Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:24 AM GMT

PDB ID	:	3EKB
Title	:	Crystal structure of the A264C mutant heme domain of cytochrome P450 BM3
Authors	:	Leys, D
Deposited on	:	2008-09-19
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:

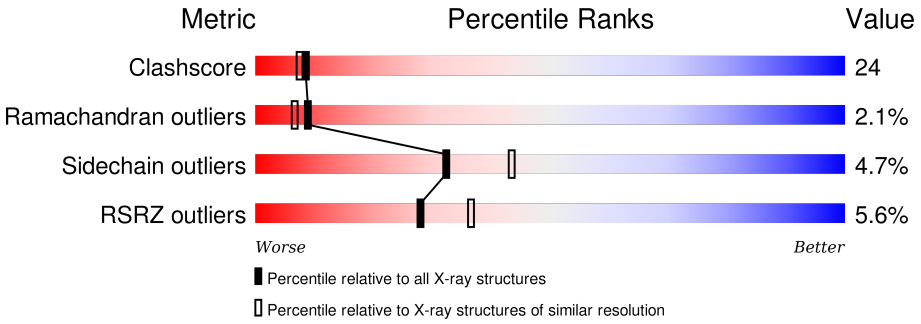
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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	470	4% 62% 28% 6%
1	B	470	7% 66% 29%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7936 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.

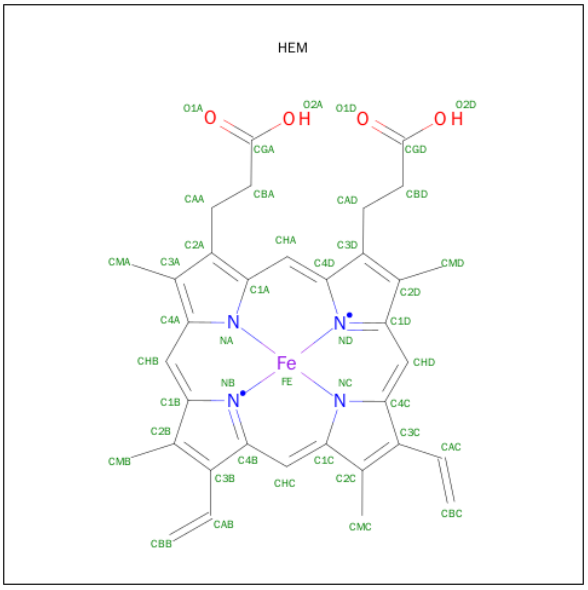
- Molecule 1 is a protein called Cytochrome P450(BM-3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	50	0
			3858	2474	653	710	21			
1	B	457	Total	C	N	O	S	0	18	0
			3698	2367	623	691	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	264	CYS	ALA	ENGINEERED	UNP P14779
B	264	CYS	ALA	ENGINEERED	UNP P14779

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



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

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

- Molecule 3 is water.

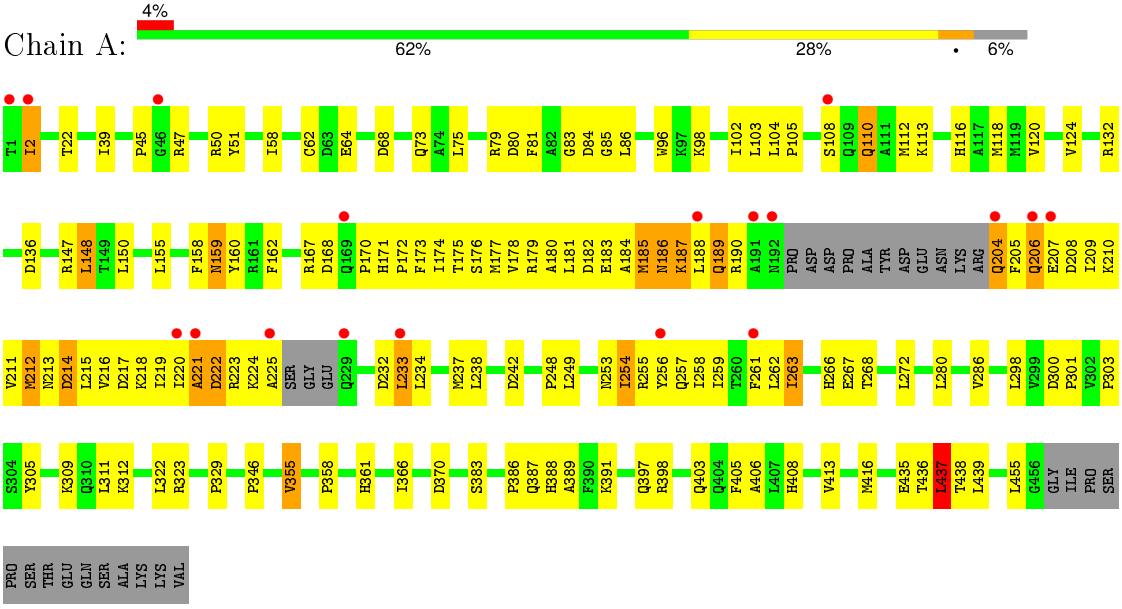
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	177	Total	O	0	0
			177	177		
3	B	117	Total	O	0	0
			117	117		

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.

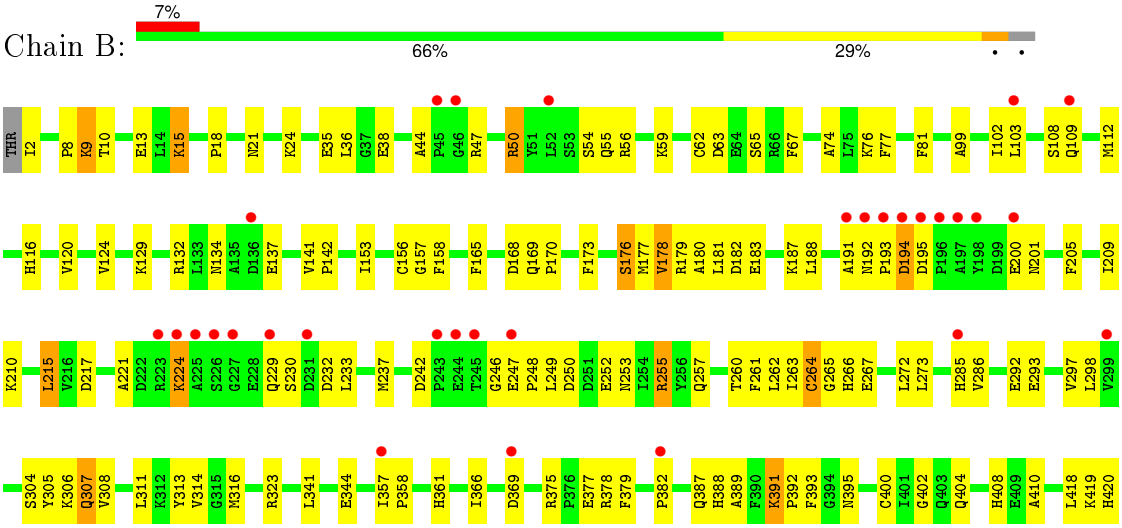
- Molecule 1: Cytochrome P450(BM-3)

