



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 04:21 am GMT

PDB ID : 2UWH
Title : CYTOCHROME P450 BM3 MUTANT IN COMPLEX WITH PALMITIC ACID
Authors : Huang, W.-C.; Joyce, M.G.; Westlake, A.C.G.; Roberts, G.C.K.; Moody, P.C.E.
Deposited on : 2007-03-21
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

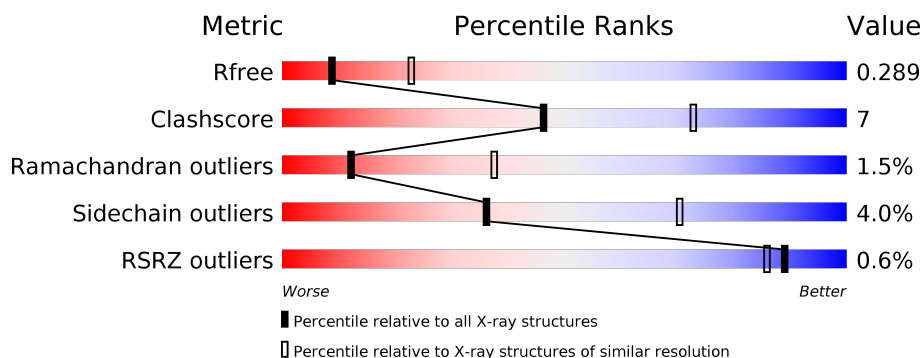
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	458	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>.</div> </div> </div>
1	B	458	<div> <div>79%</div> <div>18%</div> <div>.</div> </div>
1	C	458	<div> <div>82%</div> <div>16%</div> <div>.</div> </div>
1	D	458	<div> <div>81%</div> <div>17%</div> <div>.</div> </div>
1	E	458	<div> <div>%</div> <div>82%</div> <div>15%</div> <div>..</div> </div>
1	F	458	<div> <div>%</div> <div>78%</div> <div>20%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	PLM	F	1460	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23025 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 BIFUNCTIONAL P-450\;: NADPH-P450 REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	458	Total	C	N	O	S	0	0	0
			3690	2360	626	687	17			
1	B	458	Total	C	N	O	S	0	0	0
			3690	2360	626	687	17			
1	C	458	Total	C	N	O	S	0	0	0
			3690	2360	626	687	17			
1	D	458	Total	C	N	O	S	0	0	0
			3690	2360	626	687	17			
1	E	458	Total	C	N	O	S	0	0	0
			3690	2360	626	687	17			
1	F	458	Total	C	N	O	S	0	0	0
			3690	2360	626	687	17			

There are 6 discrepancies between the modelled and reference sequences:

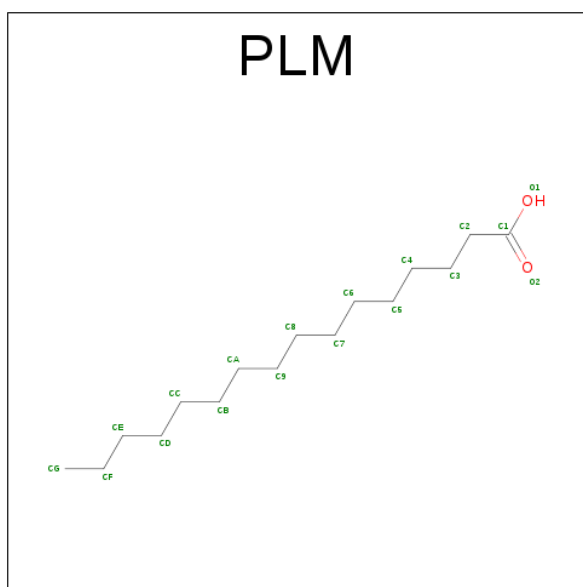
Chain	Residue	Modelled	Actual	Comment	Reference
A	82	PHE	ALA	ENGINEERED MUTATION	UNP P14779
B	82	PHE	ALA	ENGINEERED MUTATION	UNP P14779
C	82	PHE	ALA	ENGINEERED MUTATION	UNP P14779
D	82	PHE	ALA	ENGINEERED MUTATION	UNP P14779
E	82	PHE	ALA	ENGINEERED MUTATION	UNP P14779
F	82	PHE	ALA	ENGINEERED MUTATION	UNP P14779

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 3 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			18	16	2		
3	B	1	Total	C	O	0	0
			18	16	2		
3	C	1	Total	C	O	0	0
			18	16	2		
3	D	1	Total	C	O	0	0
			18	16	2		
3	E	1	Total	C	O	0	0
			18	16	2		
3	F	1	Total	C	O	0	0
			18	16	2		

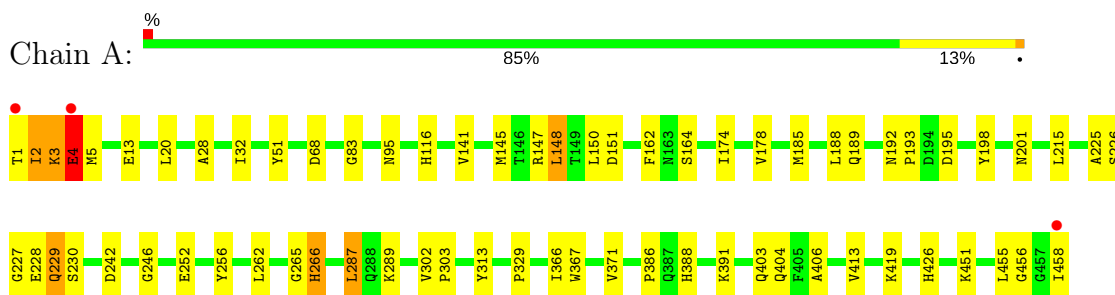
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	89	Total	O	0	0
			89	89		
4	B	94	Total	O	0	0
			94	94		
4	C	88	Total	O	0	0
			88	88		
4	D	83	Total	O	0	0
			83	83		
4	E	83	Total	O	0	0
			83	83		
4	F	82	Total	O	0	0
			82	82		

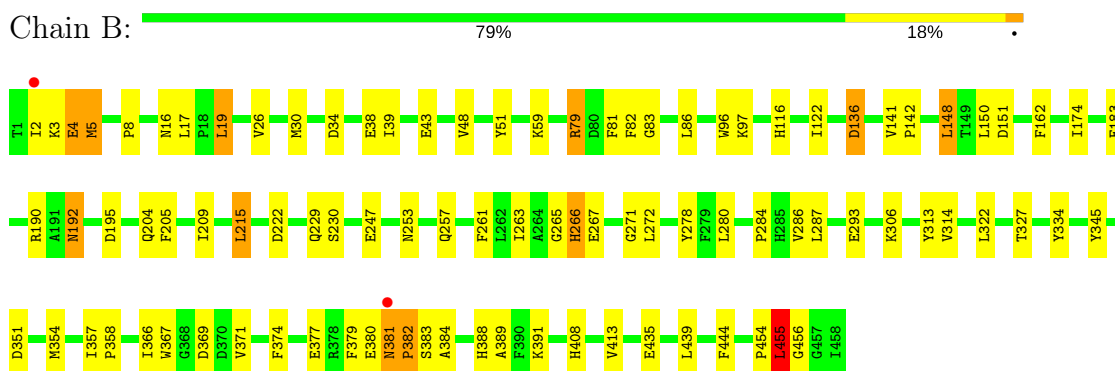
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

