Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:05 AM GMT

PDB ID	:	2PCC
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
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:

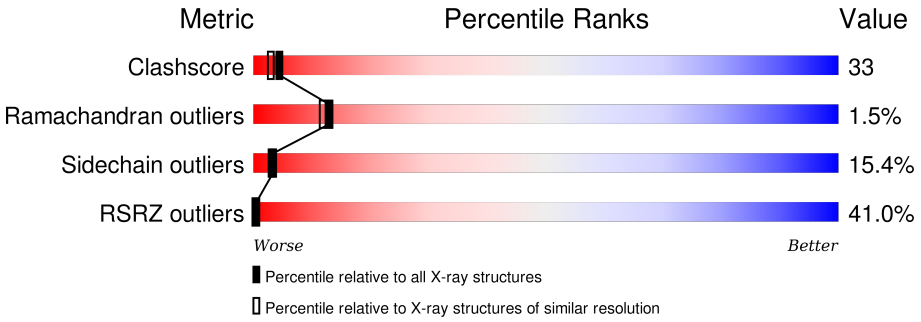
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.30 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	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (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 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	23% 44% 40% 13%
1	C	296	44% 46% 38% 13%
2	B	108	52% 39% 45% 15%
2	D	108	70% 32% 46% 19%

2 Entry composition

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
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			

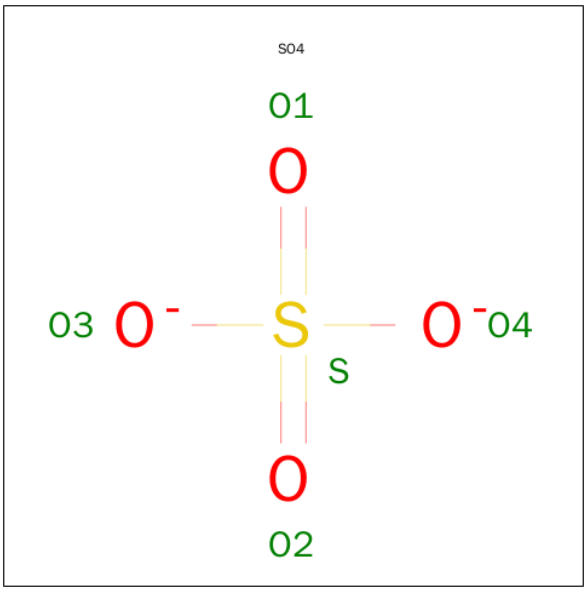
There are 4 discrepancies between the modelled and reference sequences:

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 ISO-1-CYTOCHROME C.

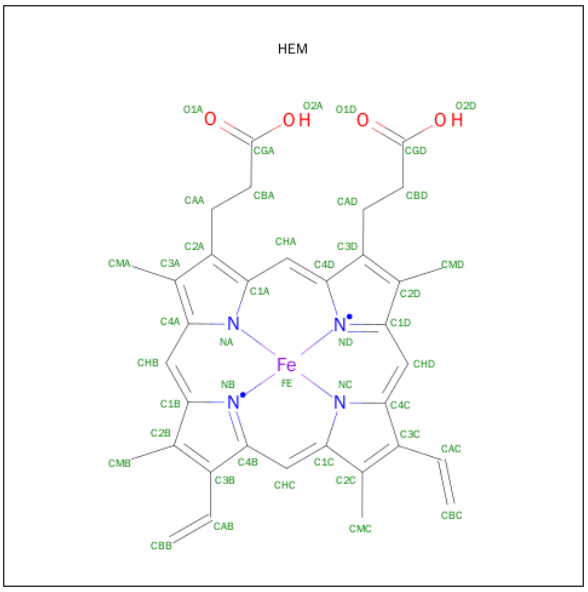
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	108	Total	C	N	O	S	0	0	0
			847	534	151	157	5			
2	D	108	Total	C	N	O	S	0	0	0
			847	534	151	157	5			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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



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

Continued on next page...

Continued from previous page...

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.

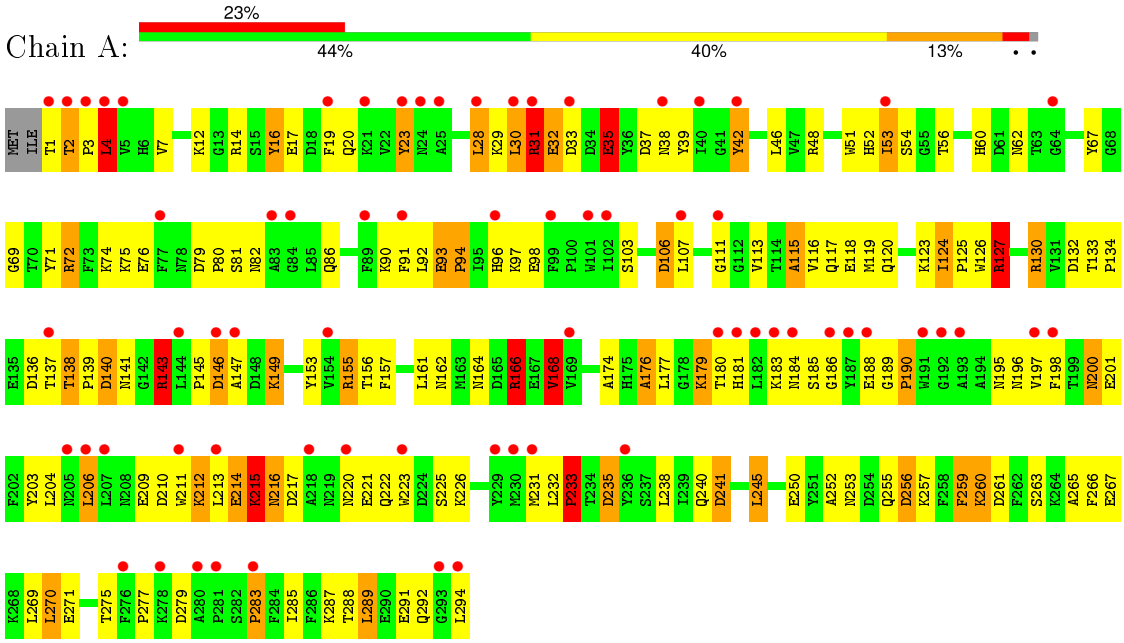
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	203	Total	O	0	0
			203	203		
5	B	46	Total	O	0	0
			46	46		
5	C	212	Total	O	0	0
			212	212		
5	D	42	Total	O	0	0
			42	42		

3 Residue-property plots (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.

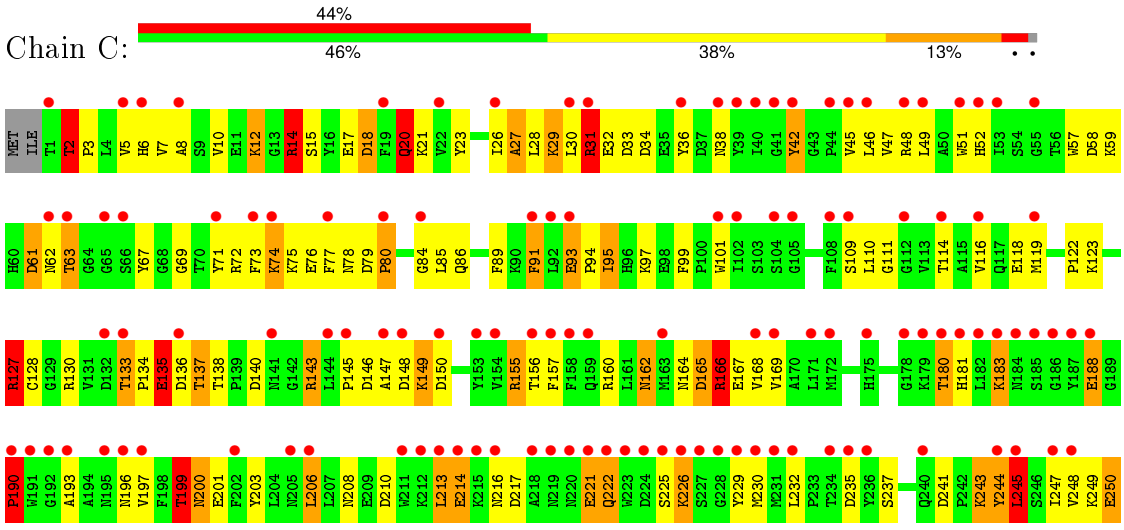
- Molecule 1: CYTOCHROME C PEROXIDASE

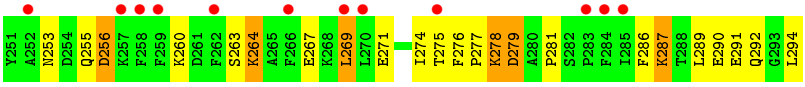
Chain A:



- Molecule 1: CYTOCHROME C PEROXIDASE

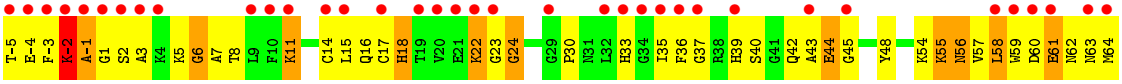
Chain C:

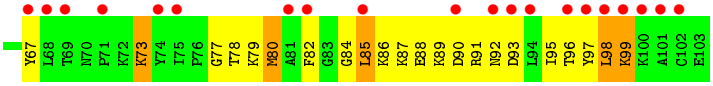




• Molecule 2: ISO-1-CYTOCHROME C

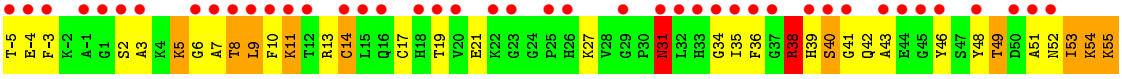
Chain B:

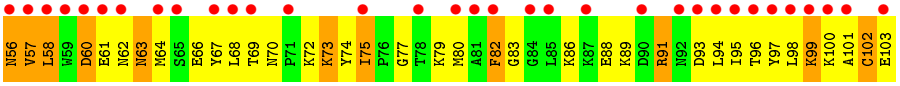




• Molecule 2: ISO-1-CYTOCHROME C

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	88.40Å 118.60Å 45.10Å 90.00° 104.60° 90.00°	Depositor
Resolution (Å)	6.00 – 2.30 35.89 – 2.25	Depositor EDS
% Data completeness (in resolution range)	(Not available) (6.00-2.30) 87.4 (35.89-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	8.10 (at 2.24Å)	Xtriage
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.167 , (Not available) 0.293 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	30.4	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 127.3	EDS
Estimated twinning fraction	0.095 for -h-l,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	2 of 37673 reflections (0.005%)	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	7115	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage'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.*

[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, 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	1.21	0/2438	2.08	74/3302 (2.2%)
1	C	1.18	2/2438 (0.1%)	2.09	97/3302 (2.9%)
2	B	0.93	0/865	1.71	4/1156 (0.3%)
2	D	0.93	0/865	1.73	11/1156 (1.0%)
All	All	1.13	2/6606 (0.0%)	2.00	186/8916 (2.1%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	225	SER	CA-CB	-5.76	1.44	1.52
1	C	181	HIS	CA-CB	5.43	1.65	1.53