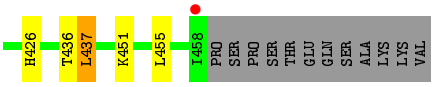
Chain A:



- Molecule 1: Cytochrome P450(BM-3)

Chain B:




H426
T436
L437
K451
L455
I458
PRO
SER
PRO
SER
THR
GLU
GLN
SER
ALA
LYS
LYS
VAL

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	60.88Å 118.69Å 146.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.68 – 2.30 19.68 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.68-2.30) 86.1 (19.68-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.46 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.215 , 0.302 0.218 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	38.5	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 57.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 54014 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7936	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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	1.04	2/3964 (0.1%)	0.99	13/5367 (0.2%)
1	B	0.98	0/3793	0.96	8/5152 (0.2%)
All	All	1.01	2/7757 (0.0%)	0.98	21/10519 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	355	VAL	CB-CG2	5.85	1.65	1.52
1	A	405	PHE	CE1-CZ	5.62	1.48	1.37

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	437	LEU	CA-CB-CG	9.85	137.95	115.30
1	A	50	ARG	NE-CZ-NH1	9.25	124.93	120.30
1	B	50	ARG	NE-CZ-NH1	9.15	124.88	120.30
1	B	50	ARG	NE-CZ-NH2	-7.89	116.36	120.30
1	A	50	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	B	437	LEU	CA-CB-CG	7.22	131.91	115.30
1	A	132	ARG	NE-CZ-NH2	-6.75	116.92	120.30
1	A	68	ASP	CB-CG-OD2	-6.35	112.58	118.30
1	B	437	LEU	CB-CG-CD2	5.93	121.08	111.00
1	A	68	ASP	CB-CG-OD1	5.83	123.54	118.30
1	A	96	TRP	CA-CB-CG	-5.83	102.63	113.70
1	A	455	LEU	CA-CB-CG	5.67	128.34	115.30
1	B	132	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	84	ASP	CB-CG-OD1	5.44	123.20	118.30
1	A	147	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	B	264	CYS	CA-CB-SG	-5.17	104.70	114.00
1	B	24	LYS	CD-CE-NZ	5.13	123.51	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	416	MET	CG-SD-CE	-5.06	92.10	100.20
1	B	455	LEU	CA-CB-CG	5.06	126.94	115.30
1	A	132	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	75	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3858	0	3738	234	1
1	B	3698	0	3517	122	0
2	A	43	0	30	3	0
2	B	43	0	30	2	0
3	A	177	0	0	26	0
3	B	117	0	0	14	1
All	All	7936	0	7315	358	1

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 24.