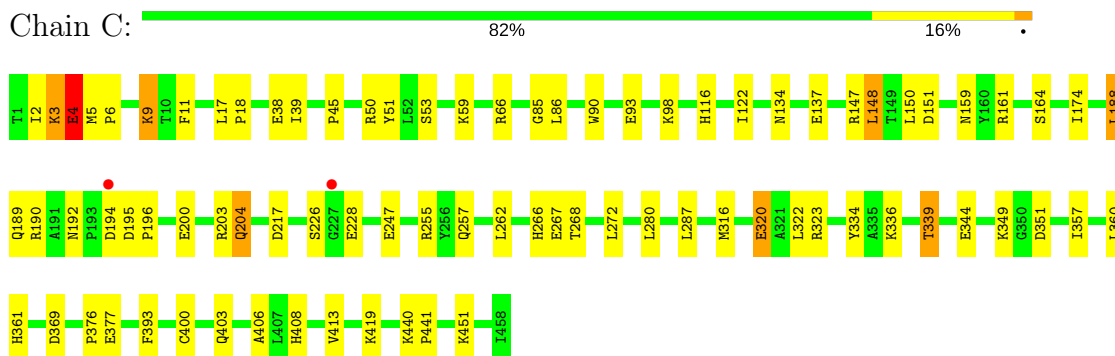
- Molecule 1: BIFUNCTIONAL P-450\; NADPH-P450 REDUCTASE



- Molecule 1: BIFUNCTIONAL P-450\; NADPH-P450 REDUCTASE



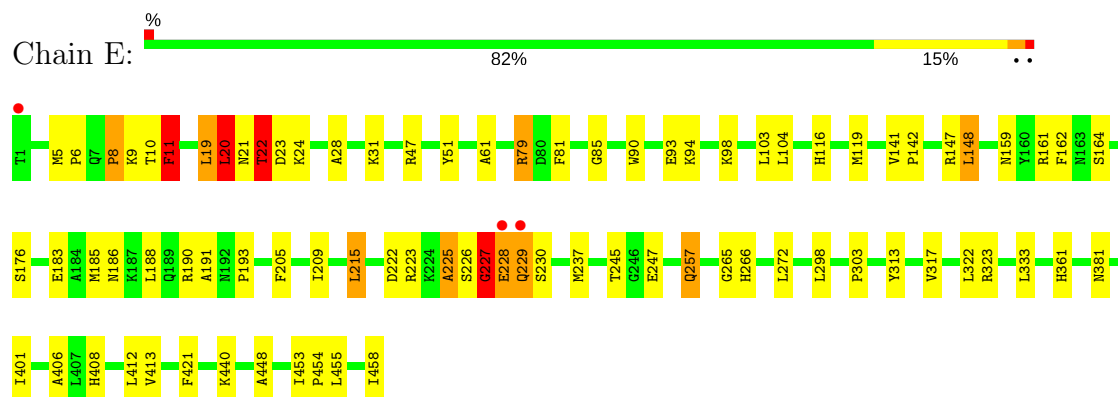
- Molecule 1: BIFUNCTIONAL P-450\; NADPH-P450 REDUCTASE



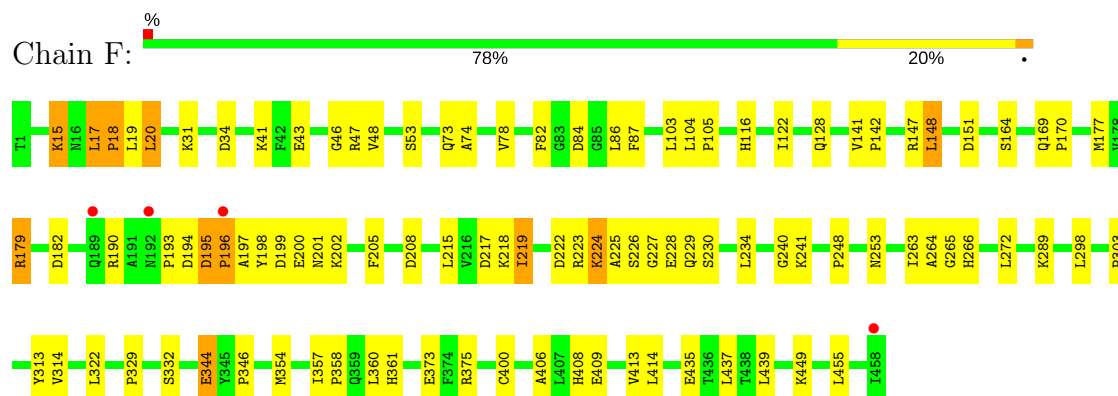
- Molecule 1: BIFUNCTIONAL P-450\; NADPH-P450 REDUCTASE



• Molecule 1: BIFUNCTIONAL P-450\; NADPH-P450 REDUCTASE



• Molecule 1: BIFUNCTIONAL P-450\; NADPH-P450 REDUCTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	116.83Å 147.03Å 183.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	114.71 – 2.80 73.52 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.8 (114.71-2.80) 97.8 (73.52-2.80)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.38 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.215 , 0.299 0.210 , 0.289	Depositor DCC
R_{free} test set	3858 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	31.8	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 26.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	23025	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.79 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.4516e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.39	0/3776	0.55	1/5104 (0.0%)
1	B	0.41	0/3776	0.55	0/5104
1	C	0.40	0/3776	0.54	0/5104
1	D	0.42	0/3776	0.57	1/5104 (0.0%)
1	E	0.41	0/3776	0.56	1/5104 (0.0%)
1	F	0.42	0/3776	0.57	1/5104 (0.0%)
All	All	0.41	0/22656	0.56	4/30624 (0.0%)

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	C	0	1
1	D	0	1
1	E	0	1
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	188	LEU	CA-CB-CG	7.08	131.60	115.30
1	A	287	LEU	CA-CB-CG	5.58	128.14	115.30
1	F	224	LYS	N-CA-C	5.42	125.63	111.00
1	E	227	GLY	N-CA-C	5.20	126.09	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	4	GLU	Peptide
1	D	21	ASN	Peptide
1	E	229	GLN	Peptide

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	3690	0	3661	46	0
1	B	3690	0	3661	48	0
1	C	3690	0	3661	50	0
1	D	3690	0	3661	57	0
1	E	3690	0	3661	52	0
1	F	3690	0	3661	65	0
2	A	43	0	30	5	0
2	B	43	0	30	2	0
2	C	43	0	30	4	0
2	D	43	0	30	6	0
2	E	43	0	30	2	0
2	F	43	0	30	6	0
3	A	18	0	31	4	0
3	B	18	0	31	1	0
3	C	18	0	31	2	0
3	D	18	0	31	1	0
3	E	18	0	31	2	0
3	F	18	0	31	2	0
4	A	89	0	0	3	0
4	B	94	0	0	2	0
4	C	88	0	0	3	0
4	D	83	0	0	0	0
4	E	83	0	0	1	0
4	F	82	0	0	3	0
All	All	23025	0	22332	321	0

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 7.

