



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:49 PM GMT

PDB ID : 1QQW  
Title : CRYSTAL STRUCTURE OF HUMAN ERYTHROCYTE CATALASE  
Authors : Ko, T.P.; Safo, M.K.; Musayev, F.N.; Wang, C.; Wu, S.H.; Abraham, D.J.  
Deposited on : 1999-06-09  
Resolution : 2.75 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](mailto: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 (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

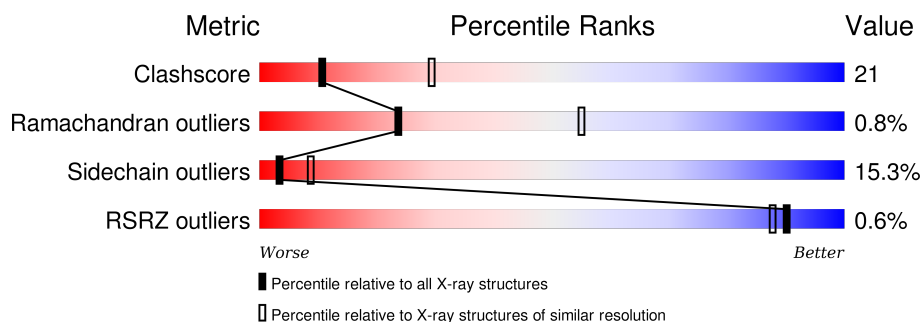
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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  $\geq 3$ , 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	527	
1	B	527	
1	C	527	
1	D	527	

## 2 Entry composition [i](#)

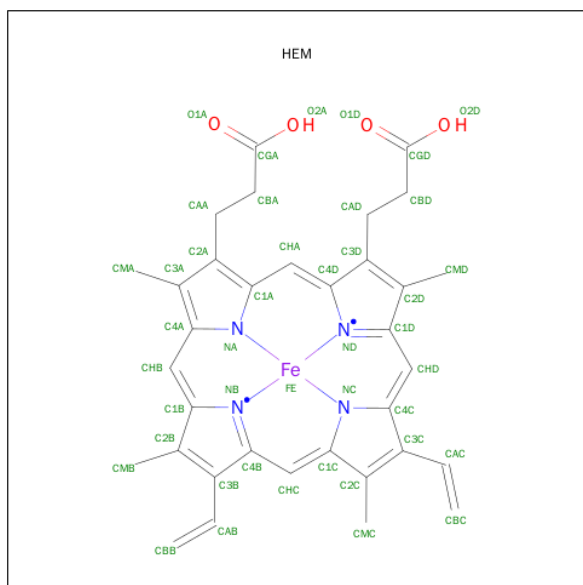
There are 3 unique types of molecules in this entry. The entry contains 16618 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CATALASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	0	0
			4012	2549	712	738	13			
1	B	500	Total	C	N	O	S	0	0	0
			4017	2552	713	739	13			
1	C	499	Total	C	N	O	S	0	0	0
			4012	2549	712	738	13			
1	D	499	Total	C	N	O	S	0	0	0
			4012	2549	712	738	13			

- 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		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

*Continued on next page...*

*Continued from previous page...*

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

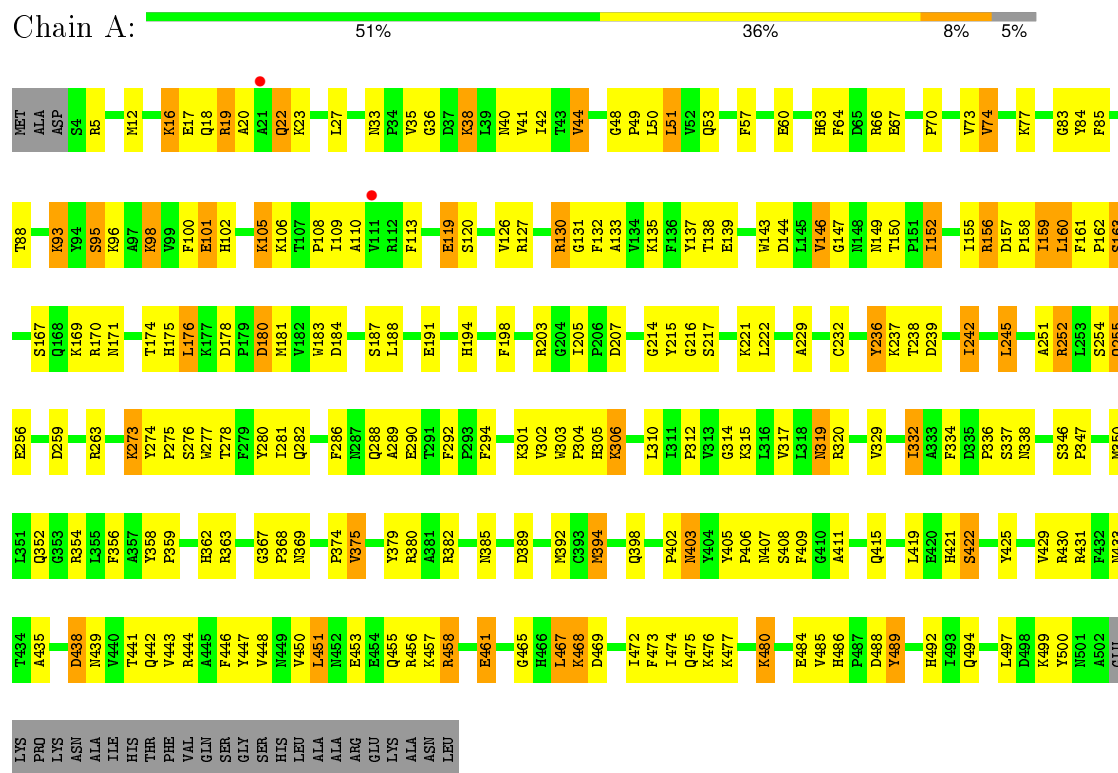
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	102	Total	O	0	0
			102	102		
3	B	119	Total	O	0	0
			119	119		
3	C	96	Total	O	0	0
			96	96		
3	D	76	Total	O	0	0
			76	76		

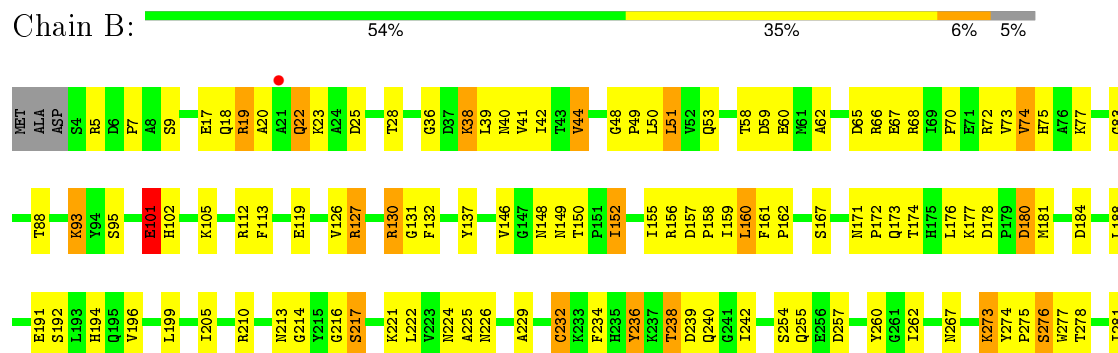
### 3 Residue-property plots

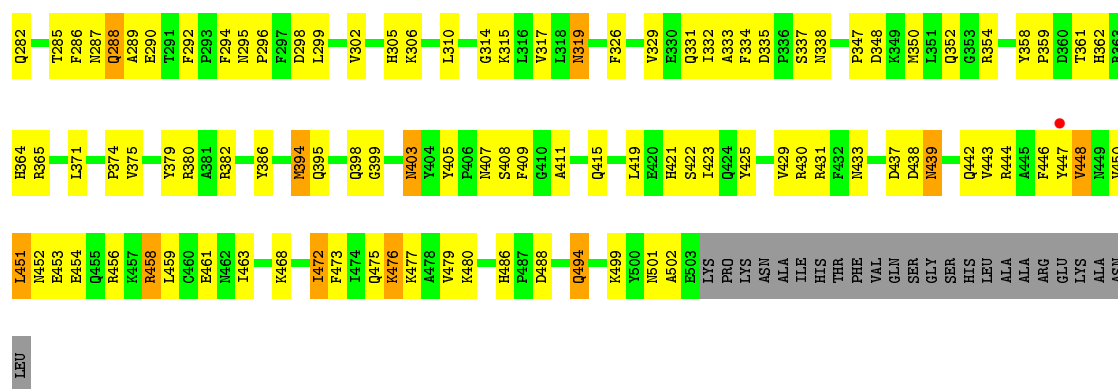
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: CATALASE