All (358) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183[A]:GLU:CB	1:A:205[A]:PHE:CE1	1.80	1.58
1:A:207[B]:GLU:O	1:A:211[B]:VAL:HG23	1.27	1.27
1:A:183[A]:GLU:CB	1:A:205[A]:PHE:CZ	2.21	1.24
1:A:186[B]:ASN:O	1:A:187[B]:LYS:CG	1.86	1.23
1:A:186[B]:ASN:O	1:A:187[B]:LYS:HG3	1.34	1.21
1:A:183[A]:GLU:CB	1:A:205[A]:PHE:HE1	1.30	1.19
1:B:248:PRO:HD3	3:B:487:HOH:O	1.43	1.17
1:A:158[B]:PHE:CZ	1:A:219[B]:ILE:CD1	2.26	1.17
1:B:173[A]:PHE:O	1:B:177[A]:MET:HE2	1.45	1.16
1:A:158[B]:PHE:CZ	1:A:219[B]:ILE:HD12	1.82	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179[A]:ARG:HA	1:B:182[A]:ASP:HB3	1.19	1.13
1:A:81:PHE:HE1	1:A:184[B]:ALA:HB2	1.04	1.12
1:A:179[A]:ARG:CZ	1:A:204[A]:GLN:OE1	1.99	1.10
1:A:207[B]:GLU:O	1:A:211[B]:VAL:CG2	1.99	1.10
1:A:213[A]:ASN:O	1:A:216[A]:VAL:N	1.86	1.06
1:B:179[A]:ARG:HA	1:B:182[A]:ASP:CB	1.86	1.05
1:A:177[B]:MET:HE2	3:A:486:HOH:O	1.56	1.03
1:A:81:PHE:CE1	1:A:184[B]:ALA:HB2	1.94	1.01
1:A:181[A]:LEU:HD22	1:A:437:LEU:HD22	1.41	1.01
1:B:388:HIS:CD2	1:B:391:LYS:HZ2	1.83	0.97
1:B:179[A]:ARG:CA	1:B:182[A]:ASP:HB3	1.94	0.96
1:A:108:SER:O	1:A:112:MET:HB2	1.65	0.96
1:A:174[B]:ILE:O	1:A:178[B]:VAL:HG23	1.67	0.94
1:B:388:HIS:HD2	1:B:391:LYS:NZ	1.65	0.94
1:A:158[B]:PHE:HZ	1:A:219[B]:ILE:HD12	1.20	0.93
1:A:158[B]:PHE:CZ	1:A:219[B]:ILE:HD13	2.01	0.92
1:A:237:MET:HE3	1:A:254:ILE:HD12	1.51	0.92
1:A:158[B]:PHE:CE2	1:A:219[B]:ILE:HD13	2.05	0.92
1:A:136:ASP:CB	3:A:633:HOH:O	2.18	0.90
1:A:179[A]:ARG:HB3	1:A:208[A]:ASP:OD2	1.72	0.89
1:B:388:HIS:HD2	1:B:391:LYS:HZ2	0.92	0.89
1:A:181[B]:LEU:HD12	1:A:185[B]:MET:HG2	1.55	0.89
1:A:213[A]:ASN:HA	1:A:216[A]:VAL:HG23	1.56	0.88
1:A:220[B]:ILE:O	1:A:223[B]:ARG:N	2.06	0.87
1:A:150:LEU:HD21	1:A:174[B]:ILE:HG12	1.55	0.87
1:A:173[B]:PHE:CE1	1:A:212[B]:MET:HG2	2.10	0.87
1:A:258:ILE:HA	3:A:478:HOH:O	1.73	0.87
1:B:173[A]:PHE:O	1:B:177[A]:MET:CE	2.23	0.87
1:A:262:LEU:O	1:A:266:HIS:HD2	1.56	0.86
1:A:213[A]:ASN:O	1:A:215[A]:LEU:N	2.08	0.85
1:B:177[A]:MET:HA	1:B:180[A]:ALA:HB3	1.58	0.85
1:A:237:MET:SD	3:A:634:HOH:O	2.35	0.84
1:A:186[B]:ASN:O	1:A:187[B]:LYS:HG2	1.74	0.84
1:A:237:MET:HE1	1:A:258:ILE:CD1	2.07	0.84
1:A:177[B]:MET:O	1:A:180[B]:ALA:HB3	1.79	0.83
1:A:174[A]:ILE:HD13	3:A:486:HOH:O	1.77	0.83
1:B:169[A]:GLN:O	1:B:170[A]:PRO:O	1.98	0.82
1:A:171[B]:HIS:CD2	3:A:639:HOH:O	2.31	0.82
1:B:9:LYS:HA	3:B:582:HOH:O	1.80	0.82
1:B:173[A]:PHE:C	1:B:177[A]:MET:HE2	2.00	0.81
1:A:177[A]:MET:CA	1:A:212[A]:MET:HE3	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176[A]:SER:O	1:B:180[A]:ALA:HB2	1.81	0.80
1:A:177[A]:MET:CG	3:A:623:HOH:O	2.29	0.80
1:A:167[B]:ARG:NH1	1:A:171[B]:HIS:HA	1.97	0.79
1:A:212[B]:MET:O	1:A:216[B]:VAL:HG23	1.82	0.79
1:A:213[A]:ASN:HA	1:A:216[A]:VAL:CG2	2.13	0.78
1:B:265:GLY:O	1:B:266:HIS:C	2.17	0.78
1:A:158[B]:PHE:CE2	1:A:219[B]:ILE:CD1	2.64	0.78
1:A:171[B]:HIS:HD2	3:A:639:HOH:O	1.64	0.78
1:A:186[B]:ASN:C	1:A:187[B]:LYS:HG3	2.04	0.78
1:A:177[A]:MET:N	1:A:212[A]:MET:HE3	1.99	0.77
1:A:179[B]:ARG:HD2	1:A:208[B]:ASP:OD2	1.85	0.77
1:B:382:PRO:HG2	3:B:578:HOH:O	1.83	0.77
1:B:173[A]:PHE:C	1:B:177[A]:MET:CE	2.53	0.77
1:B:404:GLN:HG2	3:B:538:HOH:O	1.84	0.76
1:B:247:GLU:HA	3:B:487:HOH:O	1.85	0.76
1:A:47:ARG:NH2	1:A:188[A]:LEU:O	2.19	0.75
1:A:177[A]:MET:HG3	3:A:623:HOH:O	1.83	0.74
1:B:177[A]:MET:C	1:B:179[A]:ARG:N	2.39	0.74
1:B:55:GLN:O	1:B:59:LYS:HG2	1.88	0.74
1:A:181[B]:LEU:HG	1:A:182[B]:ASP:N	2.02	0.73
1:A:180[A]:ALA:HA	1:A:205[A]:PHE:CZ	2.24	0.73
1:A:210[A]:LYS:O	1:A:214[A]:ASP:OD1	2.06	0.73
1:A:436:THR:O	1:A:437:LEU:HB3	1.89	0.72
1:B:10:THR:HB	1:B:15:LYS:HZ2	1.55	0.72
1:A:437:LEU:HD23	1:A:438:THR:H	1.55	0.71
1:A:185[B]:MET:O	1:A:186[B]:ASN:C	2.26	0.71
1:A:177[A]:MET:HB2	1:A:212[A]:MET:HE1	1.72	0.71
1:A:190:ARG:HD3	3:A:606:HOH:O	1.91	0.71
1:A:170[B]:PRO:HB2	1:A:174[B]:ILE:HB	1.73	0.70
1:A:181[B]:LEU:HB2	3:A:623:HOH:O	1.91	0.70
1:B:62:CYS:HB3	1:B:395:ASN:OD1	1.91	0.70
1:B:177[A]:MET:C	1:B:179[A]:ARG:H	1.90	0.70
1:B:305:TYR:CD1	1:B:305:TYR:C	2.63	0.70
1:B:388:HIS:CD2	1:B:391:LYS:NZ	2.50	0.70
1:A:81:PHE:HE1	1:A:184[B]:ALA:CB	1.94	0.69
1:A:221[A]:ALA:O	1:A:225[A]:ALA:N	2.24	0.69
1:A:220[B]:ILE:HB	1:A:238:LEU:HD11	1.74	0.68