All (186) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	23	TYR	CB-CG-CD2	15.44	130.26	121.00
1	A	155	ARG	NE-CZ-NH2	15.05	127.83	120.30
1	A	155	ARG	NE-CZ-NH1	-14.84	112.88	120.30
1	C	146	ASP	CB-CG-OD2	-14.44	105.31	118.30
1	A	130	ARG	NE-CZ-NH2	13.91	127.25	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	31	ARG	NE-CZ-NH2	-12.73	113.93	120.30
1	A	48	ARG	NE-CZ-NH2	-12.15	114.22	120.30
1	A	48	ARG	CD-NE-CZ	11.56	139.78	123.60
1	A	93	GLU	CA-CB-CG	11.44	138.56	113.40
1	C	18	ASP	CB-CG-OD1	-11.23	108.19	118.30
1	C	241	ASP	CB-CG-OD2	11.21	128.39	118.30
1	A	48	ARG	NE-CZ-NH1	11.13	125.86	120.30
1	A	132	ASP	CB-CG-OD1	10.65	127.89	118.30
1	A	115	ALA	CB-CA-C	9.81	124.81	110.10
1	C	23	TYR	CB-CG-CD1	-9.64	115.22	121.00
1	A	106	ASP	CB-CG-OD1	9.48	126.84	118.30
1	C	150	ASP	CB-CG-OD1	9.44	126.79	118.30
1	C	14	ARG	NE-CZ-NH1	9.39	125.00	120.30
1	A	98	GLU	CA-CB-CG	9.36	134.00	113.40
1	C	31	ARG	NE-CZ-NH1	9.32	124.96	120.30
1	A	23	TYR	CB-CG-CD2	9.32	126.59	121.00
1	C	14	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	C	61	ASP	CB-CG-OD2	8.80	126.22	118.30
1	C	269	LEU	CA-CB-CG	8.75	135.42	115.30
1	A	166	ARG	NE-CZ-NH1	-8.51	116.05	120.30
1	A	261	ASP	CB-CG-OD2	-8.51	110.64	118.30
1	A	143	ARG	CD-NE-CZ	-8.50	111.70	123.60
1	A	132	ASP	CB-CG-OD2	-8.47	110.67	118.30
1	C	127	ARG	NE-CZ-NH2	8.38	124.49	120.30
1	C	130	ARG	NE-CZ-NH2	8.11	124.36	120.30
1	A	37	ASP	CB-CG-OD1	8.01	125.50	118.30
1	C	148	ASP	CB-CG-OD1	7.93	125.44	118.30
1	A	130	ARG	NE-CZ-NH1	-7.87	116.36	120.30
1	C	146	ASP	CB-CA-C	7.87	126.14	110.40
2	B	85	LEU	CA-CB-CG	7.83	133.31	115.30
2	B	18	HIS	CA-CB-CG	7.74	126.75	113.60
1	C	58	ASP	CB-CG-OD2	-7.69	111.38	118.30
1	C	17	GLU	CB-CG-CD	7.69	134.97	114.20
1	A	30	LEU	CA-CB-CG	7.63	132.86	115.30
1	C	235	ASP	CB-CG-OD2	7.59	125.13	118.30
1	C	217	ASP	CB-CG-OD2	-7.56	111.50	118.30
1	A	217	ASP	CB-CG-OD1	7.54	125.09	118.30
1	C	146	ASP	OD1-CG-OD2	7.50	137.54	123.30
1	C	48	ARG	CD-NE-CZ	7.46	134.05	123.60
1	A	23	TYR	CB-CG-CD1	-7.46	116.52	121.00
1	C	2	THR	CA-CB-CG2	7.44	122.81	112.40
1	C	250	GLU	OE1-CD-OE2	7.42	132.21	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	14	CYS	N-CA-CB	-7.38	97.32	110.60
1	C	146	ASP	N-CA-CB	-7.34	97.39	110.60
1	C	168	VAL	CA-CB-CG1	7.29	121.83	110.90
1	C	67	TYR	CB-CG-CD2	7.27	125.36	121.00
1	C	244	TYR	CB-CG-CD1	7.25	125.35	121.00
1	C	214	GLU	CA-CB-CG	7.24	129.33	113.40
1	C	210	ASP	CB-CG-OD1	-7.21	111.81	118.30
1	A	42	TYR	CB-CG-CD1	7.19	125.31	121.00
1	C	79	ASP	CB-CG-OD1	7.15	124.73	118.30
1	C	93	GLU	CA-CB-CG	7.12	129.07	113.40
1	A	28	LEU	O-C-N	7.06	134.00	122.70
1	C	165	ASP	CB-CG-OD2	-7.05	111.95	118.30
1	A	216	ASN	CB-CA-C	7.04	124.48	110.40
1	C	225	SER	N-CA-CB	7.01	121.01	110.50
1	C	27	ALA	N-CA-CB	-6.96	100.36	110.10
1	C	181	HIS	CA-CB-CG	-6.93	101.82	113.60
1	A	289	LEU	CB-CA-C	6.84	123.20	110.20
1	C	165	ASP	CB-CG-OD1	6.79	124.41	118.30
1	C	256	ASP	CB-CG-OD1	6.69	124.32	118.30
1	A	33	ASP	CA-CB-CG	6.69	128.12	113.40
1	A	214	GLU	O-C-N	6.67	133.38	122.70
1	A	35	GLU	CA-CB-CG	6.62	127.97	113.40
1	C	28	LEU	CA-CB-CG	6.61	130.50	115.30
1	C	17	GLU	CA-CB-CG	6.60	127.91	113.40
1	A	215	LYS	CB-CA-C	-6.59	97.22	110.40
1	A	106	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	C	34	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	C	150	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	A	217	ASP	O-C-N	6.52	133.13	122.70
1	A	166	ARG	CD-NE-CZ	-6.49	114.51	123.60
1	C	130	ARG	NH1-CZ-NH2	-6.41	112.34	119.40
1	C	67	TYR	CB-CG-CD1	-6.37	117.18	121.00
1	C	263	SER	N-CA-CB	-6.34	100.99	110.50
1	A	118	GLU	CG-CD-OE2	6.34	130.97	118.30
1	C	119	MET	N-CA-CB	6.31	121.96	110.60
1	A	32	GLU	CG-CD-OE1	6.29	130.89	118.30
1	C	18	ASP	CB-CG-OD2	6.29	123.97	118.30
1	C	221	GLU	N-CA-CB	-6.29	99.29	110.60
1	C	193	ALA	CB-CA-C	6.28	119.53	110.10
1	C	201	GLU	OE1-CD-OE2	6.25	130.80	123.30
1	A	168	VAL	CA-CB-CG1	6.25	120.28	110.90
1	C	166	ARG	NE-CZ-NH2	-6.23	117.19	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	241	ASP	CB-CG-OD1	-6.23	112.69	118.30
1	A	241	ASP	CB-CG-OD1	6.17	123.86	118.30
1	C	256	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	C	58	ASP	CB-CG-OD1	6.06	123.75	118.30
1	C	210	ASP	O-C-N	6.06	132.39	122.70
1	C	229	TYR	CB-CG-CD2	-6.04	117.38	121.00
1	C	221	GLU	OE1-CD-OE2	6.03	130.54	123.30
1	C	199	THR	CA-CB-CG2	5.99	120.79	112.40
1	A	124	ILE	CB-CG1-CD1	5.96	130.58	113.90
1	C	221	GLU	CG-CD-OE1	-5.95	106.39	118.30
1	C	244	TYR	CB-CG-CD2	-5.94	117.44	121.00
1	A	118	GLU	OE1-CD-OE2	-5.94	116.18	123.30
1	C	290	GLU	CA-CB-CG	5.91	126.40	113.40
1	A	203	TYR	CB-CG-CD1	5.91	124.54	121.00
2	B	44	GLU	CA-CB-CG	5.91	126.39	113.40
1	A	33	ASP	O-C-N	-5.89	113.28	122.70
2	D	103	GLU	CA-CB-CG	5.88	126.34	113.40
1	C	229	TYR	CB-CG-CD1	5.87	124.52	121.00
1	C	135	GLU	CG-CD-OE1	-5.86	106.59	118.30
1	A	146	ASP	CB-CG-OD1	5.84	123.55	118.30
1	C	143	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	C	222	GLN	CB-CG-CD	5.79	126.64	111.60
1	C	147	ALA	N-CA-CB	-5.78	102.00	110.10
1	A	31	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	4	LEU	CA-CB-CG	5.72	128.45	115.30
1	C	29	LYS	CG-CD-CE	5.69	128.97	111.90
1	A	256	ASP	CB-CA-C	5.69	121.78	110.40
1	A	93	GLU	N-CA-CB	5.68	120.83	110.60
1	C	160	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	143	ARG	CG-CD-NE	-5.68	99.88	111.80
1	A	54	SER	CA-CB-OG	5.67	126.50	111.20
1	C	279	ASP	CB-CG-OD2	5.66	123.40	118.30
1	A	127	ARG	NE-CZ-NH1	-5.66	117.47	120.30
2	D	49	THR	N-CA-CB	5.66	121.05	110.30
1	A	209	GLU	C-N-CA	5.64	135.81	121.70
1	C	190	PRO	N-CA-CB	-5.64	96.40	102.60
1	A	168	VAL	N-CA-CB	5.63	123.89	111.50
1	C	206	LEU	CB-CA-C	5.63	120.89	110.20
1	C	23	TYR	CA-C-O	5.60	131.85	120.10
1	A	53	ILE	O-C-N	5.59	131.64	122.70
2	D	75	ILE	N-CA-CB	5.58	123.64	110.80
1	C	245	LEU	CA-CB-CG	5.55	128.07	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	33	ASP	CB-CG-OD1	-5.53	113.32	118.30
1	C	203	TYR	CB-CG-CD1	5.53	124.32	121.00
1	A	179	LYS	CA-CB-CG	-5.52	101.25	113.40
1	C	118	GLU	OE1-CD-OE2	-5.52	116.68	123.30
1	C	147	ALA	CB-CA-C	-5.51	101.84	110.10
1	A	149	LYS	CA-CB-CG	-5.50	101.31	113.40
1	A	213	LEU	CB-CA-C	5.50	120.64	110.20
1	C	180	THR	CA-CB-CG2	5.49	120.08	112.40
2	D	88	GLU	CA-CB-CG	5.46	125.42	113.40
1	A	233	PRO	N-CA-CB	-5.46	96.60	102.60
2	D	9	LEU	N-CA-CB	-5.45	99.49	110.40
1	A	111	GLY	C-N-CA	-5.43	110.89	122.30
2	D	14	CYS	N-CA-C	5.43	125.65	111.00
1	C	42	TYR	CB-CG-CD1	-5.42	117.75	121.00
1	C	95	ILE	CB-CG1-CD1	5.42	129.07	113.90
1	A	283	PRO	O-C-N	5.41	131.35	122.70
1	C	213	LEU	CB-CG-CD2	-5.40	101.82	111.00
1	A	16	TYR	CB-CA-C	5.39	121.19	110.40
1	A	213	LEU	CB-CG-CD2	-5.39	101.83	111.00
2	D	58	LEU	CB-CA-C	5.38	120.42	110.20
1	C	277	PRO	C-N-CA	5.38	135.14	121.70
1	C	250	GLU	N-CA-CB	5.37	120.26	110.60
1	A	201	GLU	CG-CD-OE2	-5.34	107.62	118.30
1	A	214	GLU	OE1-CD-OE2	5.30	129.66	123.30
1	A	185	SER	N-CA-CB	-5.28	102.58	110.50
1	A	206	LEU	CB-CA-C	5.27	120.22	110.20
1	A	215	LYS	O-C-N	5.27	131.14	122.70
1	C	17	GLU	OE1-CD-OE2	-5.27	116.97	123.30
1	C	137	THR	CA-CB-OG1	-5.25	97.97	109.00
1	A	238	LEU	CA-CB-CG	5.24	127.35	115.30
2	D	38	ARG	NE-CZ-NH2	5.20	122.90	120.30
2	D	82	PHE	CA-C-N	5.20	126.60	116.20
1	A	259	PHE	CG-CD1-CE1	5.19	126.51	120.80
1	C	29	LYS	CA-CB-CG	-5.19	101.99	113.40
1	C	188	GLU	CB-CA-C	-5.17	100.06	110.40
1	A	92	LEU	CA-CB-CG	5.15	127.14	115.30
1	C	269	LEU	CB-CG-CD2	5.14	119.74	111.00
1	C	232	LEU	CA-CB-CG	5.14	127.12	115.30
1	C	116	VAL	CA-CB-CG2	5.14	118.60	110.90
1	C	167	GLU	CG-CD-OE1	-5.13	108.03	118.30
1	A	270	LEU	O-C-N	5.12	130.90	122.70
1	A	176	ALA	C-N-CA	5.10	134.46	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	31	ASN	N-CA-C	-5.10	97.22	111.00
1	A	31	ARG	O-C-N	-5.10	114.54	122.70
1	A	31	ARG	CD-NE-CZ	-5.09	116.47	123.60
1	C	214	GLU	O-C-N	5.08	130.83	122.70
1	C	20	GLN	O-C-N	-5.05	114.61	122.70
1	A	235	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	14	ARG	CD-NE-CZ	-5.05	116.54	123.60
1	A	115	ALA	N-CA-CB	-5.04	103.05	110.10
1	C	29	LYS	CD-CE-NZ	-5.04	100.12	111.70
1	C	36	TYR	CB-CG-CD1	-5.03	117.98	121.00
1	C	130	ARG	NE-CZ-NH1	5.02	122.81	120.30
2	B	92	ASN	CB-CA-C	5.01	120.42	110.40
1	C	250	GLU	CG-CD-OE2	-5.01	108.28	118.30

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	105	1
1	C	2371	0	2252	136	5
2	B	847	0	851	75	1
2	D	847	0	851	103	0
3	A	2	0	0	1	0
3	C	2	0	0	1	0
4	A	43	0	30	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	43	0	30	16	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	423	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 33.