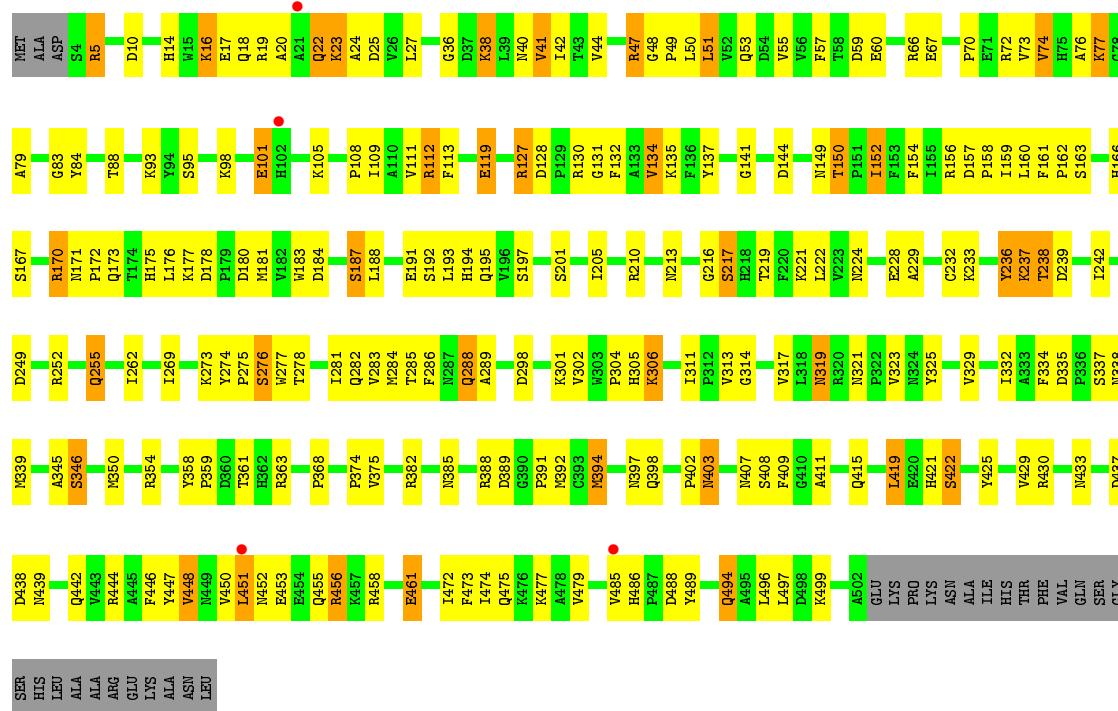


#### • Molecule 1: CATALASE

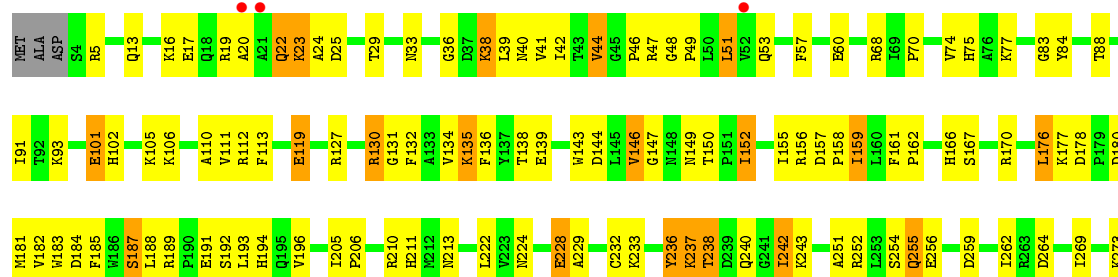




• Molecule 1: CATALASE



• Molecule 1: CATALASE



[illegible]

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.90Å 141.67Å 232.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.75 232.46 – 2.73	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.75) 80.7 (232.46-2.73)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.20 (at 2.73Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.206 , 0.272 0.226 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	17.3	Xtriage
Anisotropy	0.626	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 36.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 60778 reflections	Xtriage
$F_o, F_c$ correlation	0.80	EDS
Total number of atoms	16618	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.32	0/4131	0.49	0/5613
1	B	0.31	0/4136	0.49	0/5620
1	C	0.32	0/4131	0.49	0/5613
1	D	0.31	0/4131	0.48	0/5613
All	All	0.32	0/16529	0.49	0/22459

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	4012	0	3843	204	0
1	B	4017	0	3846	178	0
1	C	4012	0	3844	192	0
1	D	4012	0	3844	193	0
2	A	43	0	30	2	0
2	B	43	0	30	3	0
2	C	43	0	30	2	0
2	D	43	0	30	1	0
3	A	102	0	0	10	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	119	0	0	9	0
3	C	96	0	0	5	0
3	D	76	0	0	7	0
All	All	16618	0	15497	672	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 21.

All (672) 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:402:PRO:HG2	1:A:411:ALA:HB2	1.42	1.01
1:B:156:ARG:HH22	1:B:439:ASN:HD21	1.06	0.99
1:B:403:ASN:HD22	1:B:403:ASN:H	1.03	0.99
1:D:156:ARG:HH22	1:D:439:ASN:HD21	1.13	0.96
1:C:156:ARG:HH22	1:C:439:ASN:HD21	1.14	0.95
1:B:407:ASN:HD21	1:B:411:ALA:HB3	1.30	0.94
1:C:407:ASN:HD21	1:C:411:ALA:HB3	1.34	0.92
1:C:156:ARG:NH2	1:C:439:ASN:HD21	1.70	0.90
1:B:255:GLN:HB3	1:C:255:GLN:HB3	1.55	0.88
1:A:486:HIS:HD2	1:A:488:ASP:H	1.19	0.87
1:A:178:ASP:HB3	1:A:181:MET:HG3	1.56	0.86
1:A:407:ASN:HD21	1:A:411:ALA:HB3	1.42	0.85
1:D:407:ASN:HD21	1:D:411:ALA:HB3	1.42	0.84
1:C:475:GLN:HE21	1:C:497:LEU:HD13	1.41	0.84
1:A:368:PRO:HB3	1:C:66:ARG:HD3	1.60	0.83
1:D:475:GLN:HE22	1:D:501:ASN:HD21	1.23	0.83
1:B:156:ARG:HH22	1:B:439:ASN:ND2	1.76	0.83
1:B:40:ASN:HD21	1:C:433:ASN:HD22	1.23	0.82
1:D:454:GLU:HB3	1:D:458:ARG:HH21	1.44	0.82
1:B:403:ASN:N	1:B:403:ASN:HD22	1.77	0.81
1:A:255:GLN:HB3	1:D:255:GLN:HB3	1.62	0.81
1:A:329:VAL:O	1:A:332:ILE:HG22	1.80	0.80
1:B:329:VAL:O	1:B:332:ILE:HG22	1.82	0.80
1:B:19:ARG:HA	1:B:22:GLN:HE21	1.49	0.77
1:A:319:ASN:H	1:A:319:ASN:HD22	1.33	0.77
1:B:255:GLN:HG2	1:C:255:GLN:HG2	1.66	0.77
1:D:242:ILE:HD12	1:D:242:ILE:H	1.50	0.76
1:C:329:VAL:O	1:C:332:ILE:HG22	1.86	0.76
1:B:302:VAL:HG22	1:B:442:GLN:HE22	1.50	0.76
1:C:23:LYS:HE2	1:C:24:ALA:H	1.50	0.75