All (321) 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:D:1:THR:HA	1:D:2:ILE:HG23	1.25	1.18
1:A:1:THR:HA	1:A:2:ILE:HB	1.13	1.06
3:A:1460:PLM:O1	4:A:2089:HOH:O	1.81	0.97
1:A:1:THR:CA	1:A:2:ILE:HB	2.00	0.92
1:F:224:LYS:N	1:F:225:ALA:HB3	1.84	0.91
1:A:1:THR:HA	1:A:2:ILE:CB	1.97	0.90
1:C:4:GLU:HG3	1:C:6:PRO:HD3	1.52	0.88
1:F:224:LYS:H	1:F:225:ALA:HB3	1.36	0.87
1:F:196:PRO:HA	1:F:199:ASP:CG	1.97	0.85
1:D:162:PHE:HE1	1:D:215:LEU:HD21	1.42	0.84
1:C:226:SER:HB3	1:C:228:GLU:HG2	1.59	0.83
1:D:1:THR:HA	1:D:2:ILE:CG2	2.09	0.82
1:D:148:LEU:HD21	1:D:413:VAL:HG21	1.63	0.80
1:D:370:ASP:HB2	1:D:373:GLU:HG3	1.62	0.80
1:B:382:PRO:O	1:B:384:ALA:N	2.16	0.79
1:A:148:LEU:HD21	1:A:413:VAL:HG21	1.63	0.78
1:F:148:LEU:HD21	1:F:413:VAL:HG21	1.68	0.76
1:C:148:LEU:HD21	1:C:413:VAL:HG21	1.67	0.75
1:E:22:THR:HB	1:E:24:LYS:H	1.51	0.75
1:B:150:LEU:HD22	1:B:174:ILE:HD11	1.67	0.75
1:C:226:SER:CB	1:C:228:GLU:HG2	2.16	0.75
1:B:148:LEU:HD21	1:B:413:VAL:HG21	1.68	0.74
1:E:94:LYS:O	1:E:98:LYS:HB2	1.88	0.74
1:E:225:ALA:C	1:E:227:GLY:H	1.91	0.74
1:F:190:ARG:O	1:F:190:ARG:HG3	1.88	0.73
1:F:179:ARG:HB3	1:F:208:ASP:OD2	1.89	0.73
1:B:192:ASN:HB2	1:B:195:ASP:HB2	1.71	0.73
1:E:98:LYS:HE3	1:E:247:GLU:HB2	1.71	0.73
1:C:86:LEU:HB3	2:C:1459:HEM:HBD2	1.70	0.72
1:E:228:GLU:O	1:E:230:SER:N	2.20	0.72
1:B:454:PRO:HA	1:B:455:LEU:CB	2.19	0.72
1:E:148:LEU:HD21	1:E:413:VAL:HG21	1.70	0.72
1:C:90:TRP:HB2	1:C:93:GLU:HG3	1.73	0.71
1:F:18:PRO:C	1:F:20:LEU:H	1.94	0.71
1:D:162:PHE:CE1	1:D:215:LEU:HD21	2.26	0.71
1:F:373:GLU:HB3	1:F:375:ARG:HD3	1.73	0.71
1:A:20:LEU:HB2	1:A:189:GLN:NE2	2.05	0.70
1:E:147:ARG:HG2	1:E:164:SER:HB3	1.72	0.70
1:F:18:PRO:O	1:F:20:LEU:N	2.26	0.69
1:D:366:ILE:HD12	1:D:386:PRO:HG2	1.76	0.68
1:A:20:LEU:HB2	1:A:189:GLN:CD	2.15	0.67
1:E:9:LYS:HB3	1:E:11:PHE:CE2	2.30	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:VAL:HB	1:D:142:PRO:HD3	1.77	0.66
1:C:11:PHE:CD2	1:C:18:PRO:HG2	2.31	0.66
1:D:102:ILE:HD12	1:D:249:LEU:HD23	1.77	0.66
1:A:3:LYS:HB3	1:A:4:GLU:O	1.96	0.65
1:D:22:THR:HG22	1:D:23:ASP:H	1.61	0.65
1:E:79:ARG:HH11	1:E:79:ARG:HG3	1.60	0.65
1:F:47:ARG:HD3	1:F:73:GLN:HE21	1.61	0.65
1:C:255:ARG:HD3	4:C:2051:HOH:O	1.96	0.64
1:F:199:ASP:O	1:F:200:GLU:HB3	1.98	0.63
1:E:223:ARG:HH21	1:E:228:GLU:HB2	1.63	0.63
1:E:162:PHE:CE1	1:E:215:LEU:HD21	2.34	0.62
1:D:8:PRO:HB2	1:D:19:LEU:CD1	2.30	0.62
1:C:85:GLY:HA2	1:C:257:GLN:NE2	2.15	0.61
1:B:162:PHE:HE1	1:B:215:LEU:HD21	1.63	0.61
1:D:388:HIS:HD2	1:D:391:LYS:NZ	1.98	0.61
1:D:3:LYS:HD3	1:D:4:GLU:H	1.65	0.61
1:F:264:ALA:HA	3:F:1460:PLM:HG2	1.83	0.61
1:E:21:ASN:O	1:E:23:ASP:N	2.30	0.60
1:A:141:VAL:O	1:A:145:MET:HG2	2.02	0.60
1:A:426:HIS:HE1	4:A:2029:HOH:O	1.85	0.60
1:B:8:PRO:HB2	1:B:19:LEU:HD13	1.84	0.59
1:B:388:HIS:HD2	1:B:391:LYS:NZ	2.00	0.59
1:D:8:PRO:HB2	1:D:19:LEU:HD11	1.84	0.59
1:B:4:GLU:O	1:B:5:MET:HB3	2.03	0.58
1:F:193:PRO:HA	1:F:198:TYR:HD2	1.68	0.58
1:D:116:HIS:HD2	1:D:408:HIS:NE2	2.01	0.58
1:E:47:ARG:NH1	3:E:1460:PLM:O2	2.37	0.58
1:B:454:PRO:HA	1:B:455:LEU:HB2	1.86	0.57
1:F:223:ARG:O	1:F:223:ARG:HG3	2.03	0.57
1:D:53:SER:HB3	1:D:359:GLN:HB3	1.86	0.57
1:A:403:GLN:NE2	4:A:2080:HOH:O	2.37	0.57
1:D:186:ASN:O	1:D:189:GLN:HG3	2.05	0.57
1:C:11:PHE:HD2	1:C:18:PRO:HG2	1.69	0.57
1:D:22:THR:HB	1:D:24:LYS:H	1.69	0.56
1:E:28:ALA:O	1:E:31:LYS:HB3	2.05	0.56
1:E:116:HIS:HD2	1:E:408:HIS:NE2	2.04	0.56
1:C:204:GLN:HE21	1:C:204:GLN:HA	1.69	0.56
1:C:349:LYS:HE3	1:D:22:THR:HG23	1.87	0.56
1:E:141:VAL:HB	1:E:142:PRO:HD3	1.86	0.56
1:F:406:ALA:HB2	2:F:1459:HEM:HHC	1.88	0.56
1:A:3:LYS:HB3	1:A:4:GLU:HG3	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:GLU:CD	1:A:4:GLU:C	2.64	0.56
1:F:46:GLY:HA3	4:F:2008:HOH:O	2.05	0.56
1:D:154:GLY:HA3	1:D:162:PHE:HE2	1.71	0.55
1:F:195:ASP:HB2	1:F:196:PRO:C	2.25	0.55
2:A:1459:HEM:HMB2	2:A:1459:HEM:HBB2	1.88	0.55
1:D:264:ALA:HA	3:D:1460:PLM:HG1	1.88	0.55
1:A:147:ARG:HG2	1:A:164:SER:HB3	1.89	0.55
1:C:150:LEU:HD22	1:C:174:ILE:HD11	1.88	0.55
1:E:406:ALA:HB2	2:E:1459:HEM:HHC	1.87	0.55
1:F:198:TYR:O	1:F:201:ASN:HB2	2.07	0.55
1:A:192:ASN:N	1:A:193:PRO:HD3	2.22	0.55
1:C:400:CYS:HA	2:C:1459:HEM:CHA	2.37	0.55
1:C:280:LEU:HD22	1:C:287:LEU:HA	1.89	0.54
1:D:21:ASN:HB2	1:D:189:GLN:CB	2.38	0.54
1:E:225:ALA:C	1:E:227:GLY:N	2.60	0.54
1:E:272:LEU:HD13	1:E:322:LEU:HG	1.89	0.54
1:F:196:PRO:O	1:F:198:TYR:N	2.41	0.54
2:A:1459:HEM:CMB	2:A:1459:HEM:HBB2	2.38	0.54
1:C:98:LYS:HZ3	1:C:247:GLU:HB2	1.72	0.54
1:C:272:LEU:HD13	1:C:322:LEU:HG	1.90	0.54
1:E:161:ARG:HA	4:E:2035:HOH:O	2.08	0.54
1:C:38:GLU:HG3	1:C:39:ILE:HG22	1.91	0.53
1:E:22:THR:O	1:E:23:ASP:HB2	2.07	0.53
1:F:104:LEU:N	1:F:105:PRO:HD2	2.23	0.53
1:B:280:LEU:HD22	1:B:287:LEU:HA	1.90	0.53
1:B:345:TYR:HE1	4:B:2001:HOH:O	1.91	0.53
1:A:265:GLY:HA2	2:A:1459:HEM:C3C	2.44	0.53
1:D:238:LEU:HD23	1:D:254:ILE:HD13	1.90	0.53
1:F:344:GLU:O	1:F:346:PRO:HD3	2.09	0.53
1:C:188:LEU:HD23	3:C:1460:PLM:H22	1.91	0.52
1:C:440:LYS:HG3	1:C:441:PRO:HD2	1.92	0.52
1:B:293:GLU:OE1	1:B:314:VAL:HG23	2.10	0.52
1:E:10:THR:O	1:E:11:PHE:C	2.48	0.52
1:A:28:ALA:O	1:A:32:ILE:HD12	2.10	0.52
1:B:272:LEU:HD13	1:B:322:LEU:HG	1.91	0.52
1:C:406:ALA:HB2	2:C:1459:HEM:HHC	1.91	0.52
1:A:262:LEU:O	1:A:266:HIS:HD2	1.93	0.51
1:A:116:HIS:HE1	1:A:303:PRO:O	1.92	0.51
1:B:454:PRO:HA	1:B:455:LEU:HB3	1.92	0.51
1:E:103:LEU:HD21	1:E:237:MET:HG2	1.93	0.51
1:C:316:MET:CE	1:C:377:GLU:HA	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:LEU:HB3	1:D:287:LEU:HD22	1.92	0.51
1:F:141:VAL:HB	1:F:142:PRO:HD3	1.93	0.51
1:B:271:GLY:HA3	1:B:327:THR:HG21	1.93	0.51
1:A:51:TYR:OH	3:A:1460:PLM:O2	2.29	0.50
1:C:161:ARG:HA	4:C:2038:HOH:O	2.11	0.50
1:F:177:MET:HG3	1:F:263:ILE:HD13	1.92	0.50
1:F:84:ASP:OD1	1:F:253:ASN:ND2	2.40	0.50
1:E:90:TRP:HB2	1:E:93:GLU:HG3	1.93	0.50
1:F:272:LEU:HD13	1:F:322:LEU:HG	1.92	0.50
1:A:151:ASP:OD1	1:A:162:PHE:HB2	2.12	0.50
1:D:272:LEU:HD13	1:D:322:LEU:HG	1.92	0.50
1:C:9:LYS:HD3	1:C:11:PHE:CE1	2.47	0.49
1:E:323:ARG:HA	1:E:361:HIS:HD1	1.77	0.49
1:D:272:LEU:HD22	2:D:1459:HEM:HBB1	1.93	0.49
1:F:409:GLU:O	1:F:413:VAL:HG23	2.13	0.49
1:B:116:HIS:HD2	1:B:408:HIS:NE2	2.11	0.49
1:C:393:PHE:CD2	1:C:403:GLN:HG3	2.48	0.49
1:E:51:TYR:OH	3:E:1460:PLM:O1	2.26	0.49
1:A:419:LYS:O	1:A:451:LYS:HD2	2.12	0.48
1:E:191:ALA:O	1:E:193:PRO:HD3	2.13	0.48
1:F:298:LEU:HD22	1:F:303:PRO:HB3	1.95	0.48
1:B:162:PHE:CE1	1:B:215:LEU:HD21	2.45	0.48
1:A:227:GLY:O	1:A:229:GLN:N	2.46	0.48
1:A:229:GLN:HG3	1:A:230:SER:N	2.28	0.48
1:F:223:ARG:CG	1:F:223:ARG:O	2.62	0.48
1:A:188:LEU:HD13	3:A:1460:PLM:H21	1.95	0.48
1:A:265:GLY:HA2	2:A:1459:HEM:C2C	2.48	0.48
1:A:455:LEU:HG	1:A:456:GLY:H	1.79	0.48
1:A:198:TYR:HA	1:A:201:ASN:HD22	1.79	0.47
1:B:388:HIS:HD2	1:B:391:LYS:HZ2	1.61	0.47
1:C:116:HIS:HD2	1:C:408:HIS:NE2	2.13	0.47
1:E:323:ARG:HA	1:E:361:HIS:ND1	2.29	0.47
1:E:104:LEU:HA	1:E:401:ILE:HD11	1.96	0.47
1:A:406:ALA:HB2	2:A:1459:HEM:HHC	1.97	0.47
1:C:262:LEU:O	1:C:266:HIS:HD2	1.97	0.47
1:E:265:GLY:HA2	2:E:1459:HEM:C3C	2.50	0.47
1:F:240:GLY:HA2	4:F:2046:HOH:O	2.15	0.47
1:F:272:LEU:HD22	2:F:1459:HEM:HBB1	1.96	0.47
1:B:357:ILE:N	1:B:358:PRO:HD2	2.29	0.47
1:B:366:ILE:HG21	1:B:389:ALA:HB1	1.97	0.47