All (423) 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:14:CYS:HG	4:B:104:HEM:CAB	1.70	1.01
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: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:HH11	2:D:91:ARG:HG3	1.35	0.91
2:B:14:CYS:SG	4:B:104:HEM:CBB	2.59	0.91
1:C:278:LYS:H	1:C:278:LYS:HD3	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
2:D:14:CYS:SG	4:D:104:HEM:CAB	2.65	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:THR:CG2	1:C:3:PRO:HD3	2.07	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:D:17:CYS:HG	4:D:104:HEM:CAC	1.88	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:128:CYS:SG	5:C:848:HOH:O	2.38	0.81
1:C:93:GLU:HB2	1:C:94:PRO:HD3	1.63	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
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:C:3:PRO:HB2	5:C:732:HOH:O	1.86	0.75
1:A:69:GLY:O	1:A:72:ARG:HD3	1.86	0.75
1:C:133:THR:HG22	1:C:137:THR:OG1	1.86	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:C:84:GLY:N	1:C:86:GLN:HE22	1.83	0.73
1:A:17:GLU:CD	1:A:17:GLU:H	1.93	0.72
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:D:38:ARG:HH11	2:D:38:ARG:HG3	1.55	0.71
2:B:43:ALA:HB3	2:B:48:TYR:OH	1.91	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:HH11	1:C:14:ARG:HG3	1.55	0.70
1:C:74:LYS:CE	1:C:78:ASN:HD21	1.99	0.69
2:D:14:CYS:CB	4:D:104:HEM:CBB	2.69	0.69
2:B:87:LYS:O	2:B:90:ASP:HB2	1.92	0.69
2:D:39:HIS:HB3	2:D:56:ASN:ND2	2.06	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:36:PHE:CD2	2:D:99:LYS:HB3	2.27	0.69
1:C:200:ASN:HB3	1:C:255:GLN:HG3	1.73	0.69
2:B:73:LYS:HD3	5:B:446:HOH:O	1.91	0.69
2:D:38:ARG:HD3	2:D:42:GLN:HB2	1.73	0.69
1:A:166:ARG:HH22	1:A:250:GLU:CD	1.96	0.69
1:C:200:ASN:HD22	1:C:200:ASN:H	1.41	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
2:D:94:LEU:O	2:D:97:TYR:HB3	1.95	0.67
1:C:74:LYS:HG3	1:C:78:ASN:ND2	2.10	0.67
1:A:16:TYR:O	1:A:19:PHE:N	2.28	0.67
2:D:74:TYR:HB2	5:D:744:HOH:O	1.94	0.67
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
2:B:14:CYS:HG	4:B:104:HEM:CBB	2.04	0.66
1:C:216:ASN:HD22	1:C:222:GLN:NE2	1.93	0.66
1:C:29:LYS:HG3	1:C:29:LYS:O	1.95	0.65
1:C:292:GLN:C	1:C:294:LEU:H	1.99	0.65
1:C:278:LYS:HD3	1:C:278:LYS:N	2.10	0.65
1:C:80:PRO:O	5:C:664:HOH:O	2.15	0.65
1:C:264:LYS:HB3	5:C:802:HOH:O	1.96	0.65
1:C:145:PRO:HD3	1:C:157:PHE:CZ	2.32	0.65
1:C:278:LYS:H	1:C:278:LYS:CD	1.96	0.64
1:C:267:GLU:OE2	1:C:271:GLU:OE2	2.15	0.64
1:A:245:LEU:HD22	1:A:245:LEU:O	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
2:D:60:ASP:H	2:D:63:ASN:HD21	1.46	0.63
1:A:125:PRO:HG3	1:A:285:ILE:HD11	1.79	0.63
1:A:4:LEU:HD12	1:A:62:ASN:O	1.99	0.62
1:A:287:LYS:HA	1:A:291:GLU:OE1	1.99	0.62
1:A:267:GLU:OE2	1:A:271:GLU:OE2	2.16	0.62
1:A:127:ARG:HG2	1:A:283:PRO:HA	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:THR:OG1	1:A:291:GLU:HG3	2.00	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:23:TYR:CD1	1:A:23:TYR:C	2.73	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:14:CYS:HG	4:D:104:HEM:CAB	2.11	0.61
2:D:11:LYS:HD2	2:D:11:LYS:N	2.16	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
1:C:20:GLN:HE22	1:C:287:LYS:H	1.50	0.60
1:C:42:TYR:O	1:C:46:LEU:HG	2.01	0.60
2:B:91:ARG:O	2:B:95:ILE:HG12	2.00	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
2:D:51:ALA:HB1	2:D:75:ILE:CG2	2.32	0.59
1:C:71:TYR:O	1:C:77:PHE:HB2	2.01	0.59
1:A:113:VAL:O	1:A:117:GLN:HG3	2.02	0.59
2:D:64:MET:HG2	2:D:95:ILE:CD1	2.33	0.59
2:B:44:GLU:HA	5:B:444:HOH:O	2.01	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
2:D:34:GLY:HA2	2:D:102:CYS:O	2.03	0.58
1:C:133:THR:HG23	1:C:137:THR:CG2	2.33	0.58
1:A:267:GLU:O	1:A:271:GLU:HG3	2.04	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
1:C:12:LYS:HE3	5:C:696:HOH:O	2.02	0.58
2:B:37:GLY:O	2:B:58:LEU:HD11	2.04	0.58
2:D:14:CYS:SG	4:D:104:HEM:HBB2	2.43	0.58
1:C:183:LYS:N	1:C:183:LYS:HD3	2.19	0.58
1:A:123:LYS:HE2	5:A:542:HOH:O	2.03	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:A:29:LYS:HG2	1:A:29:LYS:O	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:LYS:HB2	5:C:716:HOH:O	2.03	0.57
1:A:166:ARG:NH2	1:A:250:GLU:CD	2.57	0.57
1:C:190:PRO:HG2	1:C:190:PRO:O	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
2:B:87:LYS:CB	2:B:90:ASP:OD2	2.46	0.57
1:C:63:THR:CG2	1:C:143:ARG:HH22	2.16	0.57
1:C:10:VAL:O	1:C:12:LYS:HE3	2.05	0.57
1:A:103:SER:OG	1:A:106:ASP:HB2	2.05	0.57
1:C:26:ILE:HG22	1:C:114:THR:HG21	1.86	0.57
2:B:8:THR:O	2:B:11:LYS:HD3	2.05	0.57
2:D:5:LYS:HA	2:D:8:THR:HG23	1.87	0.57
1:A:52:HIS:NE2	3:A:299:SO4:O1	2.38	0.57
2:B:16:GLN:OE1	2:B:16:GLN:N	2.35	0.57
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
1:C:29:LYS:CG	1:C:29:LYS:O	2.53	0.56
1:C:286:PHE:C	1:C:287:LYS:HE2	2.26	0.56
2:B:22:LYS:C	2:B:24:GLY:H	2.09	0.56
1:C:166:ARG:HH22	1:C:250:GLU:CD	2.09	0.56
1:A:255:GLN:NE2	1:A:259:PHE:CZ	2.73	0.56
2:D:3:ALA:HB1	2:D:97:TYR:HA	1.87	0.56
1:C:51:TRP:CD1	1:C:52:HIS:HD2	2.24	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:C:256:ASP:O	1:C:260:LYS:HG2	2.05	0.55
1:A:96:HIS:CD2	1:A:107:LEU:HD22	2.41	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:C:7:VAL:O	1:C:7:VAL:HG23	2.06	0.55
2:D:80:MET:HE1	4:D:104:HEM:NB	2.22	0.54
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
2:B:55:LYS:HD3	2:B:57:VAL:CG1	2.36	0.54
1:A:75:LYS:HE3	1:A:140:ASP:HA	1.89	0.54
2:D:60:ASP:H	2:D:63:ASN:ND2	2.04	0.54
2:D:46:TYR:C	2:D:46:TYR:CD1	2.80	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ARG:NH1	1:A:241:ASP:OD2	2.33	0.54
1:C:136:ASP:HB3	5:C:749:HOH:O	2.07	0.54
1:C:49:LEU:HB2	1:C:85:LEU:HD22	1.90	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:C:133:THR:HG22	1:C:137:THR:HG1	1.72	0.53
1:A:60:HIS:HE1	5:A:341:HOH:O	1.91	0.53
2:D:39:HIS:CE1	2:D:58:LEU:HB2	2.43	0.53
1:C:61:ASP:N	1:C:61:ASP:OD1	2.30	0.53
2:B:22:LYS:HD2	2:B:33:HIS:NE2	2.23	0.53
1:C:133:THR:CG2	1:C:137:THR:HG21	2.39	0.53
1:C:20:GLN:HG3	1:C:20:GLN:O	2.07	0.53
1:A:93:GLU:N	1:A:94:PRO:CD	2.71	0.53
1:C:63:THR:CG2	1:C:143:ARG:NH2	2.72	0.52
2:D:2:SER:O	2:D:93:ASP:HB3	2.10	0.52
1:A:216:ASN:HB2	5:A:420:HOH:O	2.10	0.52
1:A:164:ASN:O	1:A:168:VAL:HG13	2.09	0.52
2:B:8:THR:CA	2:B:11:LYS:CD	2.77	0.52
2:B:7:ALA:HB2	2:B:97:TYR:CD2	2.44	0.52
1:A:115:ALA:O	1:A:119:MET:HG3	2.09	0.52
2:D:7:ALA:HB2	2:D:97:TYR:CD1	2.44	0.52
1:A:2:THR:CG2	1:A:3:PRO:HD2	2.36	0.52
1:A:86:GLN:OE1	1:A:86:GLN:N	2.34	0.52
2:D:70:ASN:ND2	5:D:774:HOH:O	2.42	0.52
1:C:183:LYS:CE	1:C:183:LYS:H	2.23	0.52
2:B:5:LYS:O	2:B:6:GLY:C	2.48	0.51
1:C:15:SER:O	1:C:18:ASP:HB2	2.10	0.51
1:C:281:PRO:HG2	5:C:848:HOH:O	2.09	0.51
1:A:188:GLU:H	1:A:222:GLN:HE22	1.58	0.51
1:A:161:LEU:O	1:A:162:ASN:HB3	2.10	0.51
1:A:200:ASN:ND2	1:A:200:ASN:H	2.05	0.51
1:A:141:ASN:HD22	1:A:141:ASN:N	2.07	0.51
1:A:81:SER:HB3	5:A:367:HOH:O	2.11	0.51
1:A:30:LEU:HD12	1:A:42:TYR:HB2	1.92	0.51
1:C:183:LYS:H	1:C:183:LYS:CD	2.23	0.51
1:C:110:LEU:O	1:C:111:GLY:C	2.46	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:THR:CG2	1:C:137:THR:CB	2.89	0.50
1:A:52:HIS:ND1	1:A:82:ASN:OD1	2.31	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
1:C:292:GLN:O	1:C:294:LEU:N	2.44	0.50
1:A:206:LEU:HD13	1:A:231:MET:SD	2.51	0.50
1:C:63:THR:HG22	1:C:143:ARG:CZ	2.42	0.49