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:GLN:HE22	1:B:501:ASN:HD21	1.32	0.75
1:B:70:PRO:HG3	1:C:70:PRO:HD3	1.67	0.75
1:C:358:TYR:HB2	1:C:359:PRO:HD3	1.70	0.74
1:D:403:ASN:H	1:D:403:ASN:HD22	1.34	0.74
1:A:67:GLU:HG2	1:C:389:ASP:HB2	1.69	0.74
1:B:191:GLU:HA	1:B:439:ASN:HB3	1.67	0.73
1:A:83:GLY:HA2	1:A:319:ASN:ND2	2.03	0.73
1:B:486:HIS:HD2	1:B:488:ASP:H	1.36	0.73
1:B:36:GLY:HA2	1:D:415:GLN:O	1.87	0.73
1:A:403:ASN:HD22	1:A:403:ASN:H	1.34	0.73
1:B:403:ASN:H	1:B:403:ASN:ND2	1.85	0.72
1:C:298:ASP:HB3	1:C:301:LYS:HG3	1.71	0.72
1:C:72:ARG:HG2	2:C:600:HEM:CGA	2.21	0.71
1:D:158:PRO:HG3	1:D:350:MET:HA	1.72	0.71
1:A:33:ASN:HD22	1:C:141:GLY:HA3	1.56	0.70
1:D:88:THR:HG23	1:D:314:GLY:HA2	1.72	0.70
1:C:354:ARG:HG3	2:C:600:HEM:HBB2	1.74	0.70
1:D:156:ARG:NH2	1:D:439:ASN:HD21	1.88	0.69
1:A:36:GLY:HA3	1:C:419:LEU:HD23	1.75	0.69
1:D:146:VAL:HB	1:D:354:ARG:HH22	1.56	0.69
1:D:382:ARG:HH11	1:D:382:ARG:HB2	1.58	0.69
1:B:113:PHE:HA	1:B:131:GLY:O	1.93	0.68
1:A:221:LYS:HZ1	1:A:421:HIS:HB3	1.59	0.68
1:B:19:ARG:HA	1:B:22:GLN:NE2	2.08	0.68
1:A:320:ARG:HG2	1:A:320:ARG:HH11	1.56	0.68
1:B:167:SER:HA	1:B:181:MET:HE2	1.76	0.67
1:A:51:LEU:HD12	1:A:53:GLN:HB2	1.76	0.67
1:D:475:GLN:HE22	1:D:501:ASN:ND2	1.91	0.67
1:B:178:ASP:HB3	1:B:181:MET:HG3	1.76	0.67
1:D:232:CYS:HA	1:D:282:GLN:O	1.94	0.67
1:B:358:TYR:HB2	1:B:359:PRO:HD3	1.76	0.67
1:C:422:SER:OG	1:D:430:ARG:HB3	1.95	0.67
1:A:433:ASN:HA	1:D:40:ASN:ND2	2.10	0.67
1:D:38:LYS:HE3	1:D:60:GLU:OE1	1.95	0.67
1:C:53:GLN:NE2	1:D:49:PRO:HB3	2.10	0.67
1:B:156:ARG:HH12	1:B:439:ASN:HD22	1.43	0.66
1:A:486:HIS:CD2	1:A:488:ASP:H	2.09	0.66
1:A:119:GLU:HG3	1:A:170:ARG:HH21	1.58	0.66
1:A:18:GLN:NE2	1:A:19:ARG:HH21	1.93	0.66
1:D:454:GLU:HB3	1:D:458:ARG:NH2	2.10	0.66
1:C:232:CYS:HA	1:C:282:GLN:O	1.96	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:329:VAL:O	1:D:332:ILE:HG22	1.95	0.65
1:B:371:LEU:HB2	3:B:715:HOH:O	1.96	0.65
1:B:68:ARG:NH1	1:C:73:VAL:HA	2.12	0.65
1:B:448:VAL:HA	1:B:456:ARG:NH1	2.11	0.65
1:D:354:ARG:HG2	1:D:358:TYR:HE1	1.60	0.65
1:D:298:ASP:HB3	1:D:301:LYS:HG3	1.79	0.65
1:A:130:ARG:HB2	1:A:149:ASN:ND2	2.12	0.65
1:D:184:ASP:O	1:D:188:LEU:HG	1.97	0.65
1:B:156:ARG:NH2	1:B:437:ASP:H	1.94	0.64
1:D:486:HIS:HD2	1:D:488:ASP:H	1.44	0.64
1:D:75:HIS:O	1:D:112:ARG:NH2	2.30	0.64
1:D:358:TYR:HB2	1:D:359:PRO:HD3	1.79	0.64
1:C:167:SER:HA	1:C:181:MET:HE2	1.78	0.64
1:D:437:ASP:O	1:D:438:ASP:HB3	1.98	0.64
1:B:380:ARG:HH11	1:B:380:ARG:HG3	1.63	0.64
1:A:19:ARG:HA	1:A:22:GLN:HE21	1.63	0.63
1:C:479:VAL:HG11	1:C:494:GLN:HG2	1.81	0.63
1:C:486:HIS:HD2	1:C:488:ASP:H	1.46	0.63
1:A:169:LYS:NZ	3:A:615:HOH:O	2.31	0.63
1:C:452:ASN:HA	1:C:456:ARG:HH21	1.64	0.63
1:A:16:LYS:HD2	1:C:409:PHE:HA	1.80	0.63
1:C:161:PHE:HB3	1:C:162:PRO:HD3	1.81	0.63
1:D:302:VAL:H	1:D:442:GLN:HE22	1.46	0.63
1:C:302:VAL:H	1:C:442:GLN:HE22	1.45	0.63
1:C:73:VAL:HG13	1:C:74:VAL:HG22	1.80	0.63
1:A:425:TYR:CE2	1:D:49:PRO:HD3	2.34	0.62
1:D:113:PHE:HA	1:D:131:GLY:O	1.99	0.62
1:B:431:ARG:NH1	1:C:42:ILE:HG13	2.14	0.62
1:A:305:HIS:HB2	1:A:306:LYS:NZ	2.15	0.62
1:C:249:ASP:HA	1:C:252:ARG:NH1	2.15	0.62
1:D:236:TYR:HA	1:D:278:THR:O	2.00	0.62
1:C:446:PHE:HA	1:C:450:VAL:CG2	2.29	0.62
1:B:479:VAL:HG11	1:B:494:GLN:HG2	1.81	0.62
1:C:407:ASN:HD21	1:C:411:ALA:CB	2.12	0.62
1:C:392:MET:O	1:C:394:MET:HE2	1.99	0.61
1:A:468:LYS:HG3	1:A:469:ASP:N	2.14	0.61
1:A:403:ASN:HD22	1:A:403:ASN:N	1.97	0.61
1:B:38:LYS:HE2	1:B:38:LYS:O	1.99	0.61
1:B:415:GLN:O	1:D:36:GLY:HA2	2.00	0.61
1:B:429:VAL:HG11	1:C:51:LEU:HD11	1.81	0.61
1:A:12:MET:CE	1:D:180:ASP:HB3	2.31	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ASN:ND2	1:C:433:ASN:HA	2.16	0.61
1:B:174:THR:HB	1:B:176:LEU:HD12	1.81	0.61
1:D:407:ASN:HD21	1:D:411:ALA:CB	2.12	0.61
1:D:475:GLN:O	1:D:479:VAL:HG23	2.01	0.61
1:A:320:ARG:NH1	1:A:320:ARG:HG2	2.14	0.61
1:C:51:LEU:HA	1:D:51:LEU:HA	1.83	0.61
1:B:236:TYR:HA	1:B:278:THR:O	2.00	0.61
1:C:77:LYS:HE2	1:C:262:ILE:HD11	1.81	0.60
1:A:282:GLN:OE1	1:A:303:TRP:HB2	2.01	0.60
1:B:429:VAL:CG1	1:C:51:LEU:HD11	2.31	0.60
1:C:447:TYR:HA	1:C:451:LEU:HD12	1.84	0.60
1:D:467:LEU:HD11	1:D:475:GLN:HA	1.83	0.60
1:B:285:THR:OG1	1:B:288:GLN:HG2	2.01	0.60
1:D:479:VAL:HG11	1:D:494:GLN:HG2	1.82	0.60
1:A:433:ASN:HD22	1:D:40:ASN:HD21	1.49	0.60
1:A:110:ALA:HB3	1:A:135:LYS:HB3	1.83	0.60
1:B:44:VAL:O	1:B:48:GLY:HA3	2.02	0.60
1:D:191:GLU:HA	1:D:439:ASN:HB3	1.84	0.59
1:B:51:LEU:HD12	1:B:53:GLN:HB2	1.84	0.59
1:B:452:ASN:HA	1:B:456:ARG:HH21	1.66	0.59
1:A:419:LEU:HD23	1:C:36:GLY:HA3	1.83	0.59
1:A:18:GLN:HE21	1:A:19:ARG:HH21	1.49	0.59
1:B:68:ARG:HH11	1:C:73:VAL:HA	1.66	0.59
1:A:156:ARG:HH22	1:A:439:ASN:ND2	2.01	0.59
1:A:169:LYS:HE3	1:D:68:ARG:HH21	1.66	0.59
1:C:170:ARG:HD2	1:C:175:HIS:CE1	2.38	0.59
1:A:146:VAL:HG23	3:A:631:HOH:O	2.02	0.59
1:B:286:PHE:O	1:B:289:ALA:HB3	2.01	0.59
1:A:113:PHE:HA	1:A:131:GLY:O	2.03	0.59
1:D:457:LYS:HE3	1:D:461:GLU:OE1	2.03	0.59
1:A:36:GLY:HA2	1:C:415:GLN:O	2.01	0.59
1:A:431:ARG:HG3	1:D:42:ILE:HG12	1.85	0.59
1:A:93:LYS:HE2	3:A:696:HOH:O	2.03	0.59
1:A:429:VAL:HG11	1:D:51:LEU:HD11	1.84	0.59
1:A:438:ASP:OD1	1:A:441:THR:HB	2.03	0.59
1:B:157:ASP:HB3	1:B:160:LEU:HD12	1.83	0.59
1:D:38:LYS:HE2	1:D:38:LYS:O	2.03	0.59
1:A:429:VAL:CG1	1:D:51:LEU:HD11	2.32	0.59
1:D:161:PHE:HB3	1:D:162:PRO:HD3	1.84	0.59
1:D:192:SER:O	1:D:196:VAL:HG23	2.03	0.58