1:C:17:LEU:HD11	1:C:188:LEU:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:328:ALA:HB3	2:D:1459:HEM:HHB	1.96	0.47
1:D:240:GLY:O	1:D:241:LYS:HB2	2.15	0.47
1:D:332:SER:HB3	1:D:354:MET:SD	2.54	0.47
1:A:388:HIS:HA	1:A:391:LYS:HE3	1.97	0.46
1:C:419:LYS:O	1:C:451:LYS:HD2	2.14	0.46
1:F:122:ILE:HD12	1:F:151:ASP:HB3	1.97	0.46
1:B:116:HIS:CD2	1:B:408:HIS:NE2	2.83	0.46
1:B:96:TRP:CZ3	1:B:97:LYS:HD2	2.50	0.46
1:E:298:LEU:HD22	1:E:303:PRO:HB3	1.98	0.46
1:F:223:ARG:HD2	1:F:234:LEU:HD23	1.98	0.46
1:A:3:LYS:CB	1:A:4:GLU:O	2.62	0.46
1:B:26:VAL:O	1:B:30:MET:HG3	2.16	0.46
1:D:2:ILE:HG13	1:D:3:LYS:H	1.80	0.46
1:E:183:GLU:HG2	1:E:205:PHE:CD1	2.50	0.46
1:B:253:ASN:O	1:B:257:GLN:HG2	2.16	0.46
1:B:86:LEU:HB3	2:B:1459:HEM:HBD2	1.97	0.46
1:B:82:PHE:HE1	1:B:263:ILE:HD12	1.81	0.46
3:C:1460:PLM:HD1	3:C:1460:PLM:HG3	1.72	0.46
1:F:17:LEU:C	1:F:18:PRO:O	2.54	0.46
1:C:39:ILE:HA	1:C:51:TYR:O	2.16	0.45
1:F:116:HIS:HD2	1:F:408:HIS:NE2	2.13	0.45
1:F:18:PRO:C	1:F:20:LEU:N	2.60	0.45
1:D:27:GLN:NE2	1:D:433:ILE:HB	2.32	0.45
1:D:276:ALA:O	1:D:280:LEU:HG	2.16	0.45
1:F:193:PRO:HA	1:F:198:TYR:CD2	2.50	0.45
1:D:388:HIS:HD2	1:D:391:LYS:HZ1	1.63	0.45
1:C:393:PHE:CG	1:C:403:GLN:HG3	2.51	0.45
1:F:329:PRO:O	1:F:358:PRO:HD3	2.16	0.45
1:C:122:ILE:HD12	1:C:151:ASP:HB3	1.97	0.45
1:A:366:ILE:HD12	1:A:386:PRO:HG2	1.99	0.45
1:A:3:LYS:HA	1:A:4:GLU:HB3	1.99	0.45
1:B:284:PRO:HA	1:B:287:LEU:HB3	1.99	0.45
1:B:379:PHE:O	1:B:381:ASN:N	2.50	0.45
1:B:38:GLU:HG3	1:B:39:ILE:HG22	1.99	0.45
1:E:22:THR:HB	1:E:24:LYS:N	2.27	0.45
1:F:31:LYS:O	1:F:34:ASP:HB2	2.17	0.45
1:E:313:TYR:O	1:E:317:VAL:HG23	2.17	0.45
1:A:162:PHE:CE1	1:A:215:LEU:HD21	2.52	0.45
1:F:169:GLN:HB3	1:F:170:PRO:CD	2.46	0.45
1:F:265:GLY:HA2	2:F:1459:HEM:C3C	2.51	0.45
1:A:4:GLU:CD	1:A:5:MET:N	2.71	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:TYR:HA	1:B:444:PHE:CZ	2.53	0.44
1:A:329:PRO:HD2	3:A:1460:PLM:HA1	1.99	0.44
1:E:421:PHE:HB3	1:E:448:ALA:HB1	1.99	0.44
1:E:159:ASN:ND2	1:E:228:GLU:HB3	2.33	0.44
1:A:150:LEU:HD22	1:A:174:ILE:HD11	1.99	0.44
1:D:58:ILE:HD12	1:D:360:LEU:HD13	1.99	0.44
1:B:334:TYR:HA	1:B:351:ASP:O	2.18	0.44
1:C:66:ARG:HH21	1:C:339:THR:HG23	1.82	0.44
1:D:265:GLY:HA2	2:D:1459:HEM:C2C	2.53	0.44
1:E:81:PHE:HB3	1:E:209:ILE:HG12	2.00	0.44
1:F:224:LYS:CA	1:F:225:ALA:HB3	2.47	0.44
1:D:21:ASN:HB2	1:D:189:GLN:HB3	1.99	0.44
1:F:215:LEU:HA	1:F:218:LYS:HG2	1.99	0.44
1:B:51:TYR:OH	3:B:1460:PLM:O2	2.34	0.43
1:D:32:ILE:HA	1:D:35:GLU:HG2	1.99	0.43
1:F:128:GLN:HG2	4:F:2023:HOH:O	2.18	0.43
1:C:400:CYS:HA	2:C:1459:HEM:C4D	2.53	0.43
1:D:4:GLU:HA	1:D:4:GLU:OE2	2.16	0.43
1:F:435:GLU:HG2	1:F:439:LEU:CD2	2.48	0.43
1:F:82:PHE:HE2	1:F:263:ILE:HD12	1.83	0.43
1:B:286:VAL:HG11	1:B:374:PHE:HE2	1.84	0.43
1:B:81:PHE:HB3	1:B:209:ILE:HG12	1.99	0.43
1:D:265:GLY:HA2	2:D:1459:HEM:C3C	2.52	0.43
1:D:298:LEU:HB2	1:D:419:LYS:HD2	2.01	0.43
1:E:20:LEU:O	1:E:21:ASN:HB2	2.18	0.43
1:E:9:LYS:HE2	1:E:19:LEU:HD12	2.00	0.43
1:D:366:ILE:CD1	1:D:386:PRO:HG2	2.45	0.43
1:D:406:ALA:HB2	2:D:1459:HEM:HHC	1.99	0.43
1:E:5:MET:HA	1:E:6:PRO:HD3	1.92	0.43
1:F:314:VAL:HG13	1:F:414:LEU:HD23	2.00	0.43
1:A:3:LYS:CB	1:A:4:GLU:HG3	2.47	0.43
1:E:245:THR:HB	1:E:247:GLU:HG3	2.01	0.43
1:B:136:ASP:OD1	1:B:136:ASP:N	2.43	0.43
1:C:147:ARG:HG2	1:C:164:SER:HB3	2.01	0.43
1:C:217:ASP:OD1	1:C:255:ARG:NH1	2.45	0.43
1:F:87:PHE:HA	2:F:1459:HEM:HAD1	2.01	0.43
1:F:190:ARG:O	1:F:190:ARG:CG	2.61	0.43
1:A:95:ASN:HD22	1:A:95:ASN:HA	1.59	0.42
1:B:435:GLU:HG2	1:B:439:LEU:CD2	2.49	0.42
1:F:215:LEU:O	1:F:219:ILE:HG23	2.18	0.42
1:D:154:GLY:HA3	1:D:162:PHE:CE2	2.51	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:332:SER:HB3	1:F:354:MET:SD	2.59	0.42
1:A:174:ILE:O	1:A:178:VAL:HG23	2.20	0.42
1:C:357:ILE:HG22	1:C:361:HIS:CE1	2.55	0.42
1:C:3:LYS:O	1:C:4:GLU:O	2.38	0.42
1:D:177:MET:HG3	1:D:263:ILE:HG12	2.02	0.42
1:D:262:LEU:O	1:D:266:HIS:HD2	2.02	0.42
1:F:289:LYS:HD3	1:F:313:TYR:CZ	2.54	0.42
1:B:16:ASN:HB2	1:B:43:GLU:O	2.19	0.42
1:B:122:ILE:HG22	1:B:148:LEU:HD12	2.02	0.42
1:F:357:ILE:HG22	1:F:361:HIS:CE1	2.54	0.42
1:C:320:GLU:OE2	1:C:323:ARG:NE	2.44	0.42
1:E:79:ARG:HH11	1:E:79:ARG:CG	2.30	0.42
1:F:223:ARG:HH22	1:F:230:SER:HB2	1.84	0.42
1:F:86:LEU:HB3	2:F:1459:HEM:HBD2	2.01	0.42
1:D:130:TRP:CZ2	1:D:139:ILE:HG21	2.55	0.42
1:F:435:GLU:HG2	1:F:439:LEU:HD22	2.02	0.42
1:C:320:GLU:HG3	1:C:376:PRO:HA	2.01	0.42
1:F:15:LYS:HB3	1:F:43:GLU:HB3	2.01	0.42
1:F:455:LEU:HA	1:F:455:LEU:HD12	1.93	0.42
1:D:316:MET:HG2	1:D:379:PHE:HB2	2.01	0.42
1:A:302:VAL:HG21	1:A:458:ILE:HB	2.01	0.41
1:B:266:HIS:CG	1:B:267:GLU:N	2.87	0.41
1:C:200:GLU:HB3	4:C:2046:HOH:O	2.19	0.41
1:C:323:ARG:HG2	1:C:361:HIS:HB3	2.02	0.41
1:C:336:LYS:O	1:C:349:LYS:HG3	2.19	0.41
1:B:261:PHE:O	1:B:265:GLY:HA3	2.20	0.41
1:C:266:HIS:CG	1:C:267:GLU:N	2.87	0.41
1:D:102:ILE:HD12	1:D:249:LEU:CD2	2.46	0.41
1:E:119:MET:HB3	1:E:412:LEU:HD23	2.01	0.41
1:F:400:CYS:HA	2:F:1459:HEM:CHA	2.50	0.41
1:D:147:ARG:HG2	1:D:164:SER:HB3	2.02	0.41
1:D:233:LEU:O	1:D:237:MET:HG3	2.20	0.41
1:F:226:SER:HA	1:F:227:GLY:HA3	1.53	0.41
1:B:141:VAL:HB	1:B:142:PRO:CD	2.50	0.41
1:B:79:ARG:HG2	1:B:83:GLY:O	2.20	0.41
1:D:70:ASN:HB3	1:D:332:SER:OG	2.21	0.41
1:F:74:ALA:O	1:F:78:VAL:HG23	2.19	0.41
1:A:367:TRP:HB2	1:A:371:VAL:HG12	2.02	0.41
1:E:116:HIS:HE1	1:E:303:PRO:O	2.02	0.41
1:C:5:MET:SD	1:C:50:ARG:HG2	2.61	0.41
1:E:185:MET:HA	1:E:188:LEU:HD12	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:ILE:HG13	1:C:344:GLU:HA	2.03	0.41
1:E:8:PRO:C	1:E:9:LYS:HD3	2.41	0.41
1:A:242:ASP:O	1:A:246:GLY:N	2.53	0.41
1:B:38:GLU:HG2	4:B:2010:HOH:O	2.21	0.41
1:E:186:ASN:O	1:E:190:ARG:HB2	2.21	0.41
1:B:367:TRP:HB2	1:B:371:VAL:HG12	2.03	0.41
1:B:183:GLU:HG2	1:B:205:PHE:CD1	2.55	0.41
1:D:434:LYS:HB2	1:D:442:GLU:HB2	2.03	0.41
1:E:85:GLY:HA2	1:E:257:GLN:HE22	1.86	0.41
1:F:147:ARG:HG2	1:F:164:SER:HB3	2.03	0.41
1:A:185:MET:HA	1:A:188:LEU:HD12	2.03	0.40
1:B:313:TYR:HE1	1:B:377:GLU:OE2	2.04	0.40
1:C:134:ASN:O	1:C:137:GLU:HG2	2.20	0.40
1:C:53:SER:O	1:C:360:LEU:HA	2.21	0.40
1:D:102:ILE:CD1	1:D:249:LEU:HD23	2.50	0.40
1:D:309:LYS:HD3	1:D:309:LYS:HA	1.91	0.40
1:B:265:GLY:HA2	2:B:1459:HEM:C3C	2.57	0.40
1:D:116:HIS:HE1	1:D:303:PRO:O	2.04	0.40
1:E:11:PHE:CD1	1:E:11:PHE:N	2.88	0.40
1:F:53:SER:O	1:F:360:LEU:HA	2.21	0.40
1:A:229:GLN:HE21	1:A:229:GLN:HB2	1.63	0.40
1:A:289:LYS:HE3	1:A:313:TYR:CE1	2.56	0.40
1:A:83:GLY:HA3	1:A:256:TYR:CD1	2.56	0.40
1:C:334:TYR:HA	1:C:351:ASP:O	2.22	0.40
1:D:400:CYS:HA	2:D:1459:HEM:CHA	2.51	0.40
1:E:61:ALA:HB1	1:E:333:LEU:HD13	2.03	0.40
1:F:103:LEU:C	1:F:105:PRO:HD2	2.41	0.40
1:F:437:LEU:HD22	3:F:1460:PLM:H71	2.03	0.40
1:F:196:PRO:HA	1:F:199:ASP:CB	2.49	0.40
1:C:195:ASP:HA	1:C:196:PRO:HD3	1.94	0.40
1:D:60:GLU:O	1:D:63:ASP:HB2	2.22	0.40
1:E:148:LEU:CD2	1:E:413:VAL:HG21	2.46	0.40
1:E:453:ILE:HA	1:E:454:PRO:HD3	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	456/458 (100%)	426 (93%)	25 (6%)	5 (1%)	17	47
1	B	456/458 (100%)	425 (93%)	22 (5%)	9 (2%)	9	28
1	C	456/458 (100%)	429 (94%)	22 (5%)	5 (1%)	17	47
1	D	456/458 (100%)	421 (92%)	32 (7%)	3 (1%)	25	59
1	E	456/458 (100%)	410 (90%)	38 (8%)	8 (2%)	10	32
1	F	456/458 (100%)	415 (91%)	31 (7%)	10 (2%)	8	26
All	All	2736/2748 (100%)	2526 (92%)	170 (6%)	40 (2%)	12	37