2:B:23:GLY:O	2:B:24:GLY:O	2.30	0.49
2:B:-2:LYS:O	2:B:-1:ALA:HB2	2.12	0.49
2:D:55:LYS:HG3	2:D:57:VAL:HG22	1.95	0.49
1:C:21:LYS:HB2	1:C:99:PHE:CE2	2.47	0.49
1:A:180:THR:N	1:A:189:GLY:O	2.29	0.49
2:D:91:ARG:NH1	2:D:91:ARG:HG3	2.09	0.49
2:B:45:GLY:N	5:B:444:HOH:O	2.44	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: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:180:THR:HG21	1:C:230:MET:HE1	1.95	0.48
1:A:38:ASN:O	1:A:39:TYR:HB2	2.13	0.48
2:D:11:LYS:NZ	5:D:621:HOH:O	2.46	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:B:18:HIS:HE1	2:B:30:PRO:HD2	1.78	0.48
4:B:104:HEM:HMC2	4:B:104:HEM:HBC2	1.95	0.48
2:B:14:CYS:SG	4:B:104:HEM:C3B	3.02	0.48
1:C:292:GLN:C	1:C:294:LEU:N	2.66	0.48
1:C:183:LYS:N	1:C:183:LYS:CD	2.77	0.48
2:D:39:HIS:HB3	2:D:56:ASN:CG	2.33	0.48
2:B:55:LYS:O	2:B:56:ASN:C	2.52	0.48
2:D:48:TYR:CE1	4:D:104:HEM:O2A	2.66	0.48
2:B:42:GLN:O	2:B:43:ALA:C	2.50	0.48
1:C:190:PRO:CG	1:C:190:PRO:O	2.60	0.48
1:A:52:HIS:HE1	1:A:81:SER:O	1.97	0.47
2:D:63:ASN:H	2:D:63:ASN:HD22	1.61	0.47
1:A:156:THR:CG2	5:A:513:HOH:O	2.60	0.47
2:D:86:LYS:HD3	2:D:86:LYS:HA	1.72	0.47
1:C:8:ALA:HB2	1:C:274:ILE:HG22	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:34:GLY:N	2:D:102:CYS:O	2.46	0.47
1:C:38:ASN:N	1:C:38:ASN:ND2	2.63	0.47
1:C:287:LYS:NZ	1:C:287:LYS:HA	2.30	0.47
1:C:8:ALA:HB3	1:C:276:PHE:HA	1.97	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:B:57:VAL:HA	5:B:474:HOH:O	2.13	0.47
1:C:155:ARG:HB2	1:C:244:TYR:OH	2.13	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:D:60:ASP:OD1	2:D:60:ASP:C	2.54	0.46
2:D:11:LYS:CD	2:D:11:LYS:N	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: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:52:ASN:OD1	2:D:52:ASN:O	2.33	0.46
2:D:36:PHE:CE1	2:D:64:MET:HE3	2.51	0.46
1:C:127:ARG:HA	5:C:674:HOH:O	2.16	0.46
2:D:17:CYS:HG	4:D:104:HEM:CBC	2.23	0.46
1:C:93:GLU:N	1:C:94:PRO:HD2	2.31	0.46
2:B:55:LYS:O	2:B:56:ASN:O	2.34	0.46
2:D:5:LYS:O	2:D:9:LEU:HB2	2.17	0.46
2:D:60:ASP:C	2:D:62:ASN:H	2.19	0.46
1:A:23:TYR:HD1	1:A:23:TYR:C	2.18	0.46
1:C:183:LYS:H	1:C:183:LYS:HD3	1.80	0.46
1:C:26:ILE:CG2	1:C:114:THR:HG21	2.46	0.46
2:D:80:MET:HE3	4:D:104:HEM:C4B	2.51	0.45
2:B:23:GLY:O	2:B:24:GLY:C	2.55	0.45
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
1:A:141:ASN:ND2	1:A:141:ASN:N	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
2:D:56:ASN:O	2:D:57:VAL:C	2.55	0.45
1:A:130:ARG:NH1	1:A:130:ARG:HG3	2.32	0.45
1:C:69:GLY:HA2	5:C:778:HOH:O	2.16	0.45
2:D:93:ASP:N	2:D:93:ASP:OD1	2.44	0.45
1:A:119:MET:O	1:A:120:GLN:CB	2.61	0.45
1:A:29:LYS:HD3	1:A:91:PHE:CE2	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:LEU:O	2:B:16:GLN:C	2.54	0.45
1:A:232:LEU:O	1:A:235:ASP:N	2.47	0.45
1:A:7:VAL:HA	1:A:275:THR:O	2.17	0.45
1:A:294:LEU:HD11	1:C:294:LEU:CD1	2.47	0.45
1:A:211:TRP:CZ3	1:A:225:SER:HB3	2.52	0.45
2:D:14:CYS:HB2	4:D:104:HEM:HBB1	1.96	0.44
1:A:86:GLN:H	1:A:86:GLN:CD	2.18	0.44
1:A:137:THR:O	1:A:139:PRO:HD3	2.17	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
2:D:6:GLY:CA	2:D:94:LEU:HA	2.48	0.44
1:A:126:TRP:C	1:A:127:ARG:HG3	2.37	0.44
1:C:26:ILE:HA	1:C:95:ILE:HD13	1.99	0.44
2:D:100:LYS:HD3	2:D:101:ALA:CA	2.47	0.44
1:C:264:LYS:HE3	1:C:264:LYS:HB2	1.45	0.44
1:A:155:ARG:HH11	1:A:155:ARG:HD2	1.33	0.44
1:C:200:ASN:H	1:C:200:ASN:ND2	2.11	0.44
2:B:15:LEU:HA	2:B:15:LEU:HD12	1.82	0.44
2:D:13:ARG:NH1	2:D:82:PHE:CE1	2.85	0.44
1:C:84:GLY:CA	1:C:86:GLN:NE2	2.80	0.44
2:D:60:ASP:O	2:D:63:ASN:ND2	2.51	0.44
2:D:19:THR:O	2:D:31:ASN:HA	2.18	0.44
1:C:30:LEU:HD23	1:C:42:TYR:HB2	1.99	0.44
1:C:162:ASN:CG	5:C:723:HOH:O	2.56	0.44
2:B:40:SER:HA	2:B:59:TRP:HE1	1.83	0.44
2:D:93:ASP:O	2:D:94:LEU:C	2.56	0.43
2:D:42:GLN:C	2:D:43:ALA:O	2.56	0.43
2:B:43:ALA:CB	2:B:48:TYR:OH	2.62	0.43
1:A:93:GLU:N	1:A:94:PRO:HD2	2.32	0.43
2:D:36:PHE:CE1	2:D:64:MET:CE	3.02	0.43
1:C:206:LEU:HD12	1:C:206:LEU:HA	1.88	0.43
1:A:265:ALA:O	1:A:266:PHE:C	2.56	0.43
1:C:133:THR:HA	1:C:134:PRO:HD3	1.81	0.43
1:A:294:LEU:N	1:A:294:LEU:HD12	2.34	0.43
1:C:76:GLU:HB2	1:C:138:THR:CG2	2.48	0.43
2:B:79:LYS:HE3	4:B:104:HEM:HMD1	2.01	0.43
1:A:28:LEU:O	1:A:31:ARG:HB3	2.17	0.43
1:A:214:GLU:O	1:A:221:GLU:HA	2.19	0.43
1:A:116:VAL:HG11	1:A:124:ILE:HD12	2.00	0.43
1:C:74:LYS:CE	1:C:78:ASN:ND2	2.68	0.43
1:C:14:ARG:HG2	1:C:101:TRP:CZ3	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:296:HEM:HBB2	4:C:296:HEM:HMB1	2.00	0.43
1:C:38:ASN:HD22	1:C:38:ASN:H	1.67	0.43
2:D:46:TYR:C	2:D:46:TYR:HD1	2.21	0.43
1:C:8:ALA:HB2	1:C:274:ILE:CG2	2.49	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:199:THR:HG23	5:C:652:HOH:O	2.18	0.43
2:D:96:THR:O	2:D:97:TYR:C	2.57	0.43
1:C:15:SER:HB2	5:C:738:HOH:O	2.19	0.42
1:A:214:GLU:N	1:A:222:GLN:O	2.50	0.42
1:C:127:ARG:HD2	1:C:127:ARG:HH11	1.68	0.42
1:C:165:ASP:O	1:C:169:VAL:HG23	2.19	0.42
2:D:48:TYR:HE1	4:D:104:HEM:O2A	2.02	0.42
2:B:35:ILE:HG23	2:B:36:PHE:N	2.34	0.42
1:A:181:HIS:HB2	1:A:184:ASN:HB2	2.01	0.42
1:C:6:HIS:HD2	5:C:627:HOH:O	2.02	0.42
2:B:22:LYS:HZ3	2:B:33:HIS:HD2	1.66	0.42
4:B:104:HEM:HBC2	4:B:104:HEM:CMC	2.49	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
2:D:38:ARG:CD	2:D:42:GLN:HB2	2.44	0.42
1:A:190:PRO:O	1:A:190:PRO:HG2	2.20	0.42
2:B:98:LEU:O	2:B:99:LYS:C	2.57	0.42
1:A:35:GLU:HG3	5:A:552:HOH:O	2.20	0.42
5:C:838:HOH:O	2:D:13:ARG:CD	2.68	0.42
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:39:HIS:O	2:D:40:SER:C	2.58	0.42
2:D:67:TYR:HB2	2:D:74:TYR:CD2	2.55	0.42
2:B:77:GLY:O	2:B:78:THR:C	2.58	0.42
2:B:89:LYS:O	2:B:93:ASP:OD2	2.37	0.41
1:C:75:LYS:HE2	1:C:140:ASP:HA	2.02	0.41
1:A:53:ILE:HG22	1:A:71:TYR:HB2	2.01	0.41
1:C:57:TRP:HE1	1:C:62:ASN:HD22	1.68	0.41
2:B:22:LYS:HZ2	2:B:33:HIS:HD2	1.63	0.41
1:C:89:PHE:CD1	1:C:89:PHE:C	2.93	0.41
2:D:79:LYS:HG2	4:D:104:HEM:HBD2	2.01	0.41
4:C:296:HEM:HBB2	4:C:296:HEM:CMB	2.50	0.41
1:C:247:ILE:O	1:C:248:VAL:C	2.58	0.41
2:D:21:GLU:H	2:D:21:GLU:CD	2.23	0.41
1:C:243:LYS:HG2	1:C:243:LYS:HZ2	1.77	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:THR:O	1:A:143:ARG:HD2	2.21	0.41
2:B:60:ASP:O	2:B:62:ASN:N	2.54	0.41
1:A:134:PRO:C	1:A:136:ASP:N	2.73	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
2:B:5:LYS:O	2:B:8:THR:N	2.53	0.41
1:A:7:VAL:HG13	1:A:277:PRO:HD3	2.03	0.41
1:C:164:ASN:OD1	1:C:164:ASN:C	2.60	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:A:79:ASP:OD1	1:A:80:PRO:HD2	2.20	0.41
1:C:162:ASN:HD22	1:C:162:ASN:HA	1.65	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:H	2.24	0.41
2:B:97:TYR:C	2:B:97:TYR:CD1	2.94	0.40
2:D:80:MET:HE3	4:D:104:HEM:CHC	2.51	0.40
2:D:42:GLN:O	2:D:43:ALA:C	2.59	0.40
2:D:60:ASP:C	2:D:62:ASN:N	2.74	0.40
2:B:64:MET:O	2:B:67:TYR:HB3	2.21	0.40
2:D:5:LYS:C	2:D:7:ALA:H	2.24	0.40
2:B:22:LYS:HZ2	2:B:33:HIS:CD2	2.39	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
1:A:266:PHE:O	1:A:270:LEU:HG	2.21	0.40
1:A:35:GLU:CG	5:A:552:HOH:O	2.70	0.40
2:B:8:THR:CA	2:B:11:LYS:HD3	2.49	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%)	46	57
1	C	292/296 (99%)	272 (93%)	19 (6%)	1 (0%)	46	57
2	B	106/108 (98%)	91 (86%)	9 (8%)	6 (6%)	2	1
2	D	106/108 (98%)	89 (84%)	13 (12%)	4 (4%)	4	2
All	All	796/808 (98%)	716 (90%)	68 (8%)	12 (2%)	13	12