1:B:475:GLN:O	1:B:479:VAL:HG23	2.03	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:ALA:CB	3:C:693:HOH:O	2.51	0.58
1:C:55:VAL:HG22	3:C:610:HOH:O	2.03	0.58
1:D:156:ARG:HH12	1:D:439:ASN:HD22	1.49	0.58
1:A:433:ASN:HA	1:D:40:ASN:HD21	1.67	0.58
1:D:405:TYR:OH	1:D:414:GLN:HG2	2.03	0.58
1:A:49:PRO:HD3	1:D:425:TYR:CE2	2.38	0.58
1:B:184:ASP:O	1:B:188:LEU:HG	2.03	0.58
1:C:44:VAL:O	1:C:48:GLY:HA3	2.03	0.58
1:B:161:PHE:HB3	1:B:162:PRO:HD3	1.84	0.58
1:A:406:PRO:HG3	3:B:718:HOH:O	2.04	0.58
1:C:222:LEU:HG	1:C:232:CYS:SG	2.44	0.58
1:B:319:ASN:HD22	1:B:319:ASN:C	2.06	0.58
1:A:167:SER:HA	1:A:181:MET:CE	2.34	0.58
1:C:76:ALA:HB3	3:C:693:HOH:O	2.04	0.58
1:B:156:ARG:NH2	1:B:439:ASN:HD21	1.89	0.57
1:D:382:ARG:HH11	1:D:382:ARG:CB	2.17	0.57
1:C:49:PRO:HB3	1:D:53:GLN:NE2	2.19	0.57
1:C:219:THR:OG1	1:C:233:LYS:HE2	2.05	0.57
1:D:167:SER:HA	1:D:181:MET:HE2	1.86	0.57
1:C:178:ASP:HB3	1:C:181:MET:HG3	1.87	0.57
1:C:304:PRO:HB3	1:C:306:LYS:HE2	1.85	0.57
1:C:84:TYR:CA	1:C:109:ILE:HG12	2.35	0.57
1:A:358:TYR:HB2	1:A:359:PRO:HD3	1.87	0.57
1:A:457:LYS:HA	1:A:492:HIS:HE1	1.69	0.57
1:A:486:HIS:HD2	1:A:488:ASP:N	1.96	0.57
1:D:236:TYR:N	1:D:236:TYR:CD1	2.72	0.57
1:C:38:LYS:HE3	1:C:60:GLU:OE1	2.05	0.57
1:C:88:THR:HG23	1:C:314:GLY:HA2	1.86	0.57
1:A:88:THR:HG23	1:A:314:GLY:HA2	1.87	0.57
1:B:382:ARG:HD2	3:B:680:HOH:O	2.05	0.57
1:D:91:ILE:HD13	1:D:313:VAL:HG13	1.86	0.57
1:C:51:LEU:N	1:C:51:LEU:HD23	2.20	0.56
1:D:392:MET:O	1:D:394:MET:HE2	2.05	0.56
1:A:44:VAL:O	1:A:48:GLY:HA3	2.06	0.56
1:B:213:ASN:OD1	1:B:238:THR:HG22	2.04	0.56
1:D:29:THR:HG23	1:D:33:ASN:O	2.05	0.56
1:B:358:TYR:O	1:B:361:THR:HG22	2.04	0.56
1:C:446:PHE:O	1:C:450:VAL:HB	2.05	0.56
1:C:170:ARG:HD3	1:C:175:HIS:O	2.05	0.56
1:D:379:TYR:CE1	1:D:380:ARG:HG2	2.41	0.56
1:A:146:VAL:HG21	1:A:336:PRO:HG3	1.87	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:GLU:HG2	1:D:388:ARG:O	2.06	0.56
1:D:156:ARG:HH12	1:D:439:ASN:ND2	2.03	0.56
1:C:130:ARG:HB2	1:C:149:ASN:ND2	2.20	0.56
1:C:275:PRO:HB2	1:C:277:TRP:HZ3	1.71	0.56
1:A:251:ALA:O	1:A:254:SER:HB3	2.05	0.56
1:A:214:GLY:HA3	1:A:236:TYR:CE2	2.40	0.56
1:B:287:ASN:HA	3:B:665:HOH:O	2.06	0.56
1:C:84:TYR:HA	1:C:109:ILE:HG12	1.88	0.56
1:D:183:TRP:O	1:D:187:SER:HB3	2.06	0.56
1:D:475:GLN:NE2	1:D:501:ASN:HD21	1.99	0.55
1:B:444:ARG:O	1:B:448:VAL:HG23	2.06	0.55
1:B:70:PRO:HD3	1:C:70:PRO:HG3	1.88	0.55
1:D:178:ASP:OD2	1:D:180:ASP:HB2	2.05	0.55
1:A:184:ASP:O	1:A:188:LEU:HG	2.05	0.55
1:A:42:ILE:O	1:A:50:LEU:HD12	2.06	0.55
1:A:356:PHE:O	1:A:359:PRO:HD2	2.07	0.55
1:D:119:GLU:OE2	1:D:170:ARG:NH1	2.40	0.55
1:D:446:PHE:O	1:D:451:LEU:HD12	2.06	0.55
1:B:433:ASN:HA	1:C:40:ASN:ND2	2.22	0.55
1:B:49:PRO:HD3	1:C:425:TYR:CE2	2.42	0.55
1:B:335:ASP:HB2	1:B:338:ASN:OD1	2.07	0.55
1:B:475:GLN:HE22	1:B:501:ASN:ND2	2.02	0.55
1:A:222:LEU:O	1:A:229:ALA:HA	2.07	0.55
1:D:224:ASN:HD21	1:D:228:GLU:HG3	1.72	0.54
1:B:156:ARG:NH2	1:B:439:ASN:ND2	2.53	0.54
1:A:83:GLY:HA3	1:A:317:VAL:O	2.07	0.54
1:A:473:PHE:CE1	1:A:474:ILE:HG13	2.42	0.54
1:B:156:ARG:HH21	1:B:437:ASP:H	1.55	0.54
1:A:444:ARG:HD3	1:A:485:VAL:O	2.07	0.54
1:C:156:ARG:CZ	1:C:437:ASP:HB2	2.37	0.54
1:A:392:MET:O	1:A:394:MET:HE2	2.07	0.54
1:A:385:ASN:HA	1:C:27:LEU:CD1	2.37	0.54
1:C:156:ARG:HH22	1:C:439:ASN:ND2	1.95	0.54
1:B:425:TYR:CE2	1:C:49:PRO:HD3	2.43	0.54
1:C:403:ASN:OD1	1:D:166:HIS:HB3	2.07	0.54
1:A:64:PHE:HA	1:A:67:GLU:OE2	2.08	0.54
1:C:275:PRO:HB2	1:C:277:TRP:CZ3	2.42	0.54
1:D:251:ALA:O	1:D:254:SER:HB3	2.07	0.54
1:B:72:ARG:HB3	1:B:74:VAL:O	2.08	0.54
3:B:688:HOH:O	1:D:39:LEU:HD11	2.06	0.54
1:D:83:GLY:HA3	1:D:317:VAL:O	2.08	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:HIS:NE2	1:A:105:LYS:HG3	2.23	0.54
1:A:38:LYS:HE3	1:A:60:GLU:OE1	2.08	0.54
1:D:167:SER:HA	1:D:181:MET:CE	2.38	0.53
1:A:187:SER:OG	1:A:477:LYS:HD2	2.09	0.53
1:B:192:SER:O	1:B:196:VAL:HG23	2.08	0.53
1:A:457:LYS:HE3	1:A:461:GLU:OE1	2.08	0.53
1:C:389:ASP:H	1:C:397:ASN:HD21	1.57	0.53
1:A:305:HIS:HB2	1:A:306:LYS:HZ3	1.74	0.53
1:A:446:PHE:HA	1:A:450:VAL:CG2	2.39	0.53
1:C:184:ASP:O	1:C:188:LEU:HG	2.08	0.53
1:C:135:LYS:HE2	1:C:332:ILE:HD11	1.89	0.53
1:A:403:ASN:H	1:A:403:ASN:ND2	2.04	0.53
1:B:146:VAL:HB	1:B:354:ARG:HH22	1.73	0.53
1:A:394:MET:HG2	1:C:394:MET:HG2	1.90	0.53
1:D:130:ARG:NH2	1:D:206:PRO:HD2	2.24	0.53
1:A:292:PHE:CE2	1:A:294:PHE:HB2	2.43	0.53
1:D:320:ARG:HG2	1:D:320:ARG:HH11	1.74	0.53
1:C:191:GLU:HA	1:C:439:ASN:HB3	1.91	0.53
1:C:319:ASN:C	1:C:319:ASN:HD22	2.11	0.53
1:C:150:THR:HG21	1:C:195:GLN:HE22	1.73	0.53
1:B:127:ARG:HG3	1:B:199:LEU:HD11	1.89	0.53
1:A:178:ASP:OD2	1:A:180:ASP:HB2	2.09	0.53
1:A:389:ASP:HB2	1:C:67:GLU:HG2	1.91	0.53
1:B:475:GLN:NE2	1:B:501:ASN:HD21	2.02	0.53
1:A:354:ARG:HG3	2:A:600:HEM:HBB2	1.92	0.53
1:D:156:ARG:HH22	1:D:439:ASN:ND2	1.93	0.52
1:C:477:LYS:HD3	3:C:681:HOH:O	2.09	0.52
1:D:286:PHE:O	1:D:289:ALA:HB3	2.08	0.52
1:C:281:ILE:HG12	1:C:313:VAL:CG2	2.39	0.52
1:C:446:PHE:HA	1:C:450:VAL:HG23	1.91	0.52
1:A:334:PHE:O	1:A:362:HIS:HE1	1.92	0.52
1:C:269:ILE:HD12	1:C:321:ASN:ND2	2.24	0.52
1:A:431:ARG:HB3	1:D:40:ASN:HB3	1.92	0.52
1:B:446:PHE:CE2	1:B:451:LEU:HD11	2.44	0.52
1:C:444:ARG:O	1:C:448:VAL:HG23	2.10	0.52
1:A:467:LEU:HD11	1:A:475:GLN:HA	1.90	0.52
1:A:447:TYR:HA	1:A:451:LEU:HD12	1.91	0.52
1:B:395:GLN:HG2	3:B:706:HOH:O	2.09	0.52
1:C:83:GLY:HA3	1:C:317:VAL:O	2.10	0.52
1:B:302:VAL:HG22	1:B:442:GLN:NE2	2.21	0.52
1:C:354:ARG:HG2	1:C:358:TYR:HE1	1.75	0.52

