C:683:HOH:O	2.20	0.41
2:B:27:LYS:N	2:B:27:LYS:CD	2.84	0.41
1:A:32:GLU:HB3	1:A:33:ASP:OD1	2.21	0.40
2:B:2:ASP:HB2	2:B:5:LYS:N	2.29	0.40
1:C:191:TRP:HD1	1:C:231:MET:HE2	1.86	0.40
1:A:73:PHE:CD2	1:A:135:GLU:HA	2.56	0.40
2:B:40:THR:O	2:B:53:LYS:HA	2.21	0.40
1:C:214:GLU:O	1:C:222:GLN:N	2.49	0.40
1:A:92:LEU:O	1:A:95:ILE:HB	2.21	0.40
1:A:22:VAL:HG22	1:A:99:PHE:CG	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:LYS:NZ	4:A:462:HOH:O	2.53	0.40
1:A:11:GLU:H	1:A:11:GLU:HG2	1.50	0.40
1:A:88:GLY:O	1:A:92:LEU:HG	2.21	0.40
1:A:264:LYS:NZ	1:C:35:GLU:OE1	2.55	0.40
1:C:47:VAL:HG22	3:C:295:HEM:HMD3	2.04	0.40
1:C:1:THR:HG23	1:C:2:THR:H	1.87	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:444:HOH:O	4:A:444:HOH:O[8_665]	1.51	0.69
4:A:376:HOH:O	4:C:607:HOH:O[6_455]	1.61	0.59
1:C:279:ASP:CA	4:B:466:HOH:O[8_655]	2.09	0.11

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%)	23 (8%)	5 (2%)	11 36
1	C	292/296 (99%)	258 (88%)	29 (10%)	5 (2%)	11 36
2	B	102/104 (98%)	75 (74%)	19 (19%)	8 (8%)	1 2
All	All	686/696 (99%)	597 (87%)	71 (10%)	18 (3%)	7 22

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	135	GLU
1	A	277	PRO
2	B	61	GLU
2	B	65	MET

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Mol	Chain	Res	Type
2	B	100	LYS
2	B	101	ALA
1	C	85	LEU
2	B	96	ALA
2	B	97	TYR
1	C	229	TYR
1	A	12	LYS
2	B	48	TYR
1	C	59	LYS
1	C	74	LYS
1	A	34	ASP
1	C	190	PRO
1	A	33	ASP
2	B	84	GLY

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%)	215 (85%)	37 (15%)	4 11
1	C	252/254 (99%)	220 (87%)	32 (13%)	5 16
2	B	86/86 (100%)	67 (78%)	19 (22%)	1 3
All	All	590/594 (99%)	502 (85%)	88 (15%)	4 11

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	THR
1	A	4	LEU
1	A	5	VAL
1	A	7	VAL
1	A	9	SER
1	A	11	GLU
1	A	12	LYS
1	A	51	TRP

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Mol	Chain	Res	Type
1	A	74	LYS
1	A	81	SER
1	A	86	GLN
1	A	90	LYS
1	A	91	PHE
1	A	94	PRO
1	A	110	LEU
1	A	124	ILE
1	A	135	GLU
1	A	149	LYS
1	A	182	LEU
1	A	183	LYS
1	A	184	ASN
1	A	195	ASN
1	A	212	LYS
1	A	215	LYS
1	A	226	LYS
1	A	227	SER
1	A	239	ILE
1	A	243	LYS
1	A	247	ILE
1	A	257	LYS
1	A	260	LYS
1	A	263	SER
1	A	267	GLU
1	A	269	LEU
1	A	278	LYS
1	A	289	LEU
1	A	292	GLN
2	B	2	ASP
2	B	7	LYS
2	B	14	CYS
2	B	16	GLN
2	B	27	LYS
2	B	31	ASN
2	B	39	LYS
2	B	42	GLN
2	B	50	ASP
2	B	52	ASN
2	B	53	LYS
2	B	54	ASN
2	B	55	LYS

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Mol	Chain	Res	Type
2	B	57	ILE
2	B	63	THR
2	B	69	GLU
2	B	79	LYS
2	B	86	LYS
2	B	91	ARG
1	C	5	VAL
1	C	7	VAL
1	C	17	GLU
1	C	33	ASP
1	C	35	GLU
1	C	47	VAL
1	C	51	TRP
1	C	66	SER
1	C	70	THR
1	C	74	LYS
1	C	75	LYS
1	C	76	GLU
1	C	86	GLN
1	C	90	LYS
1	C	138	THR
1	C	160	ARG
1	C	181	HIS
1	C	200	ASN
1	C	217	ASP
1	C	226	LYS
1	C	227	SER
1	C	230	MET
1	C	237	SER
1	C	243	LYS
1	C	245	LEU
1	C	256	ASP
1	C	257	LYS
1	C	260	LYS
1	C	261	ASP
1	C	274	ILE
1	C	287	LYS
1	C	292	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	HIS
1	A	96	HIS
1	A	117	GLN
1	A	141	ASN
1	A	162	ASN
1	A	195	ASN
1	A	222	GLN
2	B	26	HIS
2	B	42	GLN
2	B	54	ASN
2	B	103	ASN
1	C	20	GLN
1	C	24	ASN
1	C	86	GLN
1	C	162	ASN
1	C	200	ASN
1	C	208	ASN
1	C	222	GLN
1	C	292	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	HEM	A	295	1	30,50,50	2.50	7 (23%)	24,82,82	2.62	8 (33%)
3	HEM	B	105	2	30,50,50	2.39	8 (26%)	24,82,82	2.63	13 (54%)
3	HEM	C	295	1,4	30,50,50	2.43	7 (23%)	24,82,82	3.01	14 (58%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	A	295	1	-	0/10/54/54	0/0/8/8
3	HEM	B	105	2	-	0/10/54/54	0/0/8/8
3	HEM	C	295	1,4	-	0/10/54/54	0/0/8/8