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	-2	LYS
2	B	-1	ALA
2	B	56	ASN
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%)	221 (88%)	31 (12%)	6 6
1	C	252/254 (99%)	214 (85%)	38 (15%)	3 3
2	B	89/89 (100%)	73 (82%)	16 (18%)	2 2
2	D	89/89 (100%)	69 (78%)	20 (22%)	1 1
All	All	682/686 (99%)	577 (85%)	105 (15%)	3 3

All (105) 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	12	LYS
1	A	32	GLU
1	A	35	GLU
1	A	51	TRP
1	A	72	ARG
1	A	74	LYS
1	A	94	PRO
1	A	97	LYS
1	A	138	THR
1	A	140	ASP
1	A	168	VAL
1	A	179	LYS
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	-3	PHE
2	B	-2	LYS
2	B	2	SER
2	B	11	LYS
2	B	22	LYS
2	B	55	LYS
2	B	58	LEU
2	B	61	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
1	C	2	THR
1	C	5	VAL
1	C	12	LYS
1	C	14	ARG
1	C	20	GLN
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	127	ARG
1	C	133	THR
1	C	135	GLU
1	C	149	LYS
1	C	156	THR
1	C	162	ASN
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	226	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	237	SER
1	C	243	LYS
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
2	D	8	THR
2	D	11	LYS
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	60	ASP
2	D	63	ASN
2	D	66	GLU
2	D	72	LYS
2	D	73	LYS
2	D	89	LYS
2	D	91	ARG
2	D	99	LYS
2	D	102	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	24	ASN
1	A	38	ASN
1	A	60	HIS
1	A	96	HIS
1	A	141	ASN
1	A	200	ASN
1	A	222	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	292	GLN
2	B	33	HIS
2	B	39	HIS
2	B	52	ASN
1	C	20	GLN
1	C	24	ASN
1	C	38	ASN
1	C	62	ASN
1	C	78	ASN
1	C	86	GLN
1	C	141	ASN
1	C	162	ASN
1	C	196	ASN
1	C	200	ASN
1	C	208	ASN
1	C	222	GLN
1	C	292	GLN
2	D	26	HIS
2	D	52	ASN
2	D	63	ASN

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

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	A	296	1,3	30,50,50	2.93	12 (40%)	24,82,82	4.35	11 (45%)
3	SO4	A	299	4	0,1,4	0.00	-	0,0,6	0.00	-
4	HEM	B	104	2	30,50,50	2.77	10 (33%)	24,82,82	2.76	11 (45%)
4	HEM	C	296	1,3	30,50,50	2.45	8 (26%)	24,82,82	2.60	10 (41%)
3	SO4	C	300	4	0,1,4	0.00	-	0,0,6	0.00	-
4	HEM	D	104	2	30,50,50	2.45	11 (36%)	24,82,82	2.67	13 (54%)

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	-	0/10/54/54	0/0/8/8
3	SO4	A	299	4	-	0/0/0/0	0/0/0/0
4	HEM	B	104	2	-	0/10/54/54	0/0/8/8
4	HEM	C	296	1,3	-	0/10/54/54	0/0/8/8
3	SO4	C	300	4	-	0/0/0/0	0/0/0/0
4	HEM	D	104	2	-	0/10/54/54	0/0/8/8