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ARG:NH2	1:A:439:ASN:ND2	2.58	0.52
1:A:354:ARG:HG2	1:A:358:TYR:HE1	1.75	0.52
1:C:38:LYS:HE3	1:C:60:GLU:OE2	2.10	0.52
1:A:27:LEU:CD1	1:C:385:ASN:HA	2.39	0.52
1:C:158:PRO:HD3	1:C:350:MET:HA	1.92	0.52
1:D:44:VAL:O	1:D:48:GLY:HA3	2.10	0.51
1:A:169:LYS:HE3	1:D:68:ARG:NH2	2.25	0.51
1:C:194:HIS:HE1	1:C:442:GLN:HE21	1.59	0.51
1:A:155:ILE:HG13	1:A:350:MET:HE2	1.92	0.51
1:C:286:PHE:O	1:C:289:ALA:HB3	2.09	0.51
1:B:156:ARG:HH12	1:B:439:ASN:ND2	2.08	0.51
1:D:285:THR:OG1	1:D:288:GLN:HG2	2.10	0.51
1:C:44:VAL:CG1	1:C:49:PRO:HD2	2.40	0.51
1:C:108:PRO:HG2	1:C:137:TYR:HB2	1.92	0.51
1:D:51:LEU:HD12	1:D:53:GLN:HB2	1.93	0.51
1:A:415:GLN:O	1:C:36:GLY:HA2	2.11	0.51
1:A:51:LEU:HA	1:B:51:LEU:HA	1.93	0.51
3:A:694:HOH:O	1:B:172:PRO:CD	2.58	0.51
1:A:167:SER:HA	1:A:181:MET:HE3	1.93	0.51
1:D:252:ARG:HG2	1:D:256:GLU:HG3	1.93	0.51
1:D:222:LEU:O	1:D:229:ALA:HA	2.11	0.51
1:D:194:HIS:HE1	1:D:442:GLN:HE21	1.58	0.51
1:B:433:ASN:HD22	1:C:40:ASN:HD21	1.57	0.51
1:D:144:ASP:HB2	1:D:335:ASP:O	2.11	0.51
1:D:211:HIS:HB3	1:D:243:LYS:H	1.76	0.51
1:C:249:ASP:HA	1:C:252:ARG:HH12	1.75	0.51
1:A:255:GLN:HG2	1:D:255:GLN:HG2	1.92	0.50
1:B:354:ARG:HG2	1:B:358:TYR:HE1	1.76	0.50
1:C:302:VAL:O	1:C:304:PRO:HD3	2.10	0.50
1:A:157:ASP:HB3	1:A:160:LEU:HD12	1.92	0.50
1:C:224:ASN:HD21	1:C:228:GLU:HG3	1.76	0.50
1:D:252:ARG:O	1:D:255:GLN:HG3	2.11	0.50
1:B:326:PHE:O	1:B:331:GLN:HG3	2.11	0.50
1:C:183:TRP:O	1:C:187:SER:HB3	2.12	0.50
1:C:55:VAL:O	1:C:59:ASP:HB2	2.11	0.50
1:A:385:ASN:HA	1:C:27:LEU:HD13	1.93	0.50
1:A:347:PRO:HB3	1:D:47:ARG:O	2.12	0.50
1:B:51:LEU:HD11	1:C:429:VAL:CG1	2.41	0.50
1:A:191:GLU:HA	1:A:439:ASN:HB3	1.94	0.50
1:A:475:GLN:HE21	1:A:497:LEU:HD13	1.75	0.50
1:D:19:ARG:HA	1:D:22:GLN:HE21	1.76	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:GLN:NE2	1:C:19:ARG:NH2	2.60	0.50
1:C:111:VAL:HG22	1:C:134:VAL:HG13	1.92	0.50
1:A:236:TYR:HA	1:A:278:THR:O	2.11	0.50
1:C:49:PRO:HB3	1:D:53:GLN:HE21	1.77	0.50
1:A:95:SER:HG	1:A:100:PHE:HD2	1.60	0.50
1:A:135:LYS:HG3	1:A:144:ASP:OD2	2.10	0.50
1:B:158:PRO:HD3	1:B:350:MET:HA	1.93	0.50
1:C:23:LYS:CE	1:C:24:ALA:H	2.21	0.50
1:B:364:HIS:ND1	1:C:66:ARG:HG2	2.26	0.50
1:C:14:HIS:HB3	3:C:623:HOH:O	2.11	0.50
1:D:136:PHE:HB2	1:D:143:TRP:HB3	1.93	0.49
1:D:147:GLY:HA2	2:D:600:HEM:HBC1	1.94	0.49
1:C:113:PHE:HA	1:C:131:GLY:O	2.12	0.49
1:A:119:GLU:CG	1:A:170:ARG:HH21	2.25	0.49
1:A:232:CYS:HA	1:A:282:GLN:O	2.12	0.49
1:C:144:ASP:OD1	1:C:334:PHE:HA	2.11	0.49
1:D:358:TYR:O	1:D:361:THR:HG22	2.12	0.49
1:A:480:LYS:O	1:A:484:GLU:HG2	2.12	0.49
1:A:174:THR:HB	1:A:176:LEU:HD12	1.94	0.49
1:D:354:ARG:HG2	1:D:358:TYR:CE1	2.43	0.49
1:A:170:ARG:HD2	1:A:175:HIS:CE1	2.47	0.49
1:A:176:LEU:HD21	1:D:262:ILE:CG2	2.42	0.49
1:A:275:PRO:HB2	1:A:277:TRP:CZ3	2.48	0.49
1:B:171:ASN:HB3	1:B:174:THR:OG1	2.13	0.49
1:C:144:ASP:HB2	1:C:335:ASP:O	2.12	0.49
1:D:382:ARG:HH11	1:D:382:ARG:CG	2.25	0.49
1:A:133:ALA:HB1	1:A:334:PHE:CD2	2.48	0.49
1:D:491:SER:HB2	3:D:670:HOH:O	2.12	0.49
1:C:236:TYR:HA	1:C:278:THR:O	2.11	0.49
1:D:178:ASP:HB3	1:D:181:MET:HG3	1.94	0.49
1:A:38:LYS:O	1:A:38:LYS:HE2	2.13	0.49
1:C:157:ASP:HB3	1:C:160:LEU:HD12	1.95	0.49
1:A:198:PHE:HZ	1:A:203:ARG:NH1	2.10	0.49
1:C:41:VAL:CG1	1:C:50:LEU:HD13	2.43	0.49
1:B:423:ILE:HB	1:B:425:TYR:CE1	2.48	0.49
1:A:171:ASN:HB3	1:A:174:THR:OG1	2.13	0.49
1:B:423:ILE:HB	1:B:425:TYR:HE1	1.78	0.48
1:C:163:SER:O	1:C:166:HIS:HB2	2.13	0.48
1:D:222:LEU:HG	1:D:232:CYS:SG	2.54	0.48
1:C:213:ASN:OD1	1:C:238:THR:HG22	2.14	0.48
1:D:397:ASN:O	1:D:398:GLN:HB2	2.12	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:THR:O	1:C:346:SER:HB3	2.12	0.48
1:B:295:ASN:HB3	1:B:298:ASP:HB2	1.95	0.48
1:A:380:ARG:HH11	1:A:380:ARG:HG3	1.77	0.48
1:A:33:ASN:ND2	1:C:141:GLY:HA3	2.26	0.48
1:B:319:ASN:ND2	1:B:319:ASN:C	2.67	0.48
1:B:216:GLY:O	1:B:217:SER:HB2	2.13	0.48
1:C:252:ARG:O	1:C:255:GLN:HG3	2.13	0.48
1:B:194:HIS:HE1	1:B:442:GLN:HE21	1.61	0.48
1:A:431:ARG:HG2	1:D:40:ASN:O	2.13	0.48
1:A:176:LEU:HD21	1:D:262:ILE:HG22	1.95	0.48
1:A:320:ARG:NE	3:A:693:HOH:O	2.37	0.48
1:A:183:TRP:O	1:A:187:SER:HB3	2.13	0.48
1:B:62:ALA:O	1:B:65:ASP:HB2	2.14	0.48
1:D:13:GLN:HA	1:D:13:GLN:NE2	2.29	0.48
1:D:152:ILE:HG22	1:D:299:LEU:O	2.14	0.48
1:D:433:ASN:ND2	1:D:435:ALA:H	2.11	0.48
1:D:447:TYR:HA	1:D:451:LEU:HD12	1.96	0.48
1:B:292:PHE:CE2	1:B:294:PHE:HB2	2.48	0.48
1:B:437:ASP:O	1:B:438:ASP:HB3	2.14	0.48
1:D:44:VAL:CG1	1:D:49:PRO:HD2	2.43	0.48
1:B:88:THR:HG23	1:B:314:GLY:HA2	1.94	0.48
1:D:178:ASP:O	1:D:182:VAL:HG23	2.13	0.47
1:A:446:PHE:HA	1:A:450:VAL:HG23	1.96	0.47
1:B:446:PHE:O	1:B:451:LEU:HD12	2.14	0.47
1:A:458:ARG:HB2	1:A:458:ARG:HE	1.58	0.47
1:B:156:ARG:NH2	1:B:437:ASP:HB2	2.29	0.47
1:A:312:PRO:HD3	3:A:662:HOH:O	2.14	0.47
1:C:193:LEU:HD13	1:C:485:VAL:CG2	2.44	0.47
1:A:486:HIS:CD2	1:A:488:ASP:HB2	2.50	0.47
1:C:152:ILE:HG23	1:C:302:VAL:HG12	1.95	0.47
1:A:446:PHE:O	1:A:450:VAL:HB	2.14	0.47
1:A:143:TRP:HA	1:A:338:ASN:O	2.14	0.47
1:B:130:ARG:HB2	1:B:149:ASN:ND2	2.29	0.47
1:A:161:PHE:HB3	1:A:162:PRO:HD3	1.94	0.47
1:D:403:ASN:N	1:D:403:ASN:HD22	2.04	0.47
1:A:174:THR:HB	1:A:176:LEU:CD1	2.45	0.47
1:B:40:ASN:ND2	1:C:433:ASN:HD22	2.03	0.47
1:C:135:LYS:HG3	1:C:144:ASP:OD2	2.15	0.47
1:A:152:ILE:HD13	1:A:194:HIS:CG	2.49	0.47
1:C:23:LYS:HE2	1:C:24:ALA:N	2.24	0.47
1:D:486:HIS:HB3	1:D:489:TYR:HB2	1.96	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:443:VAL:HG12	1:A:485:VAL:HG11	1.97	0.47
1:C:444:ARG:HH11	1:C:444:ARG:HB2	1.79	0.47
1:A:447:TYR:CE2	1:A:456:ARG:HG2	2.49	0.47
1:B:232:CYS:HA	1:B:282:GLN:O	2.15	0.47
1:B:75:HIS:O	1:B:112:ARG:NH2	2.48	0.47
1:D:295:ASN:HB3	1:D:298:ASP:HB2	1.97	0.47
1:C:51:LEU:H	1:C:51:LEU:HD23	1.80	0.47
1:B:275:PRO:HB2	1:B:277:TRP:HZ3	1.80	0.47
1:C:38:LYS:HE3	1:C:60:GLU:CD	2.35	0.47
1:D:380:ARG:HH11	1:D:380:ARG:HB3	1.79	0.47
1:D:130:ARG:HB2	1:D:149:ASN:ND2	2.30	0.47