1:A:181[B]:LEU:CD1	1:A:185[B]:MET:HG2	2.24	0.68
1:A:120:VAL:O	1:A:124:VAL:HG23	1.93	0.68
1:A:167[B]:ARG:HH12	1:A:171[B]:HIS:HA	1.58	0.68
1:A:403:GLN:NE2	3:A:506:HOH:O	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:GLU:OE2	1:A:397:GLN:HG2	1.93	0.67
1:A:237:MET:CE	1:A:258:ILE:CD1	2.72	0.66
1:A:177[A]:MET:HB2	1:A:212[A]:MET:CE	2.25	0.66
1:A:237:MET:CE	1:A:258:ILE:HD11	2.26	0.66
1:A:212[A]:MET:O	1:A:213[A]:ASN:O	2.13	0.66
1:A:181[A]:LEU:HD13	1:A:267:GLU:OE2	1.96	0.66
1:B:420:HIS:NE2	3:B:508:HOH:O	2.28	0.66
1:A:177[A]:MET:HG2	3:A:623:HOH:O	1.93	0.65
1:A:237:MET:HB3	1:A:254:ILE:HD12	1.79	0.65
1:A:162:PHE:HE1	1:A:215[A]:LEU:HD21	1.62	0.65
1:A:102:ILE:C	3:A:517:HOH:O	2.34	0.65
1:A:175[B]:THR:N	3:A:535:HOH:O	2.29	0.64
1:A:104:LEU:HB3	1:A:105:PRO:HD3	1.80	0.64
1:B:304:SER:OG	1:B:307:GLN:NE2	2.31	0.64
1:A:160:TYR:OH	1:A:171[B]:HIS:NE2	2.31	0.64
1:B:388:HIS:HA	1:B:391:LYS:HD2	1.80	0.63
1:B:10:THR:HB	1:B:15:LYS:NZ	2.13	0.63
1:B:8:PRO:O	1:B:9:LYS:CB	2.46	0.63
1:A:213[A]:ASN:CA	1:A:216[A]:VAL:HG23	2.28	0.63
1:A:73:GLN:HB2	1:A:188[A]:LEU:HD23	1.81	0.62
1:B:103:LEU:HD13	1:B:261:PHE:HZ	1.63	0.62
1:B:177[A]:MET:O	1:B:179[A]:ARG:N	2.33	0.62
1:A:158[B]:PHE:HZ	1:A:219[B]:ILE:CD1	1.89	0.62
1:A:186[B]:ASN:C	1:A:187[B]:LYS:CG	2.65	0.61
1:A:216[B]:VAL:HG11	1:A:258:ILE:HG13	1.83	0.61
1:A:183[A]:GLU:O	1:A:185[A]:MET:N	2.33	0.61
1:B:116:HIS:HD2	1:B:408:HIS:NE2	1.99	0.61
1:B:252:GLU:HG3	1:B:255:ARG:HH21	1.66	0.60
1:A:173[B]:PHE:CD1	1:A:212[B]:MET:HG2	2.36	0.60
1:A:262:LEU:O	1:A:266:HIS:CD2	2.48	0.60
1:A:162:PHE:CE1	1:A:215[A]:LEU:HD21	2.36	0.60
1:A:185[B]:MET:O	1:A:187[B]:LYS:N	2.34	0.60
1:B:205:PHE:CE2	1:B:209:ILE:HD11	2.37	0.60
1:A:103:LEU:HD22	1:A:233:LEU:HD12	1.84	0.60
1:A:158[B]:PHE:CZ	1:A:216[B]:VAL:HG13	2.37	0.60
1:A:280:LEU:HD23	1:A:286:VAL:HG12	1.84	0.59
1:A:148:LEU:HD21	1:A:413:VAL:HG21	1.84	0.59
1:A:206[A]:GLN:O	1:A:210[A]:LYS:CB	2.51	0.59
1:A:184[B]:ALA:O	1:A:185[B]:MET:O	2.21	0.59
1:A:179[A]:ARG:NH2	1:A:204[A]:GLN:OE1	2.35	0.59
1:A:173[B]:PHE:HD1	1:A:215[B]:LEU:HD23	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:PHE:HB3	1:B:400:CYS:HB3	1.83	0.59
1:A:167[B]:ARG:NH1	1:A:171[B]:HIS:CA	2.64	0.59
1:A:176[B]:SER:N	3:A:535:HOH:O	1.96	0.59
1:A:237:MET:HB3	1:A:254:ILE:CD1	2.32	0.59
1:B:266:HIS:CE1	1:B:267:GLU:HB2	2.38	0.59
1:A:177[A]:MET:CB	1:A:212[A]:MET:HE1	2.33	0.58
1:A:436:THR:O	1:A:437:LEU:CB	2.49	0.58
1:A:183[A]:GLU:O	1:A:186[A]:ASN:N	2.36	0.58
1:A:158[B]:PHE:CD1	1:A:234:LEU:HD22	2.38	0.58
1:B:181[A]:LEU:HD11	1:B:263:ILE:HG23	1.85	0.58
1:B:179[A]:ARG:HA	1:B:182[A]:ASP:HB2	1.82	0.58
1:B:103:LEU:HD21	1:B:237:MET:HG2	1.85	0.58
1:B:99:ALA:HB2	1:B:249:LEU:HD21	1.86	0.58
1:B:177[A]:MET:O	1:B:181[A]:LEU:N	2.22	0.57
1:A:237:MET:HE1	1:A:258:ILE:HD13	1.86	0.57
1:A:216[B]:VAL:HG11	1:A:258:ILE:HG21	1.87	0.57
1:B:179[A]:ARG:C	1:B:182[A]:ASP:HB3	2.25	0.57
1:A:249:LEU:HD12	1:A:254:ILE:HD11	1.85	0.57
1:A:177[A]:MET:CB	1:A:212[A]:MET:CE	2.83	0.56
1:B:316:MET:HE3	1:B:377:GLU:HA	1.88	0.56
1:A:216[B]:VAL:C	1:A:218[B]:LYS:H	2.08	0.56
1:B:436:THR:O	1:B:437:LEU:HB2	2.05	0.56
1:B:285:HIS:HB2	3:B:506:HOH:O	2.05	0.56
1:A:177[B]:MET:HE3	1:A:263:ILE:HG12	1.88	0.56
1:A:177[A]:MET:HA	1:A:212[A]:MET:HE3	1.84	0.56
1:A:179[B]:ARG:HD3	1:A:204[B]:GLN:HG2	1.87	0.56
1:B:249:LEU:HD22	1:B:253:ASN:OD1	2.06	0.56
1:A:254:ILE:O	1:A:258:ILE:HG12	2.06	0.55
1:A:216[B]:VAL:CG1	1:A:258:ILE:HG21	2.37	0.55
1:A:216[B]:VAL:O	1:A:218[B]:LYS:N	2.37	0.55
1:A:221[A]:ALA:HA	1:A:224[A]:LYS:HB2	1.89	0.55
1:B:18:PRO:O	1:B:21:ASN:HB2	2.05	0.55
1:A:181[B]:LEU:CD1	1:A:185[B]:MET:CG	2.85	0.55
1:B:191:ALA:HB2	3:B:569:HOH:O	2.07	0.55
1:A:268:THR:OG1	3:A:647:HOH:O	2.04	0.54
1:A:237:MET:HE2	1:A:258:ILE:HD11	1.88	0.54
1:A:105:PRO:HD2	3:A:517:HOH:O	2.06	0.54
1:B:286:VAL:HG13	1:B:313:TYR:OH	2.07	0.54
1:B:242:ASP:O	1:B:246:GLY:N	2.40	0.54
1:A:300:ASP:HB3	1:A:301:PRO:HD2	1.89	0.54
1:B:173[A]:PHE:C	1:B:177[A]:MET:HE1	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179[B]:ARG:CD	1:A:208[B]:ASP:OD2	2.54	0.54
1:A:177[B]:MET:CE	1:A:263:ILE:HG12	2.38	0.53
1:A:237:MET:HE1	1:A:258:ILE:HD11	1.89	0.53
1:A:185[A]:MET:HG3	3:A:622:HOH:O	2.07	0.53
1:A:257:GLN:O	1:A:261:PHE:HD1	1.92	0.53