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	104	HEM	C3B-C4B	-8.46	1.44	1.51
4	A	296	HEM	C3B-C4B	-7.89	1.44	1.51
4	A	296	HEM	C2D-C3D	-7.58	1.31	1.54
4	B	104	HEM	C3D-C4D	-7.54	1.41	1.51
4	D	104	HEM	C2D-C3D	-6.82	1.34	1.54
4	C	296	HEM	C2D-C3D	-6.38	1.35	1.54
4	C	296	HEM	C3B-C4B	-6.34	1.46	1.51
4	B	104	HEM	C2D-C3D	-6.11	1.36	1.54
4	D	104	HEM	C3D-C4D	-5.78	1.44	1.51
4	D	104	HEM	C3B-C4B	-5.29	1.47	1.51
4	C	296	HEM	C2C-C1C	-4.95	1.43	1.52
4	A	296	HEM	C3D-C4D	-4.89	1.45	1.51
4	A	296	HEM	C2C-C1C	-4.07	1.44	1.52
4	C	296	HEM	C3D-C4D	-4.06	1.46	1.51
4	B	104	HEM	C2C-C1C	-3.89	1.45	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	104	HEM	C2C-C1C	-3.71	1.45	1.52
4	D	104	HEM	C2D-C1D	-2.53	1.43	1.51
4	A	296	HEM	C3C-CAC	-2.40	1.46	1.51
4	D	104	HEM	C2B-C1B	-2.37	1.44	1.51
4	B	104	HEM	C2D-C1D	-2.34	1.44	1.51
4	B	104	HEM	C2B-C1B	-2.22	1.44	1.51
4	C	296	HEM	C2B-C1B	-2.07	1.45	1.51
4	D	104	HEM	C3B-CAB	2.01	1.55	1.51
4	B	104	HEM	CMA-C3A	2.03	1.55	1.51
4	C	296	HEM	CMA-C3A	2.21	1.56	1.51
4	D	104	HEM	CAA-C2A	2.30	1.56	1.52
4	A	296	HEM	CHC-C1C	2.33	1.41	1.36
4	A	296	HEM	C3B-CAB	2.37	1.55	1.51
4	B	104	HEM	FE-NC	2.37	2.05	1.95
4	A	296	HEM	FE-NB	2.51	2.10	1.97
4	D	104	HEM	C3C-CAC	2.63	1.56	1.51
4	A	296	HEM	CMA-C3A	2.64	1.57	1.51
4	B	104	HEM	C3C-CAC	2.71	1.56	1.51
4	C	296	HEM	C4C-NC	2.80	1.39	1.36
4	B	104	HEM	CAA-C2A	2.93	1.57	1.52
4	A	296	HEM	CAA-C2A	2.98	1.57	1.52
4	D	104	HEM	C4C-NC	3.02	1.39	1.36
4	D	104	HEM	C1C-NC	3.02	1.39	1.36
4	A	296	HEM	C1C-NC	4.19	1.41	1.36
4	C	296	HEM	C1C-NC	4.59	1.41	1.36
4	A	296	HEM	C4C-NC	4.73	1.41	1.36

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	296	HEM	CAA-C2A-C1A	-7.16	119.24	127.01
4	B	104	HEM	CAA-C2A-C1A	-4.55	122.06	127.01
4	C	296	HEM	CMA-C3A-C4A	-3.86	121.98	128.36
4	D	104	HEM	CAA-C2A-C1A	-3.79	122.90	127.01
4	A	296	HEM	CMA-C3A-C4A	-3.70	122.25	128.36
4	B	104	HEM	CBA-CAA-C2A	-3.02	107.12	112.53
4	C	296	HEM	C3B-CAB-CBB	-2.86	120.06	124.46
4	B	104	HEM	CBD-CAD-C3D	-2.50	106.28	113.55
4	B	104	HEM	C3C-CAC-CBC	-2.23	121.04	124.46
4	D	104	HEM	CMA-C3A-C4A	-2.23	124.68	128.36
4	D	104	HEM	CBA-CAA-C2A	-2.06	108.83	112.53
4	B	104	HEM	C3B-CAB-CBB	2.06	127.62	124.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	296	HEM	CMA-C3A-C2A	2.11	129.65	125.24
4	D	104	HEM	CAA-CBA-CGA	2.26	116.88	112.75
4	D	104	HEM	C3B-C4B-CHC	2.38	126.52	123.16
4	A	296	HEM	CMA-C3A-C2A	2.57	130.61	125.24
4	C	296	HEM	CAD-C3D-C4D	2.76	122.20	112.47
4	D	104	HEM	CAD-C3D-C4D	2.92	122.78	112.47
4	A	296	HEM	CAD-C3D-C4D	2.97	122.96	112.47
4	A	296	HEM	C3B-C4B-CHC	3.00	127.38	123.16
4	D	104	HEM	CMD-C2D-C3D	3.00	127.64	114.35
4	B	104	HEM	CAD-C3D-C4D	3.22	123.81	112.47
4	B	104	HEM	CMD-C2D-C3D	3.22	128.60	114.35
4	D	104	HEM	C2C-C1C-CHC	3.29	128.68	123.68
4	C	296	HEM	CBA-CAA-C2A	3.36	118.55	112.53
4	C	296	HEM	CMD-C2D-C3D	3.64	130.45	114.35
4	C	296	HEM	CMC-C2C-C3C	3.79	125.98	116.53
4	D	104	HEM	C3C-CAC-CBC	3.80	130.28	124.46
4	C	296	HEM	C2D-C3D-C4D	3.83	107.99	101.50
4	A	296	HEM	CMD-C2D-C3D	3.96	131.85	114.35
4	D	104	HEM	CMB-C2B-C3B	4.22	127.07	116.53
4	B	104	HEM	C2D-C3D-C4D	4.31	108.80	101.50
4	D	104	HEM	C2D-C3D-C4D	4.41	108.98	101.50
4	A	296	HEM	C2D-C3D-C4D	4.44	109.02	101.50
4	B	104	HEM	CAD-C3D-C2D	4.77	126.93	113.22
4	A	296	HEM	CMC-C2C-C3C	4.77	128.44	116.53
4	D	104	HEM	CMC-C2C-C3C	4.87	128.68	116.53
4	A	296	HEM	CAD-C3D-C2D	5.12	127.95	113.22
4	D	104	HEM	CAD-C3D-C2D	5.22	128.24	113.22
4	C	296	HEM	CMB-C2B-C3B	5.27	129.69	116.53
4	B	104	HEM	CMB-C2B-C3B	5.50	130.25	116.53
4	B	104	HEM	CMC-C2C-C3C	5.61	130.54	116.53
4	C	296	HEM	CAD-C3D-C2D	5.73	129.70	113.22
4	A	296	HEM	CMB-C2B-C3B	5.90	131.25	116.53
4	A	296	HEM	C3C-CAC-CBC	15.32	147.95	124.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	299	SO4	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	104	HEM	16	0
4	C	296	HEM	4	0
3	C	300	SO4	1	0
4	D	104	HEM	19	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%)	1.38	68 (23%)	1	1	10, 24, 48, 90	0
1	C	294/296 (99%)	1.93	130 (44%)	0	0	8, 24, 42, 72	0
2	B	108/108 (100%)	2.77	56 (51%)	0	0	16, 43, 73, 118	0
2	D	108/108 (100%)	3.28	76 (70%)	0	0	22, 54, 83, 119	0
All	All	804/808 (99%)	2.02	330 (41%)	0	0	8, 29, 67, 119	0