1:D:19:ARG:HA	1:D:22:GLN:HG3	1.96	0.47
1:A:242:ILE:H	1:A:242:ILE:HD12	1.79	0.47
1:B:102:HIS:O	1:B:105:LYS:HB2	2.14	0.47
1:A:319:ASN:N	1:A:319:ASN:HD22	1.99	0.47
1:B:101:GLU:OE2	1:B:102:HIS:HD2	1.97	0.47
1:D:23:LYS:HE2	1:D:24:ALA:HB3	1.97	0.47
1:C:154:PHE:O	1:C:192:SER:HA	2.15	0.47
1:C:472:ILE:O	1:C:475:GLN:HB2	2.15	0.47
1:D:44:VAL:HG13	1:D:49:PRO:HD2	1.96	0.47
1:A:119:GLU:H	1:A:119:GLU:HG2	1.52	0.47
1:B:137:TYR:O	1:B:380:ARG:NH1	2.48	0.47
1:D:447:TYR:HA	1:D:451:LEU:CD1	2.45	0.47
1:D:210:ARG:HH21	1:D:264:ASP:CG	2.18	0.47
1:C:156:ARG:NH2	1:C:439:ASN:ND2	2.51	0.46
1:B:51:LEU:HD11	1:C:429:VAL:HG11	1.97	0.46
1:A:57:PHE:HD1	1:D:159:ILE:HD12	1.80	0.46
1:D:237:LYS:HG3	1:D:280:TYR:CE1	2.50	0.46
1:B:83:GLY:HA3	1:B:317:VAL:O	2.15	0.46
1:D:403:ASN:ND2	3:D:607:HOH:O	2.47	0.46
1:B:178:ASP:OD2	1:B:180:ASP:HB2	2.16	0.46
1:B:379:TYR:CE1	1:B:380:ARG:HG2	2.51	0.46
1:D:233:LYS:HG3	1:D:303:TRP:CE3	2.50	0.46
1:A:51:LEU:HD11	1:D:429:VAL:CG1	2.44	0.46
1:D:433:ASN:HD21	1:D:435:ALA:HB2	1.81	0.46
1:A:95:SER:HB2	1:A:222:LEU:HD22	1.97	0.46
1:B:210:ARG:HB3	1:B:240:GLN:HE21	1.81	0.46
1:D:102:HIS:NE2	1:D:105:LYS:HG3	2.29	0.46
1:B:472:ILE:O	1:B:476:LYS:HG2	2.15	0.46
1:C:284:MET:SD	1:C:289:ALA:HA	2.55	0.46
1:D:44:VAL:O	1:D:44:VAL:HG22	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:TYR:CD1	1:C:319:ASN:HA	2.51	0.46
1:C:325:TYR:CE1	1:C:329:VAL:HG11	2.51	0.46
1:A:51:LEU:HD11	1:D:429:VAL:HG11	1.98	0.46
1:B:214:GLY:HA3	1:B:236:TYR:CE2	2.51	0.46
1:A:178:ASP:CB	1:A:181:MET:HG3	2.36	0.46
1:D:139:GLU:HG3	1:D:380:ARG:HH12	1.81	0.46
1:A:63:HIS:HE1	1:C:388:ARG:O	1.98	0.46
1:B:446:PHE:O	1:B:450:VAL:HB	2.16	0.46
1:B:294:PHE:O	1:B:296:PRO:HD3	2.16	0.46
1:A:70:PRO:HG3	1:D:70:PRO:HD3	1.99	0.45
1:D:411:ALA:HB1	1:D:412:PRO:HD2	1.98	0.45
1:B:210:ARG:HD3	1:B:275:PRO:HG3	1.97	0.45
1:A:409:PHE:HA	1:C:16:LYS:HD2	1.98	0.45
1:D:288:GLN:HG2	1:D:288:GLN:H	1.48	0.45
1:B:348:ASP:O	1:B:352:GLN:HG2	2.16	0.45
1:B:347:PRO:HB3	1:C:47:ARG:O	2.15	0.45
1:D:110:ALA:HB3	1:D:135:LYS:HB3	1.99	0.45
1:C:339:MET:HE1	1:C:345:ALA:HB2	1.99	0.45
1:C:302:VAL:N	1:C:442:GLN:HE22	2.13	0.45
1:B:240:GLN:NE2	1:B:275:PRO:HB3	2.31	0.45
1:B:262:ILE:HG22	1:C:176:LEU:HD21	1.99	0.45
1:B:167:SER:HA	1:B:181:MET:CE	2.45	0.45
1:A:139:GLU:OE1	1:A:139:GLU:N	2.39	0.45
1:D:180:ASP:O	1:D:184:ASP:HB2	2.17	0.45
1:B:236:TYR:CD1	1:B:236:TYR:N	2.84	0.45
1:A:147:GLY:HA2	2:A:600:HEM:HBC1	1.98	0.45
1:A:273:LYS:HB2	1:A:273:LYS:HE3	1.82	0.45
1:B:18:GLN:NE2	1:B:19:ARG:HH21	2.15	0.45
1:C:359:PRO:O	1:C:363:ARG:HD2	2.16	0.45
1:A:444:ARG:O	1:A:448:VAL:HG23	2.16	0.45
1:D:193:LEU:HD11	1:D:481:ASN:HB3	1.99	0.45
1:D:472:ILE:O	1:D:476:LYS:HG2	2.17	0.45
1:B:72:ARG:HG2	2:B:600:HEM:CGA	2.46	0.45
1:A:379:TYR:CE1	1:A:380:ARG:HG2	2.52	0.45
1:A:40:ASN:ND2	1:D:433:ASN:HA	2.32	0.45
1:B:93:LYS:HD2	3:B:629:HOH:O	2.16	0.45
1:D:327:ALA:HA	1:D:331:GLN:HE21	1.81	0.45
1:D:452:ASN:O	1:D:456:ARG:HG3	2.16	0.45
1:B:386:TYR:CE1	1:B:405:TYR:HB2	2.51	0.45
1:B:425:TYR:CD2	1:C:49:PRO:HD3	2.53	0.44
1:D:433:ASN:HD22	1:D:434:THR:N	2.15	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:319:ASN:HD22	1:D:319:ASN:H	1.65	0.44
1:B:51:LEU:HD23	1:B:51:LEU:N	2.31	0.44
1:A:369:ASN:O	1:C:392:MET:HE1	2.17	0.44
1:A:222:LEU:HG	1:A:232:CYS:SG	2.58	0.44
1:A:472:ILE:HG22	1:A:473:PHE:N	2.31	0.44
1:B:221:LYS:HZ1	1:B:421:HIS:HB3	1.82	0.44
1:B:257:ASP:OD2	1:B:260:TYR:HA	2.16	0.44
1:B:72:ARG:NH1	1:B:112:ARG:NH1	2.65	0.44
1:B:73:VAL:HG13	1:B:74:VAL:HG22	1.99	0.44
1:B:38:LYS:HE3	1:B:60:GLU:OE1	2.16	0.44
1:C:461:GLU:HA	1:C:496:LEU:HD13	2.00	0.44
1:B:157:ASP:HA	1:B:158:PRO:HD2	1.82	0.44
1:C:285:THR:OG1	1:C:288:GLN:HG2	2.17	0.44
1:D:111:VAL:HG22	1:D:134:VAL:HG13	2.00	0.44
1:D:292:PHE:CD1	1:D:293:PRO:HD2	2.52	0.44
1:A:407:ASN:ND2	1:A:411:ALA:HB3	2.23	0.44
1:C:284:MET:CG	1:C:288:GLN:HG3	2.47	0.44
1:A:274:TYR:HA	1:A:275:PRO:HD3	1.90	0.44
1:B:173:GLN:NE2	1:C:323:VAL:HA	2.32	0.44
1:B:156:ARG:CZ	1:B:437:ASP:HB2	2.47	0.44
1:C:335:ASP:HB2	1:C:338:ASN:OD1	2.17	0.44
1:D:194:HIS:CE1	1:D:442:GLN:HE21	2.36	0.44
1:B:66:ARG:O	1:D:390:GLY:HA2	2.17	0.44
1:C:403:ASN:ND2	1:C:403:ASN:H	2.14	0.44
1:A:98:LYS:O	1:A:101:GLU:HB2	2.17	0.44
1:A:27:LEU:O	1:A:35:VAL:HG23	2.18	0.44
1:C:5:ARG:HD2	1:C:10:ASP:OD2	2.18	0.44
1:B:409:PHE:HA	1:D:16:LYS:HD2	2.00	0.44
1:D:170:ARG:NH2	3:D:602:HOH:O	2.39	0.44
1:B:262:ILE:CG2	1:C:176:LEU:HD21	2.48	0.44
1:A:159:ILE:HD12	1:D:57:PHE:HD1	1.82	0.44
1:D:269:ILE:HD12	1:D:321:ASN:ND2	2.33	0.43
1:C:156:ARG:NH2	1:C:437:ASP:H	2.15	0.43
1:B:148:ASN:CG	2:B:600:HEM:HAC	2.39	0.43
1:C:41:VAL:HG13	1:C:50:LEU:HD13	2.00	0.43
1:C:472:ILE:HG22	1:C:473:PHE:N	2.34	0.43
1:A:237:LYS:O	1:A:277:TRP:HA	2.17	0.43
1:D:102:HIS:O	1:D:105:LYS:HB2	2.18	0.43
1:B:239:ASP:OD2	1:B:276:SER:HB3	2.19	0.43
1:B:407:ASN:HD21	1:B:411:ALA:CB	2.16	0.43
1:A:486:HIS:HB3	1:A:489:TYR:HB2	1.99	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ALA:HB3	1:D:363:ARG:NH2	2.34	0.43
1:A:252:ARG:O	1:A:255:GLN:HG3	2.18	0.43
1:C:288:GLN:H	1:C:288:GLN:HG2	1.60	0.43
1:A:280:TYR:HB3	1:A:310:LEU:HB3	2.00	0.43
1:A:146:VAL:HB	1:A:354:ARG:HH22	1.82	0.43
1:B:382:ARG:HG3	1:B:382:ARG:O	2.18	0.43
1:D:84:TYR:CE1	1:D:106:LYS:HD3	2.54	0.43
1:A:301:LYS:HA	1:A:442:GLN:HE22	1.83	0.43
1:D:156:ARG:NH2	1:D:437:ASP:H	2.17	0.43
1:C:274:TYR:HA	1:C:275:PRO:HD3	1.91	0.43
1:D:280:TYR:HB3	1:D:310:LEU:HB3	2.00	0.43
1:B:419:LEU:HA	1:B:419:LEU:HD23	1.80	0.43
1:D:46:PRO:HD2	3:D:620:HOH:O	2.19	0.43
1:B:40:ASN:HD21	1:C:433:ASN:HA	1.83	0.43
1:A:465:GLY:O	1:A:468:LYS:HG2	2.18	0.43
1:B:333:ALA:HB1	1:B:362:HIS:CE1	2.54	0.43
1:D:326:PHE:HA	1:D:330:GLU:HB3	2.01	0.43
1:A:332:ILE:HD12	1:A:375:VAL:HB	2.01	0.43
1:B:194:HIS:HA	1:B:443:VAL:HG22	2.00	0.43
1:C:210:ARG:CD	1:C:275:PRO:HG3	2.49	0.43
1:A:451:LEU:HD22	1:A:455:GLN:HB3	2.00	0.43
1:D:259:ASP:HB3	1:D:262:ILE:HD12	2.01	0.43