1:B:81:PHE:HB3	1:B:209:ILE:HG12	1.91	0.53
1:B:298:LEU:HB2	1:B:419:LYS:HD2	1.90	0.53
1:A:224[A]:LYS:NZ	3:A:602:HOH:O	2.31	0.53
1:B:179[A]:ARG:O	1:B:182[A]:ASP:HB3	2.09	0.53
1:A:223[B]:ARG:HG3	3:A:569:HOH:O	2.09	0.53
1:B:392:PRO:HD2	3:B:565:HOH:O	2.07	0.53
1:A:150:LEU:HD21	1:A:174[B]:ILE:CG1	2.35	0.52
1:A:213[B]:ASN:HB3	1:A:255:ARG:NE	2.25	0.52
1:B:377:GLU:OE1	1:B:377:GLU:N	2.39	0.52
1:A:272:LEU:HD13	1:A:322:LEU:HG	1.92	0.52
1:B:103:LEU:HD21	1:B:237:MET:CG	2.39	0.52
1:A:179[A]:ARG:NE	1:A:204[A]:GLN:OE1	2.41	0.52
1:A:249:LEU:HD12	1:A:254:ILE:CD1	2.40	0.52
1:A:187[A]:LYS:HA	1:A:190:ARG:HD2	1.91	0.52
1:A:209[A]:ILE:O	1:A:211[A]:VAL:N	2.43	0.52
1:A:103:LEU:HD22	1:A:233:LEU:CD1	2.39	0.52
1:A:280:LEU:CD2	1:A:286:VAL:HG12	2.40	0.51
1:A:98:LYS:CE	1:A:248:PRO:O	2.59	0.51
1:B:168[B]:ASP:N	3:B:580:HOH:O	1.94	0.51
1:B:176[A]:SER:O	1:B:180[A]:ALA:CB	2.54	0.51
1:A:81:PHE:CE1	1:A:184[B]:ALA:CB	2.79	0.51
1:B:44:ALA:HB3	1:B:47:ARG:HG3	1.93	0.51
1:A:220[B]:ILE:HA	1:A:223[B]:ARG:HB3	1.93	0.51
1:A:223[A]:ARG:CZ	1:A:234:LEU:HD23	2.41	0.51
1:A:220[B]:ILE:C	1:A:222[B]:ASP:N	2.63	0.51
1:A:173[B]:PHE:CZ	1:A:262:LEU:HD13	2.45	0.51
1:B:419:LYS:O	1:B:451:LYS:HD2	2.11	0.51
1:B:81:PHE:CE2	1:B:263:ILE:HD11	2.46	0.50
1:A:175[B]:THR:CA	3:A:535:HOH:O	2.59	0.50
1:A:366:ILE:HG21	1:A:389:ALA:HB1	1.92	0.50
1:A:116:HIS:HD2	1:A:408:HIS:NE2	2.09	0.50
1:A:179[A]:ARG:NH1	1:A:204[A]:GLN:OE1	2.40	0.50
1:B:156:CYS:O	1:B:232:ASP:HB2	2.11	0.50
1:A:183[B]:GLU:CB	1:A:205[B]:PHE:HD1	2.25	0.50
1:A:237:MET:HE1	1:A:258:ILE:CG1	2.41	0.49
1:A:183[B]:GLU:CB	1:A:205[B]:PHE:CD1	2.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181[B]:LEU:HD12	1:A:185[B]:MET:CG	2.35	0.49
1:A:183[A]:GLU:O	1:A:184[A]:ALA:C	2.49	0.49
1:A:2:ILE:HG12	1:A:346:PRO:HD3	1.93	0.49
1:A:176[B]:SER:O	1:A:180[B]:ALA:HB2	2.11	0.49
1:B:55:GLN:O	1:B:59:LYS:CG	2.59	0.49
1:A:255:ARG:O	1:A:259:ILE:HG13	2.13	0.49
1:A:173[B]:PHE:HB2	1:A:215[B]:LEU:CD2	2.42	0.49
1:B:109:GLN:HB2	1:B:404:GLN:HG3	1.94	0.49
1:B:38:GLU:HB3	1:B:54:SER:HB3	1.93	0.49
1:A:220[B]:ILE:C	1:A:222[B]:ASP:H	2.16	0.49
1:A:85:GLY:HA2	1:A:257:GLN:NE2	2.27	0.49
1:B:375:ARG:HG2	1:B:375:ARG:HH11	1.78	0.49
1:A:237:MET:HE1	1:A:258:ILE:HG12	1.95	0.49
1:A:176[B]:SER:O	1:A:180[B]:ALA:CB	2.60	0.49
1:A:176[B]:SER:O	1:A:180[B]:ALA:N	2.38	0.49
1:A:177[B]:MET:HE1	1:A:263:ILE:HA	1.93	0.49
1:B:102:ILE:HG22	1:B:102:ILE:O	2.13	0.49
1:A:177[A]:MET:CA	1:A:212[A]:MET:CE	2.88	0.48
1:B:177[A]:MET:HA	1:B:180[A]:ALA:CB	2.37	0.48
1:A:406:ALA:HB2	2:A:471:HEM:HHC	1.95	0.48
2:A:471:HEM:HBB2	2:A:471:HEM:CMB	2.43	0.48
1:B:194:ASP:HA	3:B:579:HOH:O	2.13	0.48
1:A:183[A]:GLU:CB	1:A:205[A]:PHE:HZ	2.11	0.48
1:A:207[B]:GLU:O	1:A:211[B]:VAL:CB	2.58	0.48
1:A:150:LEU:CD2	1:A:174[B]:ILE:HG12	2.37	0.48
1:A:213[A]:ASN:O	1:A:214[A]:ASP:C	2.51	0.48
1:A:220[B]:ILE:O	1:A:222[B]:ASP:N	2.46	0.48
1:B:35:GLU:HB3	1:B:36:LEU:HD23	1.95	0.48
1:A:300:ASP:HB3	1:A:301:PRO:CD	2.43	0.47
1:A:181[B]:LEU:HD11	1:A:185[B]:MET:HG3	1.96	0.47
1:A:220[B]:ILE:HB	1:A:238:LEU:HD21	1.97	0.47
1:B:157:GLY:C	1:B:158:PHE:CG	2.88	0.47
1:B:304:SER:O	1:B:308:VAL:HG23	2.15	0.47
1:B:141:VAL:HB	1:B:142:PRO:HD3	1.97	0.47
1:A:173[B]:PHE:C	1:A:173[B]:PHE:CD2	2.88	0.47
1:B:177[A]:MET:O	1:B:178[A]:VAL:C	2.53	0.47
1:B:387:GLN:HG2	1:B:388:HIS:ND1	2.29	0.47
1:B:217:ASP:OD1	1:B:255:ARG:HD3	2.15	0.47
1:B:311:LEU:HB3	1:B:314:VAL:HB	1.96	0.47
1:A:162:PHE:HB3	1:A:174[B]:ILE:HD11	1.96	0.47
1:B:286:VAL:HG23	3:B:506:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:HIS:HD2	1:A:391:LYS:NZ	2.13	0.47
1:A:215[A]:LEU:O	1:A:216[A]:VAL:C	2.53	0.46
1:B:253:ASN:O	1:B:257:GLN:HG2	2.14	0.46
1:A:118:MET:HG2	3:A:615:HOH:O	2.15	0.46
1:B:272:LEU:HD12	1:B:272:LEU:C	2.35	0.46
1:A:58:ILE:HD13	1:A:355:VAL:HG13	1.96	0.46
1:A:204[A]:GLN:HG3	1:A:207[A]:GLU:HB3	1.97	0.46
1:A:437:LEU:HD23	1:A:438:THR:HG23	1.98	0.46
1:B:400:CYS:HB2	2:B:471:HEM:NA	2.31	0.46
1:B:120:VAL:O	1:B:124:VAL:HG23	2.16	0.46
1:B:2:ILE:HA	1:B:344:GLU:O	2.16	0.46
1:B:178[A]:VAL:O	1:B:182[A]:ASP:HB2	2.14	0.46
1:B:76:LYS:HD3	3:B:584:HOH:O	2.15	0.46
1:A:162:PHE:HA	3:A:639:HOH:O	2.15	0.46
1:A:167[B]:ARG:NH1	1:A:171[B]:HIS:N	2.63	0.46