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3	LYS
1	B	380	GLU
1	B	383	SER
1	C	4	GLU
1	D	2	ILE
1	E	8	PRO
1	E	227	GLY
1	E	229	GLN
1	F	196	PRO
1	F	197	ALA
1	A	2	ILE
1	A	225	ALA
1	B	229	GLN
1	C	3	LYS
1	D	21	ASN
1	E	11	PHE
1	E	20	LEU
1	E	22	THR
1	E	226	SER
1	F	19	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	226	SER
1	B	381	ASN
1	B	382	PRO
1	E	225	ALA
1	F	18	PRO
1	F	194	ASP
1	F	195	ASP
1	B	455	LEU
1	C	159	ASN
1	C	192	ASN
1	F	248	PRO
1	F	344	GLU
1	A	4	GLU
1	A	228	GLU
1	B	5	MET
1	F	222	ASP
1	D	240	GLY
1	F	229	GLN
1	C	45	PRO
1	B	456	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	400/401 (100%)	389 (97%)	11 (3%)	49	82
1	B	400/401 (100%)	377 (94%)	23 (6%)	23	55
1	C	400/401 (100%)	386 (96%)	14 (4%)	41	75
1	D	400/401 (100%)	383 (96%)	17 (4%)	33	67
1	E	400/401 (100%)	384 (96%)	16 (4%)	36	70
1	F	400/401 (100%)	384 (96%)	16 (4%)	36	70
All	All	2400/2406 (100%)	2303 (96%)	97 (4%)	36	70