1:D:127:ARG:HA	1:D:205:ILE:HG12	2.00	0.43
1:B:152:ILE:HG22	1:B:299:LEU:O	2.19	0.43
1:B:273:LYS:HB2	1:B:273:LYS:HE3	1.88	0.43
1:D:185:PHE:O	1:D:189:ARG:HG2	2.19	0.43
1:C:23:LYS:HE2	1:C:24:ALA:HB3	2.01	0.43
1:B:274:TYR:CD1	1:B:319:ASN:HA	2.54	0.43
1:A:108:PRO:HD2	1:A:380:ARG:NH1	2.34	0.43
1:A:155:ILE:HB	3:A:699:HOH:O	2.18	0.42
1:C:319:ASN:ND2	1:C:319:ASN:C	2.72	0.42
1:B:433:ASN:HA	1:C:40:ASN:HD21	1.82	0.42
1:D:213:ASN:OD1	1:D:238:THR:HG22	2.18	0.42
1:B:42:ILE:O	1:B:50:LEU:HD12	2.19	0.42
1:C:358:TYR:O	1:C:361:THR:HG22	2.19	0.42
1:A:137:TYR:O	1:A:380:ARG:NH1	2.52	0.42
1:B:275:PRO:HB2	1:B:277:TRP:CZ3	2.54	0.42
1:C:236:TYR:CD1	1:C:236:TYR:N	2.88	0.42
1:D:472:ILE:HG22	1:D:473:PHE:N	2.33	0.42
1:C:283:VAL:HG23	1:C:311:ILE:HD12	2.01	0.42
1:B:222:LEU:O	1:B:229:ALA:HA	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:ARG:HG3	2:B:600:HEM:HBB2	2.00	0.42
1:D:332:ILE:HG12	1:D:334:PHE:CE1	2.55	0.42
1:A:155:ILE:HG22	1:A:191:GLU:OE2	2.19	0.42
1:A:48:GLY:HA2	1:D:425:TYR:CE2	2.55	0.42
1:A:275:PRO:HB2	1:A:277:TRP:HZ3	1.85	0.42
1:B:332:ILE:HG12	1:B:334:PHE:CE1	2.55	0.42
1:A:319:ASN:ND2	1:A:319:ASN:N	2.68	0.42
1:D:382:ARG:CG	1:D:382:ARG:NH1	2.82	0.42
1:C:222:LEU:O	1:C:229:ALA:HA	2.18	0.42
1:B:274:TYR:HA	1:B:275:PRO:HD3	1.86	0.42
1:A:422:SER:OG	1:B:430:ARG:HB3	2.19	0.42
1:D:242:ILE:CD1	1:D:242:ILE:H	2.20	0.42
1:C:446:PHE:CE2	1:C:451:LEU:HD11	2.55	0.42
1:A:127:ARG:HA	1:A:205:ILE:HG12	2.01	0.42
1:B:161:PHE:O	1:B:162:PRO:C	2.58	0.42
1:A:363:ARG:HA	1:A:367:GLY:O	2.20	0.42
1:B:305:HIS:HD2	1:B:310:LEU:HG	1.84	0.42
1:B:382:ARG:CD	3:B:680:HOH:O	2.67	0.42
1:D:274:TYR:CD1	1:D:319:ASN:HA	2.55	0.42
1:D:480:LYS:O	1:D:484:GLU:HG3	2.20	0.42
1:B:7:PRO:HG2	1:B:267:ASN:OD1	2.20	0.42
1:B:458:ARG:HB2	1:B:458:ARG:HE	1.78	0.42
1:D:277:TRP:HB2	1:D:316:LEU:HB3	2.02	0.42
1:C:473:PHE:CZ	1:C:474:ILE:HG13	2.54	0.42
1:C:446:PHE:HA	1:C:450:VAL:HG21	2.01	0.42
1:D:472:ILE:N	3:D:667:HOH:O	2.52	0.42
1:C:127:ARG:HA	1:C:205:ILE:HG12	2.02	0.42
1:A:468:LYS:HD3	1:A:500:TYR:CD2	2.54	0.42
1:C:237:LYS:O	1:C:277:TRP:HA	2.19	0.42
1:B:394:MET:O	1:B:395:GLN:HB2	2.20	0.42
1:A:302:VAL:H	1:A:442:GLN:HE22	1.67	0.42
1:B:459:LEU:HD11	1:B:463:ILE:HD11	2.01	0.42
1:B:234:PHE:CD1	1:B:281:ILE:HG22	2.55	0.42
1:D:294:PHE:HB3	3:D:649:HOH:O	2.18	0.42
1:B:226:ASN:ND2	3:B:652:HOH:O	2.53	0.42
1:C:452:ASN:HA	1:C:456:ARG:NH2	2.32	0.41
1:C:305:HIS:HB2	1:C:306:LYS:HZ3	1.84	0.41
1:A:438:ASP:HA	3:A:680:HOH:O	2.20	0.41
1:A:259:ASP:HB3	1:D:176:LEU:HD23	2.02	0.41
1:C:451:LEU:HD22	1:C:455:GLN:HB3	2.01	0.41
1:C:79:ALA:O	1:C:112:ARG:HA	2.20	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:ASN:N	1:A:403:ASN:ND2	2.66	0.41
1:A:158:PRO:HD3	1:A:350:MET:HA	2.01	0.41
1:D:135:LYS:HG3	1:D:144:ASP:OD2	2.20	0.41
1:C:73:VAL:HG13	1:C:74:VAL:CG2	2.48	0.41
1:C:239:ASP:HB2	1:C:276:SER:HB3	2.01	0.41
1:A:239:ASP:HB2	1:A:276:SER:HB3	2.01	0.41
1:D:327:ALA:O	1:D:375:VAL:HG21	2.19	0.41
1:B:399:GLY:O	1:D:324:ASN:ND2	2.44	0.41
1:C:171:ASN:CG	1:C:172:PRO:HD2	2.41	0.41
1:D:339:MET:CE	1:D:345:ALA:HB2	2.51	0.41
1:D:306:LYS:H	1:D:306:LYS:HG2	1.53	0.41
1:A:66:ARG:HH12	1:D:360:ASP:CG	2.23	0.41
1:C:402:PRO:HB2	1:C:411:ALA:HB2	2.02	0.41
1:A:302:VAL:O	1:A:304:PRO:HD3	2.21	0.41
1:A:83:GLY:HA2	1:A:319:ASN:HD21	1.79	0.41
1:A:163:SER:HB3	1:B:405:TYR:H	1.86	0.41
1:C:221:LYS:HE3	1:C:421:HIS:CD2	2.55	0.41
1:D:388:ARG:O	1:D:389:ASP:HB2	2.21	0.41
1:A:473:PHE:CZ	1:A:474:ILE:HG13	2.56	0.41
1:A:286:PHE:O	1:A:289:ALA:HB3	2.21	0.41
1:C:119:GLU:H	1:C:119:GLU:HG2	1.42	0.41
1:D:252:ARG:HE	1:D:252:ARG:HB3	1.76	0.41
1:A:352:GLN:NE2	1:C:53:GLN:HE21	2.18	0.41
1:A:425:TYR:CE2	1:D:48:GLY:HA2	2.56	0.41
1:A:405:TYR:HA	1:A:406:PRO:HA	1.90	0.41
1:D:119:GLU:HG3	1:D:170:ARG:HH12	1.86	0.41
1:C:403:ASN:HD22	1:C:403:ASN:H	1.68	0.41
1:A:60:GLU:HG2	3:A:609:HOH:O	2.21	0.41
1:D:70:PRO:O	1:D:365:ARG:HG3	2.20	0.41
1:D:373:ILE:HG22	1:D:375:VAL:HG23	2.02	0.41
1:D:321:ASN:ND2	3:D:624:HOH:O	2.54	0.41
1:B:159:ILE:HD12	1:C:57:PHE:HD1	1.85	0.41
1:A:216:GLY:O	1:A:217:SER:HB2	2.20	0.41
1:A:85:PHE:O	1:A:106:LYS:HA	2.21	0.41
1:C:368:PRO:HG2	1:C:391:PRO:HG2	2.02	0.41
1:A:22:GLN:HG2	1:A:22:GLN:H	1.56	0.41
1:A:19:ARG:HA	1:A:22:GLN:HG3	2.02	0.41
1:B:431:ARG:HH11	1:B:431:ARG:HG2	1.86	0.41
1:C:284:MET:HG3	1:C:288:GLN:HG3	2.01	0.41
1:B:499:LYS:O	1:B:502:ALA:HB3	2.20	0.41
1:B:58:THR:O	1:B:59:ASP:C	2.59	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ASP:O	1:D:412:PRO:HA	2.21	0.40
1:A:433:ASN:HD21	1:A:435:ALA:HB2	1.85	0.40
1:A:352:GLN:HE22	1:C:53:GLN:HE21	1.68	0.40
1:D:389:ASP:HB3	1:D:390:GLY:H	1.72	0.40
1:B:127:ARG:HA	1:B:205:ILE:HG12	2.02	0.40
1:B:447:TYR:HA	1:B:451:LEU:HD12	2.03	0.40
1:C:157:ASP:HA	1:C:158:PRO:HD2	1.82	0.40
1:A:66:ARG:NH2	1:D:360:ASP:OD1	2.54	0.40
1:A:207:ASP:HA	1:A:245:LEU:HG	2.03	0.40
1:A:419:LEU:HD23	1:A:419:LEU:HA	1.88	0.40
3:A:694:HOH:O	1:B:172:PRO:HD2	2.19	0.40
1:A:40:ASN:HA	1:D:157:ASP:OD2	2.22	0.40
1:A:84:TYR:N	1:A:109:ILE:HG12	2.35	0.40
1:A:44:VAL:CG1	1:A:49:PRO:HD2	2.51	0.40
1:B:442:GLN:HB3	1:B:442:GLN:HE21	1.62	0.40
1:A:431:ARG:HB3	1:D:40:ASN:CB	2.50	0.40
1:C:194:HIS:CE1	1:C:442:GLN:HE21	2.38	0.40
1:B:224:ASN:O	1:B:226:ASN:N	2.55	0.40
1:C:216:GLY:O	1:C:217:SER:HB2	2.21	0.40
1:B:70:PRO:O	1:B:365:ARG:HG3	2.22	0.40
1:D:325:TYR:CE1	1:D:329:VAL:HG11	2.56	0.40
1:A:130:ARG:H	1:A:149:ASN:CG	2.25	0.40
1:B:39:LEU:HD21	1:D:405:TYR:CD2	2.56	0.40
1:C:237:LYS:H	1:C:237:LYS:HG2	1.63	0.40
1:B:315:LYS:HB2	1:B:315:LYS:HE2	1.90	0.40
1:C:22:GLN:HG2	1:C:22:GLN:H	1.66	0.40
1:A:73:VAL:HG13	1:A:74:VAL:HG22	2.03	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	497/527 (94%)	443 (89%)	51 (10%)	3 (1%)	30	62
1	B	498/527 (94%)	445 (89%)	48 (10%)	5 (1%)	19	48
1	C	497/527 (94%)	445 (90%)	47 (10%)	5 (1%)	19	48
1	D	497/527 (94%)	455 (92%)	39 (8%)	3 (1%)	30	62
All	All	1989/2108 (94%)	1788 (90%)	185 (9%)	16 (1%)	24	55