1:B:357:ILE:HG22	1:B:361:HIS:CE1	2.49	0.46
1:A:204[B]:GLN:HG3	1:A:208[B]:ASP:OD2	2.15	0.46
1:A:209[A]:ILE:C	1:A:211[A]:VAL:N	2.70	0.46
1:A:437:LEU:CD2	1:A:438:THR:HG23	2.46	0.46
1:B:323:ARG:HG2	1:B:361:HIS:HB3	1.98	0.46
1:A:81:PHE:CD1	1:A:205[B]:PHE:HZ	2.34	0.46
1:B:38:GLU:CB	1:B:54:SER:HB3	2.46	0.46
1:A:305:TYR:O	1:A:309:LYS:HG2	2.16	0.46
1:A:215[B]:LEU:HG	1:A:216[B]:VAL:N	2.30	0.45
1:A:183[A]:GLU:C	1:A:185[A]:MET:N	2.70	0.45
1:B:377:GLU:C	1:B:379:PHE:H	2.19	0.45
1:B:74:ALA:HB2	1:B:188:LEU:HD11	1.98	0.45
1:A:103:LEU:HD21	1:A:237:MET:HG3	1.99	0.45
1:A:221[A]:ALA:O	1:A:224[A]:LYS:N	2.49	0.45
1:A:181[A]:LEU:HB3	1:A:436:THR:HB	1.99	0.45
1:B:377:GLU:C	1:B:379:PHE:N	2.70	0.45
1:B:436:THR:O	1:B:437:LEU:CB	2.65	0.45
1:A:170[B]:PRO:O	1:A:171[B]:HIS:C	2.55	0.44
1:A:329:PRO:O	1:A:358:PRO:HD3	2.17	0.44
1:A:209[A]:ILE:C	1:A:211[A]:VAL:H	2.20	0.44
1:A:298:LEU:HD21	1:A:311:LEU:HD11	1.99	0.44
1:B:63:ASP:OD1	1:B:65:SER:OG	2.35	0.44
1:B:77:PHE:CD1	1:B:187:LYS:HE3	2.52	0.44
1:A:216[A]:VAL:HG22	1:A:259:ILE:HG12	1.99	0.44
1:A:216[B]:VAL:HA	1:A:219[B]:ILE:HD12	1.98	0.44
1:B:366:ILE:HG21	1:B:389:ALA:HB1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220[A]:ILE:O	1:A:224[A]:LYS:HB2	2.17	0.44
1:B:129:LYS:HD2	1:B:165[A]:PHE:HD1	1.82	0.44
1:A:232:ASP:O	1:A:233:LEU:C	2.56	0.44
1:A:79:ARG:HG3	1:A:83:GLY:O	2.18	0.44
1:B:316:MET:CE	1:B:377:GLU:HA	2.48	0.43
1:A:98:LYS:HE3	1:A:248:PRO:O	2.18	0.43
1:A:179[A]:ARG:O	1:A:182[A]:ASP:HB3	2.18	0.43
1:A:221[A]:ALA:O	1:A:222[A]:ASP:C	2.57	0.43
1:A:22:THR:H	1:A:189:GLN:HE22	1.66	0.43
1:B:169[A]:GLN:C	1:B:170[A]:PRO:O	2.55	0.43
1:B:10:THR:H	1:B:10:THR:HG23	1.56	0.43
1:B:273:LEU:HD11	1:B:410:ALA:HA	2.00	0.43
1:B:418:LEU:HA	1:B:418:LEU:HD23	1.72	0.43
1:A:179[B]:ARG:HD3	1:A:204[B]:GLN:CG	2.49	0.43
1:A:204[A]:GLN:HB2	1:A:204[A]:GLN:HE21	1.60	0.43
1:A:223[B]:ARG:CG	3:A:569:HOH:O	2.65	0.43
1:A:254:ILE:HA	1:A:254:ILE:HD13	1.56	0.43
1:B:293:GLU:O	1:B:297:VAL:HG23	2.19	0.43
1:A:220[B]:ILE:C	1:A:223[B]:ARG:H	2.16	0.43
1:A:62:CYS:SG	1:A:391:LYS:HE2	2.58	0.43
1:B:305:TYR:HD1	1:B:306:LYS:N	2.17	0.42
1:B:35:GLU:CB	1:B:36:LEU:HD23	2.48	0.42
1:A:177[A]:MET:CB	1:A:212[A]:MET:HE3	2.49	0.42
1:A:220[B]:ILE:O	1:A:223[B]:ARG:HB3	2.18	0.42
1:B:173[B]:PHE:CD1	1:B:215:LEU:HD22	2.54	0.42
1:A:253:ASN:O	1:A:256:TYR:HB2	2.19	0.42
1:B:153:ILE:HG13	3:B:553:HOH:O	2.19	0.42
1:A:207[A]:GLU:O	1:A:211[A]:VAL:CG2	2.68	0.42
1:A:220[B]:ILE:HA	1:A:223[B]:ARG:CB	2.49	0.42
1:B:134:ASN:N	1:B:137:GLU:OE1	2.34	0.42
1:A:222[B]:ASP:O	1:A:225[B]:ALA:HB3	2.20	0.42
1:A:173[B]:PHE:HE2	1:A:177[B]:MET:SD	2.43	0.42
1:A:207[A]:GLU:O	1:A:211[A]:VAL:HG23	2.19	0.42
1:A:73:GLN:HB2	1:A:188[A]:LEU:CD2	2.49	0.42
1:B:357:ILE:N	1:B:358:PRO:CD	2.82	0.42
1:A:323:ARG:HG2	1:A:361:HIS:HB3	2.02	0.42
2:A:471:HEM:HBB2	2:A:471:HEM:HMB2	2.02	0.42
1:B:108:SER:O	1:B:112:MET:CE	2.68	0.42
1:A:259:ILE:H	1:A:259:ILE:HG13	1.65	0.41
1:A:98:LYS:HG3	1:A:242:ASP:HB2	2.03	0.41
1:A:116:HIS:HE1	1:A:303:PRO:O	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:THR:O	1:B:264:CYS:HB2	2.21	0.41
1:B:221:ALA:O	1:B:224:LYS:HG3	2.19	0.41
1:B:67:PHE:CZ	1:B:341:LEU:HD13	2.55	0.41
1:A:81:PHE:HD1	1:A:205[B]:PHE:HZ	1.69	0.41
1:B:183:GLU:OE2	1:B:201:ASN:HB3	2.21	0.41
1:A:86:LEU:O	1:A:398:ARG:NH2	2.54	0.41
1:A:172[B]:PRO:O	3:A:535:HOH:O	2.22	0.41
1:A:213[A]:ASN:O	1:A:215[A]:LEU:CA	2.68	0.41
1:A:222[A]:ASP:O	1:A:223[A]:ARG:C	2.57	0.41
1:B:173[B]:PHE:CE2	1:B:262:LEU:HD13	2.56	0.41
1:B:229:GLN:NE2	1:B:229:GLN:HA	2.35	0.41
1:A:435:GLU:HG2	1:A:439:LEU:CD2	2.51	0.41
1:B:377:GLU:O	1:B:379:PHE:N	2.54	0.41
1:B:108:SER:O	1:B:112:MET:HE3	2.21	0.40
1:B:173[A]:PHE:CB	1:B:177[A]:MET:HE1	2.37	0.40
1:A:39:ILE:HA	1:A:51:TYR:O	2.22	0.40
1:B:402:GLY:HA3	2:B:471:HEM:C3C	2.56	0.40
1:A:110:GLN:H	1:A:113:LYS:HG3	1.87	0.40
1:A:181[A]:LEU:HD22	1:A:437:LEU:CD2	2.30	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168[B]:ASP:OD2	3:B:580:HOH:O[3_545]	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	484/470 (103%)	423 (87%)	43 (9%)	18 (4%)	4 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	473/470 (101%)	421 (89%)	45 (10%)	7 (2%)	13 12
All	All	957/940 (102%)	844 (88%)	88 (9%)	25 (3%)	9 4