All (330) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	-4	GLU	12.8
2	D	-5	THR	12.5
2	B	-5	THR	11.6
2	D	94	LEU	9.7
2	D	44	GLU	9.1
1	A	193	ALA	8.4
2	D	-3	PHE	8.2
1	A	1	THR	8.1
2	D	36	PHE	7.7
2	B	32	LEU	7.6
2	B	-2	LYS	7.6
1	A	2	THR	7.3
2	B	35	ILE	7.0
2	D	85	LEU	7.0
2	B	1	GLY	6.4
2	D	39	HIS	6.4
2	D	33	HIS	6.3
2	B	-4	GLU	6.3
2	B	71	PRO	6.3
2	D	8	THR	6.2
2	B	10	PHE	6.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	57	VAL	5.9
2	D	64	MET	5.7
2	B	68	LEU	5.6
2	D	43	ALA	5.6
1	C	228	GLY	5.6
2	D	-1	ALA	5.5
2	D	32	LEU	5.5
2	B	74	TYR	5.4
1	C	186	GLY	5.4
2	D	41	GLY	5.1
2	D	7	ALA	5.1
2	B	3	ALA	5.1
1	C	45	VAL	5.1
2	D	67	TYR	5.0
2	B	-3	PHE	5.0
1	C	147	ALA	5.0
2	B	37	GLY	5.0
2	B	22	LYS	4.9
2	D	14	CYS	4.9
2	B	59	TRP	4.9
1	C	202	PHE	4.9
1	C	215	LYS	4.9
2	D	22	LYS	4.8
1	C	187	TYR	4.8
2	B	20	VAL	4.6
2	B	-1	ALA	4.6
2	B	64	MET	4.5
1	C	144	LEU	4.5
1	C	53	ILE	4.4
2	B	36	PHE	4.4
2	B	43	ALA	4.4
2	B	67	TYR	4.4
2	D	96	THR	4.4
1	C	108	PHE	4.4
1	C	205	ASN	4.4
1	C	5	VAL	4.4
2	D	35	ILE	4.4
2	D	31	ASN	4.4
1	C	219	ASN	4.4
1	A	28	LEU	4.3
1	A	5	VAL	4.3
2	B	93	ASP	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	58	LEU	4.3
1	C	223	TRP	4.2
2	B	9	LEU	4.1
2	D	3	ALA	4.1
2	B	60	ASP	4.0
1	C	191	TRP	4.0
2	D	2	SER	4.0
1	A	198	PHE	4.0
2	D	20	VAL	4.0
1	C	104	SER	4.0
2	B	85	LEU	3.9
2	B	39	HIS	3.9
1	A	213	LEU	3.8
1	C	229	TYR	3.8
1	C	193	ALA	3.8
1	C	154	VAL	3.8
1	C	42	TYR	3.8
2	D	34	GLY	3.8
2	D	29	GLY	3.8
1	C	19	PHE	3.7
2	B	11	LYS	3.7
2	B	75	ILE	3.7
1	C	182	LEU	3.7
1	C	230	MET	3.7
2	B	2	SER	3.7
2	D	26	HIS	3.7
1	C	169	VAL	3.7
2	D	52	ASN	3.7
1	C	248	VAL	3.6
2	D	101	ALA	3.6
1	C	206	LEU	3.6
1	C	211	TRP	3.6
2	D	15	LEU	3.6
1	C	105	GLY	3.6
2	B	45	GLY	3.6
1	A	192	GLY	3.6
2	D	71	PRO	3.6
2	B	100	LYS	3.6
1	C	168	VAL	3.5
1	A	186	GLY	3.5
2	B	90	ASP	3.5
1	A	31	ARG	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	11	LYS	3.5
2	D	37	GLY	3.5
1	C	8	ALA	3.5
1	C	197	VAL	3.5
1	A	183	LYS	3.5
1	C	145	PRO	3.4
2	D	98	LEU	3.4
2	D	19	THR	3.4
1	A	99	PHE	3.4
1	C	38	ASN	3.4
1	C	275	THR	3.4
1	C	40	ILE	3.4
1	C	180	THR	3.4
1	C	212	LYS	3.4
2	D	100	LYS	3.4
2	D	69	THR	3.4
2	D	45	GLY	3.4
1	C	44	PRO	3.4
2	B	69	THR	3.3
1	C	196	ASN	3.3
1	C	262	PHE	3.3
2	D	51	ALA	3.3
2	B	94	LEU	3.3
1	C	156	THR	3.3
1	A	38	ASN	3.3
2	D	25	PRO	3.3
2	B	34	GLY	3.3
2	D	59	TRP	3.2
1	A	197	VAL	3.2
1	C	232	LEU	3.2
2	D	23	GLY	3.2
1	C	136	ASP	3.2
2	D	65	SER	3.2
1	A	182	LEU	3.2
1	A	4	LEU	3.1
1	C	181	HIS	3.1
2	D	84	GLY	3.1
2	D	40	SER	3.1
1	A	207	LEU	3.1
1	A	169	VAL	3.1
1	C	73	PHE	3.1
1	A	294	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	185	SER	3.1
2	D	68	LEU	3.0
1	C	284	PHE	3.0
1	C	71	TYR	3.0
1	A	181	HIS	3.0
1	C	46	LEU	3.0
2	B	96	THR	3.0
1	C	39	TYR	3.0
1	C	172	MET	3.0
1	A	187	TYR	3.0
2	D	10	PHE	3.0
1	C	225	SER	3.0
1	C	220	ASN	2.9
1	C	157	PHE	2.9
2	B	15	LEU	2.9
1	C	227	SER	2.9
1	C	92	LEU	2.9
2	D	16	GLN	2.9
1	C	214	GLU	2.9
2	D	99	LYS	2.9
1	A	236	TYR	2.9
1	C	236	TYR	2.9
2	D	82	PHE	2.9
1	C	91	PHE	2.8
1	A	144	LEU	2.8
2	D	95	ILE	2.8
1	C	231	MET	2.8
2	D	6	GLY	2.8
1	C	221	GLU	2.8
1	A	223	TRP	2.8
2	D	90	ASP	2.8
1	C	141	ASN	2.8
1	C	66	SER	2.8
1	A	89	PHE	2.8
2	D	97	TYR	2.8
2	B	21	GLU	2.8
1	C	148	ASP	2.7
1	C	102	ILE	2.7
2	B	4	LYS	2.7
1	C	26	ILE	2.7
2	B	81	ALA	2.7
2	B	19	THR	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	46	TYR	2.7
2	D	48	TYR	2.7
1	A	154	VAL	2.7
1	C	51	TRP	2.7
1	C	84	GLY	2.6
1	C	80	PRO	2.6
1	A	280	ALA	2.6
1	C	36	TYR	2.6
1	C	192	GLY	2.6
1	C	195	ASN	2.6
2	D	18	HIS	2.6
2	D	87	LYS	2.6
1	C	30	LEU	2.6
1	C	218	ALA	2.6
2	D	81	ALA	2.6
2	D	93	ASP	2.6
1	C	270	LEU	2.6
2	D	58	LEU	2.6
1	C	247	ILE	2.6
1	A	281	PRO	2.6
2	B	99	LYS	2.6
2	D	60	ASP	2.5
1	A	211	TRP	2.5
1	A	218	ALA	2.5
1	C	62	ASN	2.5
1	C	188	GLU	2.5
1	C	49	LEU	2.5
1	C	74	LYS	2.5
1	C	266	PHE	2.5
1	C	153	TYR	2.5
2	D	103	GLU	2.5
1	C	41	GLY	2.5
1	C	269	LEU	2.5
1	A	283	PRO	2.5
1	C	52	HIS	2.5
2	D	92	ASN	2.5
1	A	91	PHE	2.5
1	C	48	ARG	2.5
2	B	61	GLU	2.5
1	C	114	THR	2.4
1	A	205	ASN	2.4
1	C	213	LEU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	24	ASN	2.4
2	D	78	THR	2.4
1	C	93	GLU	2.4
1	C	133	THR	2.4
1	A	101	TRP	2.4
1	C	101	TRP	2.4
1	C	258	PHE	2.4
1	C	183	LYS	2.4
2	D	56	ASN	2.4
1	C	216	ASN	2.4
1	A	53	ILE	2.4
1	A	102	ILE	2.4
1	C	22	VAL	2.4
1	C	116	VAL	2.4
2	B	82	PHE	2.4
1	C	179	LYS	2.4
1	A	33	ASP	2.3
1	A	111	GLY	2.3
1	A	188	GLU	2.3
1	C	55	GLY	2.3
1	C	65	GLY	2.3
1	C	252	ALA	2.3
2	D	50	ASP	2.3
1	C	184	ASN	2.3
1	A	107	LEU	2.3
1	A	278	LYS	2.3
2	D	75	ILE	2.3
1	C	158	PHE	2.3
1	A	191	TRP	2.3
2	B	23	GLY	2.3
1	C	119	MET	2.3
1	C	150	ASP	2.3
2	D	61	GLU	2.3
1	A	30	LEU	2.3
1	A	206	LEU	2.3
2	B	33	HIS	2.3
1	A	21	LYS	2.3
2	D	9	LEU	2.3
1	A	19	PHE	2.3
1	C	224	ASP	2.3
1	C	31	ARG	2.3
1	C	190	PRO	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	112	GLY	2.2
1	C	285	ILE	2.2
2	B	98	LEU	2.2
1	C	63	THR	2.2
1	C	132	ASP	2.2
1	C	235	ASP	2.2
1	A	23	TYR	2.2
1	C	6	HIS	2.2
2	B	101	ALA	2.2
1	C	222	GLN	2.2
1	C	77	PHE	2.2
1	A	3	PRO	2.2
1	C	257	LYS	2.2
1	A	40	ILE	2.2
1	A	84	GLY	2.2
1	A	146	ASP	2.2
2	D	1	GLY	2.2
1	C	259	PHE	2.2
2	B	97	TYR	2.2
1	A	77	PHE	2.1
1	A	230	MET	2.1
1	A	231	MET	2.1
1	C	163	MET	2.1
1	C	175	HIS	2.1
1	A	180	THR	2.1
2	B	17	CYS	2.1
1	A	96	HIS	2.1
1	C	109	SER	2.1
1	C	171	LEU	2.1
2	D	80	MET	2.1
1	A	276	PHE	2.1
1	A	42	TYR	2.1
1	C	244	TYR	2.1
1	C	234	THR	2.1
1	C	226	LYS	2.1
1	C	240	GLN	2.1
1	A	229	TYR	2.1
1	C	1	THR	2.1
1	A	25	ALA	2.1
1	A	64	GLY	2.1
2	B	92	ASN	2.1
1	C	159	GLN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	14	CYS	2.1
1	C	245	LEU	2.1
2	D	12	THR	2.1
1	C	283	PRO	2.1
1	A	137	THR	2.0
1	A	220	ASN	2.0
1	A	293	GLY	2.0
2	B	29	GLY	2.0
1	A	147	ALA	2.0
1	A	184	ASN	2.0
2	B	63	ASN	2.0
2	D	62	ASN	2.0
1	C	178	GLY	2.0
1	A	83	ALA	2.0
2	B	102	CYS	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 carbohydrates 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. 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
4	HEM	B	104	43/43	0.77	0.29	-0.02	24,30,33,35	0
4	HEM	D	104	43/43	0.81	0.30	-0.20	26,32,42,48	0
4	HEM	A	296	43/43	0.91	0.20	-0.72	9,18,20,24	0
4	HEM	C	296	43/43	0.82	0.24	-0.83	7,16,20,24	0
3	SO4	A	299	2/5	0.82	0.26	-	28,28,28,29	0
3	SO4	C	300	2/5	0.84	0.25	-	22,22,22,25	0

6.5 Other polymers (i)

There are no such residues in this entry.