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	4	GLU
1	A	13	GLU
1	A	68	ASP
1	A	148	LEU
1	A	195	ASP
1	A	229	GLN
1	A	252	GLU
1	A	266	HIS
1	A	287	LEU
1	A	404	GLN
1	B	2	ILE
1	B	4	GLU
1	B	17	LEU
1	B	19	LEU
1	B	34	ASP
1	B	48	VAL
1	B	59	LYS
1	B	79	ARG
1	B	136	ASP
1	B	148	LEU
1	B	151	ASP
1	B	190	ARG
1	B	192	ASN
1	B	204	GLN
1	B	215	LEU
1	B	222	ASP
1	B	230	SER
1	B	247	GLU
1	B	266	HIS
1	B	306	LYS
1	B	354	MET
1	B	369	ASP
1	B	455	LEU
1	C	4	GLU
1	C	9	LYS
1	C	59	LYS
1	C	148	LEU
1	C	188	LEU
1	C	189	GLN
1	C	190	ARG
1	C	194	ASP
1	C	203	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	204	GLN
1	C	268	THR
1	C	320	GLU
1	C	339	THR
1	C	369	ASP
1	D	3	LYS
1	D	10	THR
1	D	95	ASN
1	D	97	LYS
1	D	148	LEU
1	D	188	LEU
1	D	222	ASP
1	D	229	GLN
1	D	244	GLU
1	D	266	HIS
1	D	287	LEU
1	D	306	LYS
1	D	339	THR
1	D	369	ASP
1	D	449	LYS
1	D	452	LYS
1	D	455	LEU
1	E	11	PHE
1	E	19	LEU
1	E	20	LEU
1	E	22	THR
1	E	79	ARG
1	E	148	LEU
1	E	176	SER
1	E	215	LEU
1	E	222	ASP
1	E	228	GLU
1	E	257	GLN
1	E	266	HIS
1	E	381	ASN
1	E	440	LYS
1	E	455	LEU
1	E	458	ILE
1	F	15	LYS
1	F	17	LEU
1	F	20	LEU
1	F	41	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	48	VAL
1	F	148	LEU
1	F	179	ARG
1	F	182	ASP
1	F	202	LYS
1	F	205	PHE
1	F	217	ASP
1	F	219	ILE
1	F	228	GLU
1	F	241	LYS
1	F	266	HIS
1	F	449	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	73	GLN
1	A	95	ASN
1	A	109	GLN
1	A	116	HIS
1	A	189	GLN
1	A	201	ASN
1	A	204	GLN
1	A	266	HIS
1	A	388	HIS
1	A	403	GLN
1	A	426	HIS
1	B	92	HIS
1	B	116	HIS
1	B	189	GLN
1	B	201	ASN
1	B	204	GLN
1	B	388	HIS
1	B	403	GLN
1	B	426	HIS
1	C	21	ASN
1	C	95	ASN
1	C	109	GLN
1	C	116	HIS
1	C	204	GLN
1	C	266	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	388	HIS
1	C	426	HIS
1	D	27	GLN
1	D	73	GLN
1	D	92	HIS
1	D	95	ASN
1	D	109	GLN
1	D	116	HIS
1	D	201	ASN
1	D	204	GLN
1	D	239	ASN
1	D	266	HIS
1	D	285	HIS
1	D	388	HIS
1	D	403	GLN
1	E	95	ASN
1	E	109	GLN
1	E	116	HIS
1	E	189	GLN
1	E	201	ASN
1	E	204	GLN
1	E	359	GLN
1	E	381	ASN
1	E	388	HIS
1	E	403	GLN
1	E	426	HIS
1	F	27	GLN
1	F	73	GLN
1	F	95	ASN
1	F	116	HIS
1	F	169	GLN
1	F	189	GLN
1	F	266	HIS
1	F	388	HIS
1	F	403	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