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	GLN
1	A	185[A]	MET
1	A	185[B]	MET
1	A	186[A]	ASN
1	A	186[B]	ASN
1	A	187[A]	LYS
1	A	187[B]	LYS
1	A	217[A]	ASP
1	A	217[B]	ASP
1	A	159[A]	ASN
1	A	159[B]	ASN
1	A	189	GLN
1	A	221[A]	ALA
1	A	221[B]	ALA
1	A	233	LEU
1	A	437	LEU
1	B	250	ASP
1	B	378	ARG
1	B	9	LYS
1	B	194	ASP
1	B	193	PRO
1	B	426	HIS
1	A	263	ILE
1	B	215	LEU
1	A	386	PRO

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	405/412 (98%)	383 (95%)	22 (5%)	27 36
1	B	380/412 (92%)	360 (95%)	20 (5%)	28 37
All	All	785/824 (95%)	743 (95%)	42 (5%)	32 36

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	45	PRO
1	A	80	ASP
1	A	148	LEU
1	A	159[A]	ASN
1	A	159[B]	ASN
1	A	204[A]	GLN
1	A	204[B]	GLN
1	A	206[A]	GLN
1	A	206[B]	GLN
1	A	212[A]	MET
1	A	212[B]	MET
1	A	214[A]	ASP
1	A	214[B]	ASP
1	A	222[A]	ASP
1	A	222[B]	ASP
1	A	254	ILE
1	A	312	LYS
1	A	370	ASP
1	A	383	SER
1	A	387	GLN
1	A	437	LEU
1	B	13	GLU
1	B	15	LYS
1	B	50	ARG
1	B	56	ARG
1	B	176[A]	SER
1	B	176[B]	SER
1	B	178[A]	VAL
1	B	178[B]	VAL
1	B	192	ASN
1	B	195	ASP
1	B	200	GLU
1	B	210	LYS
1	B	224	LYS