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	295	HEM	C3B-C4B	-8.04	1.44	1.51
3	C	295	HEM	C2D-C3D	-7.34	1.32	1.54
3	A	295	HEM	C2D-C3D	-7.09	1.33	1.54
3	C	295	HEM	C3B-C4B	-6.96	1.45	1.51
3	B	105	HEM	C2D-C3D	-6.71	1.34	1.54
3	B	105	HEM	C3B-C4B	-6.37	1.46	1.51
3	B	105	HEM	C3D-C4D	-5.65	1.44	1.51
3	C	295	HEM	C2C-C1C	-4.12	1.44	1.52
3	A	295	HEM	C3D-C4D	-4.11	1.46	1.51
3	A	295	HEM	C2C-C1C	-3.91	1.45	1.52
3	B	105	HEM	C2C-C1C	-3.90	1.45	1.52
3	C	295	HEM	C3D-C4D	-3.50	1.47	1.51
3	A	295	HEM	C2B-C1B	-2.14	1.44	1.51
3	A	295	HEM	C2D-C1D	-2.11	1.45	1.51
3	B	105	HEM	C2B-C1B	-2.07	1.45	1.51
3	B	105	HEM	C4C-NC	2.10	1.38	1.36
3	B	105	HEM	C1C-NC	2.10	1.38	1.36
3	C	295	HEM	CAD-C3D	2.14	1.58	1.54
3	B	105	HEM	CAA-C2A	2.34	1.56	1.52
3	C	295	HEM	C1C-NC	2.45	1.39	1.36
3	A	295	HEM	C4C-NC	2.79	1.39	1.36
3	C	295	HEM	CAA-C2A	3.10	1.57	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	295	HEM	CAA-C2A-C1A	-4.39	122.24	127.01
3	B	105	HEM	CMA-C3A-C4A	-4.10	121.57	128.36
3	C	295	HEM	CMA-C3A-C4A	-3.46	122.64	128.36
3	C	295	HEM	CAA-C2A-C1A	-2.65	124.14	127.01
3	C	295	HEM	C1D-CHD-C4C	-2.55	121.56	125.82
3	B	105	HEM	C4B-CHC-C1C	-2.45	121.73	125.82
3	C	295	HEM	CBD-CAD-C3D	-2.12	107.40	113.55
3	B	105	HEM	CAA-C2A-C1A	-2.11	124.72	127.01
3	B	105	HEM	CBA-CAA-C2A	2.06	116.22	112.53
3	B	105	HEM	CBD-CAD-C3D	2.20	119.96	113.55
3	A	295	HEM	CAD-C3D-C4D	2.49	121.25	112.47
3	B	105	HEM	CAA-CBA-CGA	2.59	117.49	112.75
3	C	295	HEM	CAD-CBD-CGD	2.62	123.70	113.02
3	A	295	HEM	C3C-CAC-CBC	2.80	128.75	124.46
3	B	105	HEM	CMA-C3A-C2A	2.87	131.25	125.24
3	C	295	HEM	CAD-C3D-C4D	3.14	123.53	112.47
3	C	295	HEM	CMD-C2D-C3D	3.30	128.96	114.35
3	A	295	HEM	CMD-C2D-C3D	3.41	129.44	114.35
3	B	105	HEM	CAD-C3D-C4D	3.44	124.62	112.47
3	C	295	HEM	CBA-CAA-C2A	3.53	118.85	112.53
3	B	105	HEM	CMD-C2D-C3D	3.65	130.50	114.35
3	B	105	HEM	C2D-C3D-C4D	4.14	108.52	101.50
3	C	295	HEM	C2D-C3D-C4D	4.16	108.56	101.50
3	A	295	HEM	CMB-C2B-C3B	4.34	127.36	116.53
3	C	295	HEM	CAA-CBA-CGA	4.37	120.76	112.75
3	B	105	HEM	CMC-C2C-C3C	4.49	127.75	116.53
3	B	105	HEM	CMB-C2B-C3B	4.53	127.84	116.53
3	B	105	HEM	CAD-C3D-C2D	4.74	126.85	113.22
3	C	295	HEM	CMC-C2C-C3C	4.88	128.72	116.53
3	C	295	HEM	CMB-C2B-C3B	4.98	128.96	116.53
3	A	295	HEM	C2D-C3D-C4D	5.00	109.98	101.50
3	C	295	HEM	CAD-C3D-C2D	5.06	127.77	113.22
3	A	295	HEM	CMC-C2C-C3C	5.17	129.44	116.53
3	C	295	HEM	C3C-CAC-CBC	5.34	132.65	124.46
3	A	295	HEM	CAD-C3D-C2D	5.37	128.65	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	295	HEM	5	0
3	B	105	HEM	19	0
3	C	295	HEM	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	294/296 (99%)	-1.25	1 (0%) 94 92	10, 25, 47, 92	0
1	C	294/296 (99%)	-1.26	0 100 100	12, 26, 44, 62	0
2	B	104/104 (100%)	-0.27	1 (0%) 84 77	29, 68, 92, 107	0
All	All	692/696 (99%)	-1.11	2 (0%) 94 92	10, 27, 75, 107	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	THR	2.8
2	B	3	VAL	2.1

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	HEM	A	295	43/43	0.98	0.09	0.42	13,26,35,38	0
3	HEM	C	295	43/43	0.98	0.09	-0.35	15,23,26,28	0
3	HEM	B	105	43/43	0.97	0.12	-1.03	41,47,58,65	0

6.5 Other polymers (i)

There are no such residues in this entry.