12 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	1459	1	28,50,50	2.16	11 (39%)	17,82,82	4.02	10 (58%)
3	PLM	A	1460	-	14,17,17	0.15	0	13,17,17	0.50	0
2	HEM	B	1459	1	28,50,50	2.15	11 (39%)	17,82,82	3.77	12 (70%)
3	PLM	B	1460	-	14,17,17	0.17	0	13,17,17	0.42	0
2	HEM	C	1459	1	28,50,50	2.12	9 (32%)	17,82,82	3.59	11 (64%)
3	PLM	C	1460	-	14,17,17	0.14	0	13,17,17	0.56	0
2	HEM	D	1459	1	28,50,50	2.17	10 (35%)	17,82,82	3.59	10 (58%)
3	PLM	D	1460	-	14,17,17	0.11	0	13,17,17	0.64	0
2	HEM	E	1459	1	28,50,50	2.17	10 (35%)	17,82,82	3.86	10 (58%)
3	PLM	E	1460	-	14,17,17	0.14	0	13,17,17	0.56	0
2	HEM	F	1459	1	28,50,50	2.11	10 (35%)	17,82,82	3.82	10 (58%)
3	PLM	F	1460	-	14,17,17	0.18	0	13,17,17	0.57	0

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	1459	1	-	0/6/54/54	0/0/8/8
3	PLM	A	1460	-	-	0/13/15/15	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	1459	1	-	0/6/54/54	0/0/8/8
3	PLM	B	1460	-	-	0/13/15/15	0/0/0/0
2	HEM	C	1459	1	-	0/6/54/54	0/0/8/8
3	PLM	C	1460	-	-	0/13/15/15	0/0/0/0
2	HEM	D	1459	1	-	0/6/54/54	0/0/8/8
3	PLM	D	1460	-	-	0/13/15/15	0/0/0/0
2	HEM	E	1459	1	-	0/6/54/54	0/0/8/8
3	PLM	E	1460	-	-	0/13/15/15	0/0/0/0
2	HEM	F	1459	1	-	0/6/54/54	0/0/8/8
3	PLM	F	1460	-	-	0/13/15/15	0/0/0/0

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1459	HEM	C3B-CAB	2.01	1.51	1.47
2	F	1459	HEM	C1A-CHA	2.02	1.45	1.40
2	B	1459	HEM	C3C-CAC	2.09	1.51	1.47
2	D	1459	HEM	C4A-CHB	2.10	1.45	1.40
2	D	1459	HEM	C1A-CHA	2.12	1.45	1.40
2	D	1459	HEM	C3B-CAB	2.13	1.52	1.47
2	B	1459	HEM	C1D-CHD	2.17	1.45	1.40
2	F	1459	HEM	C3B-CAB	2.19	1.52	1.47
2	B	1459	HEM	C3B-CAB	2.23	1.52	1.47
2	A	1459	HEM	C1A-CHA	2.25	1.46	1.40
2	E	1459	HEM	C3B-CAB	2.25	1.52	1.47
2	B	1459	HEM	C1A-CHA	2.25	1.46	1.40
2	B	1459	HEM	C4B-CHC	2.27	1.46	1.40
2	A	1459	HEM	C3C-CAC	2.32	1.52	1.47
2	A	1459	HEM	C1D-CHD	2.34	1.46	1.40
2	C	1459	HEM	C1A-CHA	2.35	1.46	1.40
2	F	1459	HEM	C4A-CHB	2.36	1.46	1.40
2	C	1459	HEM	C4A-CHB	2.38	1.46	1.40
2	E	1459	HEM	C4B-CHC	2.45	1.46	1.40
2	E	1459	HEM	C4A-CHB	2.47	1.46	1.40
2	E	1459	HEM	C1A-CHA	2.48	1.46	1.40
2	F	1459	HEM	C4B-CHC	2.48	1.46	1.40
2	C	1459	HEM	C4B-CHC	2.49	1.46	1.40
2	A	1459	HEM	C4A-CHB	2.49	1.46	1.40
2	B	1459	HEM	C4A-CHB	2.55	1.46	1.40
2	F	1459	HEM	C1D-CHD	2.56	1.46	1.40
2	E	1459	HEM	C1D-CHD	2.63	1.47	1.40
2	D	1459	HEM	C4B-CHC	2.64	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1459	HEM	C4B-CHC	2.65	1.47	1.40
2	D	1459	HEM	C1D-CHD	2.68	1.47	1.40
2	C	1459	HEM	C1D-CHD	2.78	1.47	1.40
2	B	1459	HEM	C3D-C2D	3.04	1.46	1.37
2	E	1459	HEM	C3D-C2D	3.10	1.46	1.37
2	C	1459	HEM	CBB-CAB	3.14	1.51	1.28
2	D	1459	HEM	CBB-CAB	3.15	1.51	1.28
2	E	1459	HEM	CBB-CAB	3.15	1.51	1.28
2	A	1459	HEM	CBB-CAB	3.17	1.51	1.28
2	B	1459	HEM	CBC-CAC	3.21	1.51	1.28
2	D	1459	HEM	CBC-CAC	3.22	1.51	1.28
2	C	1459	HEM	C3D-C2D	3.23	1.47	1.37
2	C	1459	HEM	CBC-CAC	3.24	1.51	1.28
2	F	1459	HEM	CBB-CAB	3.24	1.51	1.28
2	E	1459	HEM	CBC-CAC	3.24	1.51	1.28
2	A	1459	HEM	CBC-CAC	3.25	1.51	1.28
2	F	1459	HEM	CBC-CAC	3.26	1.51	1.28
2	B	1459	HEM	CBB-CAB	3.26	1.51	1.28
2	A	1459	HEM	C3D-C2D	3.34	1.47	1.37
2	D	1459	HEM	C3D-C2D	3.35	1.47	1.37
2	F	1459	HEM	C3D-C2D	3.42	1.47	1.37
2	F	1459	HEM	C3C-C2C	5.03	1.47	1.40
2	C	1459	HEM	C3B-C2B	5.06	1.47	1.40
2	A	1459	HEM	C3C-C2C	5.24	1.47	1.40
2	B	1459	HEM	C3B-C2B	5.32	1.47	1.40
2	E	1459	HEM	C3C-C2C	5.41	1.47	1.40
2	F	1459	HEM	C3B-C2B	5.44	1.47	1.40
2	D	1459	HEM	C3B-C2B	5.53	1.47	1.40
2	C	1459	HEM	C3C-C2C	5.54	1.47	1.40
2	B	1459	HEM	C3C-C2C	5.62	1.47	1.40
2	D	1459	HEM	C3C-C2C	5.63	1.47	1.40
2	A	1459	HEM	C3B-C2B	5.69	1.47	1.40
2	E	1459	HEM	C3B-C2B	5.88	1.48	1.40