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Mol	Chain	Res	Type
1	B	230	SER
1	B	233	LEU
1	B	255	ARG
1	B	292	GLU
1	B	307	GLN
1	B	369	ASP
1	B	391	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	HIS
1	A	189	GLN
1	A	388	HIS
1	A	426	HIS
1	A	428	ASN
1	B	27	GLN
1	B	95	ASN
1	B	116	HIS
1	B	186	ASN
1	B	201	ASN
1	B	229	GLN
1	B	266	HIS
1	B	307	GLN
1	B	388	HIS
1	B	403	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 (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEM	A	471	1,3	30,50,50	2.73	9 (30%)	24,82,82	2.80	13 (54%)
2	HEM	B	471	1	30,50,50	1.81	5 (16%)	24,82,82	2.52	11 (45%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	471	1,3	-	0/10/54/54	0/0/8/8
2	HEM	B	471	1	-	0/10/54/54	0/0/8/8

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	471	HEM	C3B-C4B	-9.22	1.43	1.51
2	B	471	HEM	C3B-C4B	-6.15	1.46	1.51
2	A	471	HEM	C3D-C4D	-4.61	1.45	1.51
2	B	471	HEM	C3D-C4D	-3.24	1.47	1.51
2	B	471	HEM	C2C-C1C	-2.94	1.47	1.52
2	A	471	HEM	C2C-C1C	-2.45	1.47	1.52
2	A	471	HEM	C2D-C1D	-2.38	1.44	1.51
2	B	471	HEM	CMA-C3A	2.13	1.56	1.51
2	A	471	HEM	CMA-C3A	2.83	1.57	1.51
2	B	471	HEM	FE-NC	2.84	2.07	1.95
2	A	471	HEM	FE-ND	2.92	2.13	1.97
2	A	471	HEM	FE-NB	3.67	2.16	1.97
2	A	471	HEM	C3C-CAC	4.30	1.59	1.51
2	A	471	HEM	C4C-NC	5.65	1.43	1.36

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	471	HEM	CBD-CAD-C3D	-4.63	100.07	113.55
2	A	471	HEM	C3B-CAB-CBB	-4.33	117.82	124.46
2	A	471	HEM	C3C-CAC-CBC	-4.02	118.28	124.46
2	B	471	HEM	C3C-CAC-CBC	-3.33	119.35	124.46
2	B	471	HEM	CBA-CAA-C2A	-3.12	106.94	112.53
2	B	471	HEM	CBD-CAD-C3D	-2.48	106.33	113.55
2	A	471	HEM	C3B-C4B-NB	-2.46	106.93	111.63
2	B	471	HEM	CMA-C3A-C4A	-2.21	124.70	128.36
2	B	471	HEM	C3B-CAB-CBB	2.09	127.67	124.46
2	A	471	HEM	C2D-C3D-C4D	2.16	105.16	101.50
2	A	471	HEM	C3B-C4B-CHC	2.23	126.30	123.16
2	A	471	HEM	C1D-CHD-C4C	2.31	129.68	125.82
2	B	471	HEM	CMD-C2D-C3D	2.44	125.14	114.35
2	A	471	HEM	C2C-C1C-CHC	2.84	128.01	123.68
2	B	471	HEM	C2C-C1C-CHC	3.26	128.64	123.68
2	A	471	HEM	CMD-C2D-C3D	3.46	129.64	114.35
2	B	471	HEM	CAD-C3D-C2D	3.48	123.21	113.22
2	B	471	HEM	CMB-C2B-C3B	3.57	125.45	116.53
2	A	471	HEM	CAD-C3D-C4D	3.64	125.30	112.47
2	A	471	HEM	CMB-C2B-C3B	3.88	126.22	116.53
2	A	471	HEM	CMC-C2C-C3C	4.11	126.79	116.53
2	B	471	HEM	CMC-C2C-C3C	5.01	129.04	116.53
2	B	471	HEM	CAD-C3D-C4D	5.65	132.40	112.47
2	A	471	HEM	CAD-C3D-C2D	5.68	129.54	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	471	HEM	3	0
2	B	471	HEM	2	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	442/470 (94%)	-0.10	18 (4%)	41	50	19, 36, 57, 67	0
1	B	457/470 (97%)	0.14	32 (7%)	19	27	28, 43, 68, 86	0
All	All	899/940 (95%)	0.02	50 (5%)	28	36	19, 40, 63, 86	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	225	ALA	7.8
1	B	191	ALA	6.2
1	B	243	PRO	5.2
1	A	225[A]	ALA	4.7
1	A	191	ALA	4.3
1	A	1	THR	4.3
1	A	192	ASN	4.1
1	A	204[A]	GLN	4.0
1	B	223	ARG	3.8
1	B	136	ASP	3.8
1	A	188[A]	LEU	3.8
1	B	226	SER	3.7
1	A	2	ILE	3.5
1	B	196	PRO	3.3
1	B	244	GLU	3.3
1	B	229	GLN	3.1
1	A	108	SER	3.0
1	B	458	ILE	3.0
1	B	247	GLU	2.8
1	B	382	PRO	2.7
1	B	299	VAL	2.7
1	A	46	GLY	2.6
1	B	46	GLY	2.6
1	B	231	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	221[A]	ALA	2.5
1	B	195	ASP	2.5
1	A	169[A]	GLN	2.5
1	A	233	LEU	2.5
1	B	285	HIS	2.5
1	A	207[A]	GLU	2.4
1	B	198	TYR	2.4
1	B	109	GLN	2.4
1	B	245	THR	2.3
1	B	224	LYS	2.3
1	A	229	GLN	2.3
1	B	194	ASP	2.3
1	B	369	ASP	2.2
1	B	200	GLU	2.2
1	B	192	ASN	2.2
1	A	261	PHE	2.1
1	B	357	ILE	2.1
1	B	193	PRO	2.1
1	B	227	GLY	2.0
1	B	45	PRO	2.0
1	A	220[A]	ILE	2.0
1	A	206[A]	GLN	2.0
1	B	52	LEU	2.0
1	B	103	LEU	2.0
1	B	197	ALA	2.0
1	A	256	TYR	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
2	HEM	B	471	43/43	0.97	0.10	-0.50	27,31,35,41	0
2	HEM	A	471	43/43	0.98	0.09	-0.51	17,23,26,31	0

6.5 Other polymers (i)

There are no such residues in this entry.