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1459	HEM	C1D-C2D-C3D	-7.91	101.49	107.00
2	F	1459	HEM	C1D-C2D-C3D	-7.41	101.84	107.00
2	C	1459	HEM	C1D-C2D-C3D	-7.21	101.98	107.00
2	B	1459	HEM	C1D-C2D-C3D	-7.07	102.08	107.00
2	E	1459	HEM	C1D-C2D-C3D	-6.88	102.21	107.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1459	HEM	C1D-C2D-C3D	-6.85	102.23	107.00
2	B	1459	HEM	C4A-C3A-C2A	-6.67	102.35	107.00
2	D	1459	HEM	C4A-C3A-C2A	-6.46	102.50	107.00
2	A	1459	HEM	C4A-C3A-C2A	-6.19	102.69	107.00
2	C	1459	HEM	C4A-C3A-C2A	-6.07	102.77	107.00
2	F	1459	HEM	C4A-C3A-C2A	-5.81	102.95	107.00
2	E	1459	HEM	C4A-C3A-C2A	-5.57	103.12	107.00
2	A	1459	HEM	C4C-C3C-C2C	-5.37	103.15	106.90
2	B	1459	HEM	C4C-C3C-C2C	-4.69	103.62	106.90
2	E	1459	HEM	C4C-C3C-C2C	-4.29	103.90	106.90
2	D	1459	HEM	C4C-C3C-C2C	-4.19	103.97	106.90
2	F	1459	HEM	C4C-C3C-C2C	-3.79	104.25	106.90
2	C	1459	HEM	C4C-C3C-C2C	-3.74	104.28	106.90
2	E	1459	HEM	CBD-CAD-C3D	-2.38	107.93	112.47
2	B	1459	HEM	CMA-C3A-C2A	2.10	128.91	124.94
2	B	1459	HEM	CBA-CAA-C2A	2.13	116.56	112.48
2	C	1459	HEM	CMA-C3A-C2A	2.13	128.96	124.94
2	F	1459	HEM	CMD-C2D-C3D	2.15	128.99	124.94
2	C	1459	HEM	CMD-C2D-C3D	2.17	129.03	124.94
2	D	1459	HEM	CMD-C2D-C3D	2.23	129.14	124.94
2	B	1459	HEM	CMD-C2D-C3D	2.24	129.17	124.94
2	F	1459	HEM	CMC-C2C-C3C	2.50	129.53	124.89
2	A	1459	HEM	CMC-C2C-C3C	2.64	129.79	124.89
2	D	1459	HEM	CMC-C2C-C3C	2.71	129.93	124.89
2	E	1459	HEM	CMC-C2C-C3C	2.80	130.09	124.89
2	C	1459	HEM	CMB-C2B-C3B	2.82	130.13	124.89
2	A	1459	HEM	CMD-C2D-C3D	2.99	130.58	124.94
2	C	1459	HEM	CMC-C2C-C3C	3.02	130.50	124.89
2	B	1459	HEM	CMB-C2B-C3B	3.03	130.52	124.89
2	F	1459	HEM	CMB-C2B-C3B	3.04	130.53	124.89
2	B	1459	HEM	CMC-C2C-C3C	3.05	130.55	124.89
2	E	1459	HEM	CMB-C2B-C3B	3.19	130.81	124.89
2	D	1459	HEM	CMB-C2B-C3B	3.20	130.84	124.89
2	A	1459	HEM	CMB-C2B-C3B	3.22	130.87	124.89
2	C	1459	HEM	C3C-C4C-NC	3.38	117.33	110.94
2	D	1459	HEM	C3C-C4C-NC	3.48	117.51	110.94
2	D	1459	HEM	CAA-CBA-CGA	3.53	118.69	112.66
2	F	1459	HEM	C3C-C4C-NC	3.56	117.67	110.94
2	B	1459	HEM	CAA-CBA-CGA	3.58	118.78	112.66
2	E	1459	HEM	C3C-C4C-NC	3.65	117.83	110.94
2	B	1459	HEM	C3C-C4C-NC	3.67	117.87	110.94
2	A	1459	HEM	C3C-C4C-NC	4.09	118.66	110.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1459	HEM	CAA-CBA-CGA	4.19	119.82	112.66
2	C	1459	HEM	CAD-CBD-CGD	4.36	120.11	112.66
2	B	1459	HEM	CAD-CBD-CGD	4.88	121.00	112.66
2	D	1459	HEM	CAD-CBD-CGD	5.34	121.78	112.66
2	A	1459	HEM	CAD-CBD-CGD	5.46	122.00	112.66
2	A	1459	HEM	CAA-CBA-CGA	5.49	122.03	112.66
2	E	1459	HEM	CAA-CBA-CGA	5.56	122.16	112.66
2	D	1459	HEM	C3B-C4B-NB	5.61	116.47	109.21
2	F	1459	HEM	CAD-CBD-CGD	5.86	122.67	112.66
2	F	1459	HEM	CAA-CBA-CGA	6.05	122.99	112.66
2	A	1459	HEM	C3B-C4B-NB	6.08	117.07	109.21
2	E	1459	HEM	C3B-C4B-NB	6.08	117.07	109.21
2	F	1459	HEM	C3B-C4B-NB	6.11	117.10	109.21
2	B	1459	HEM	C3B-C4B-NB	6.31	117.37	109.21
2	C	1459	HEM	C3B-C4B-NB	6.34	117.40	109.21
2	E	1459	HEM	CAD-CBD-CGD	6.55	123.86	112.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1459	HEM	5	0
3	A	1460	PLM	4	0
2	B	1459	HEM	2	0
3	B	1460	PLM	1	0
2	C	1459	HEM	4	0
3	C	1460	PLM	2	0
2	D	1459	HEM	6	0
3	D	1460	PLM	1	0
2	E	1459	HEM	2	0
3	E	1460	PLM	2	0
2	F	1459	HEM	6	0
3	F	1460	PLM	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	458/458 (100%)	-0.34	3 (0%) 87 83	13, 21, 36, 46	0
1	B	458/458 (100%)	-0.35	2 (0%) 92 90	13, 21, 36, 46	0
1	C	458/458 (100%)	-0.32	2 (0%) 92 90	13, 21, 36, 46	0
1	D	458/458 (100%)	-0.29	2 (0%) 92 90	13, 21, 36, 46	0
1	E	458/458 (100%)	-0.26	3 (0%) 87 83	13, 21, 36, 46	0
1	F	458/458 (100%)	-0.26	4 (0%) 84 79	13, 21, 36, 46	0
All	All	2748/2748 (100%)	-0.30	16 (0%) 89 86	13, 21, 36, 46	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	ILE	4.8
1	B	381	ASN	3.9
1	A	1	THR	3.7
1	F	192	ASN	3.6
1	D	1	THR	3.5
1	C	227	GLY	3.0
1	A	4	GLU	2.7
1	F	196	PRO	2.6
1	E	229	GLN	2.5
1	A	458	ILE	2.5
1	E	228	GLU	2.4
1	D	21	ASN	2.3
1	F	458	ILE	2.3
1	C	194	ASP	2.3
1	E	1	THR	2.2
1	F	189	GLN	2.1

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	PLM	F	1460	18/18	0.88	0.30	3.07	19,19,19,19	0
3	PLM	D	1460	18/18	0.89	0.20	1.61	19,19,19,19	0
3	PLM	A	1460	18/18	0.83	0.23	1.48	20,20,20,20	0
3	PLM	C	1460	18/18	0.87	0.21	1.35	19,19,19,19	0
3	PLM	B	1460	18/18	0.88	0.18	1.12	19,19,19,19	0
2	HEM	A	1459	43/43	0.97	0.18	0.85	13,16,18,28	0
2	HEM	B	1459	43/43	0.97	0.17	0.60	13,16,18,28	0
2	HEM	F	1459	43/43	0.96	0.17	0.37	13,16,18,28	0
3	PLM	E	1460	18/18	0.92	0.18	0.14	20,20,20,20	0
2	HEM	C	1459	43/43	0.97	0.15	-0.01	13,16,18,28	0
2	HEM	E	1459	43/43	0.97	0.15	-0.53	13,16,18,28	0
2	HEM	D	1459	43/43	0.96	0.15	-0.76	13,16,18,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.