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	ALA
1	C	20	ALA
1	D	20	ALA
1	B	20	ALA
1	B	101	GLU
1	D	101	GLU
1	A	438	ASP
1	B	225	ALA
1	C	101	GLU
1	C	448	VAL
1	B	448	VAL
1	C	438	ASP
1	D	374	PRO
1	B	374	PRO
1	C	374	PRO
1	A	374	PRO

### 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	429/451 (95%)	358 (83%)	71 (17%)	3	7
1	B	429/451 (95%)	370 (86%)	59 (14%)	4	11
1	C	429/451 (95%)	366 (85%)	63 (15%)	4	10
1	D	429/451 (95%)	360 (84%)	69 (16%)	3	7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1716/1804 (95%)	1454 (85%)	262 (15%)	<b>3</b> <b>9</b>

All (262) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	16	LYS
1	A	17	GLU
1	A	19	ARG
1	A	22	GLN
1	A	23	LYS
1	A	38	LYS
1	A	41	VAL
1	A	44	VAL
1	A	51	LEU
1	A	74	VAL
1	A	77	LYS
1	A	93	LYS
1	A	95	SER
1	A	96	LYS
1	A	98	LYS
1	A	101	GLU
1	A	105	LYS
1	A	119	GLU
1	A	120	SER
1	A	126	VAL
1	A	130	ARG
1	A	132	PHE
1	A	138	THR
1	A	146	VAL
1	A	150	THR
1	A	152	ILE
1	A	156	ARG
1	A	159	ILE
1	A	160	LEU
1	A	163	SER
1	A	176	LEU
1	A	180	ASP
1	A	215	TYR
1	A	236	TYR
1	A	238	THR
1	A	242	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	245	LEU
1	A	252	ARG
1	A	255	GLN
1	A	256	GLU
1	A	263	ARG
1	A	273	LYS
1	A	281	ILE
1	A	288	GLN
1	A	290	GLU
1	A	306	LYS
1	A	315	LYS
1	A	319	ASN
1	A	332	ILE
1	A	337	SER
1	A	346	SER
1	A	375	VAL
1	A	382	ARG
1	A	394	MET
1	A	398	GLN
1	A	403	ASN
1	A	408	SER
1	A	422	SER
1	A	430	ARG
1	A	451	LEU
1	A	453	GLU
1	A	458	ARG
1	A	461	GLU
1	A	467	LEU
1	A	468	LYS
1	A	476	LYS
1	A	480	LYS
1	A	489	TYR
1	A	494	GLN
1	A	499	LYS
1	B	5	ARG
1	B	9	SER
1	B	17	GLU
1	B	19	ARG
1	B	22	GLN
1	B	23	LYS
1	B	28	THR
1	B	38	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	41	VAL
1	B	44	VAL
1	B	51	LEU
1	B	74	VAL
1	B	77	LYS
1	B	93	LYS
1	B	95	SER
1	B	101	GLU
1	B	119	GLU
1	B	126	VAL
1	B	127	ARG
1	B	130	ARG
1	B	132	PHE
1	B	150	THR
1	B	152	ILE
1	B	155	ILE
1	B	160	LEU
1	B	177	LYS
1	B	180	ASP
1	B	217	SER
1	B	232	CYS
1	B	236	TYR
1	B	238	THR
1	B	242	ILE
1	B	254	SER
1	B	273	LYS
1	B	276	SER
1	B	288	GLN
1	B	290	GLU
1	B	306	LYS
1	B	319	ASN
1	B	337	SER
1	B	375	VAL
1	B	394	MET
1	B	398	GLN
1	B	403	ASN
1	B	408	SER
1	B	422	SER
1	B	439	ASN
1	B	451	LEU
1	B	453	GLU
1	B	454	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	458	ARG
1	B	461	GLU
1	B	468	LYS
1	B	472	ILE
1	B	473	PHE
1	B	476	LYS
1	B	477	LYS
1	B	480	LYS
1	B	494	GLN
1	C	5	ARG
1	C	16	LYS
1	C	17	GLU
1	C	22	GLN
1	C	23	LYS
1	C	25	ASP
1	C	38	LYS
1	C	41	VAL
1	C	47	ARG
1	C	51	LEU
1	C	74	VAL
1	C	77	LYS
1	C	93	LYS
1	C	95	SER
1	C	98	LYS
1	C	101	GLU
1	C	105	LYS
1	C	112	ARG
1	C	119	GLU
1	C	127	ARG
1	C	128	ASP
1	C	132	PHE
1	C	134	VAL
1	C	150	THR
1	C	152	ILE
1	C	159	ILE
1	C	170	ARG
1	C	173	GLN
1	C	177	LYS
1	C	180	ASP
1	C	187	SER
1	C	197	SER
1	C	201	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	217	SER
1	C	236	TYR
1	C	237	LYS
1	C	238	THR
1	C	242	ILE
1	C	255	GLN
1	C	273	LYS
1	C	276	SER
1	C	288	GLN
1	C	306	LYS
1	C	319	ASN
1	C	337	SER
1	C	346	SER
1	C	375	VAL
1	C	382	ARG
1	C	394	MET
1	C	398	GLN
1	C	403	ASN
1	C	408	SER
1	C	419	LEU
1	C	422	SER
1	C	430	ARG
1	C	451	LEU
1	C	453	GLU
1	C	456	ARG
1	C	458	ARG
1	C	461	GLU
1	C	489	TYR
1	C	494	GLN
1	C	499	LYS
1	D	5	ARG
1	D	17	GLU
1	D	22	GLN
1	D	23	LYS
1	D	25	ASP
1	D	38	LYS
1	D	41	VAL
1	D	44	VAL
1	D	51	LEU
1	D	74	VAL
1	D	77	LYS
1	D	93	LYS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	D	101	GLU
1	D	119	GLU
1	D	130	ARG
1	D	132	PHE
1	D	135	LYS
1	D	138	THR
1	D	146	VAL
1	D	150	THR
1	D	152	ILE
1	D	155	ILE
1	D	159	ILE
1	D	176	LEU
1	D	177	LYS
1	D	187	SER
1	D	228	GLU
1	D	236	TYR
1	D	237	LYS
1	D	238	THR
1	D	240	GLN
1	D	242	ILE
1	D	255	GLN
1	D	273	LYS
1	D	276	SER
1	D	281	ILE
1	D	288	GLN
1	D	290	GLU
1	D	302	VAL
1	D	306	LYS
1	D	319	ASN
1	D	337	SER
1	D	346	SER
1	D	354	ARG
1	D	375	VAL
1	D	377	CYS
1	D	380	ARG
1	D	382	ARG
1	D	394	MET
1	D	395	GLN
1	D	403	ASN
1	D	408	SER
1	D	417	SER
1	D	419	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	422	SER
1	D	424	GLN
1	D	430	ARG
1	D	433	ASN
1	D	436	ASN
1	D	444	ARG
1	D	451	LEU
1	D	453	GLU
1	D	458	ARG
1	D	468	LYS
1	D	476	LYS
1	D	477	LYS
1	D	480	LYS
1	D	489	TYR
1	D	494	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	18	GLN
1	A	22	GLN
1	A	33	ASN
1	A	226	ASN
1	A	287	ASN
1	A	319	ASN
1	A	321	ASN
1	A	338	ASN
1	A	362	HIS
1	A	403	ASN
1	A	415	GLN
1	A	421	HIS
1	A	433	ASN
1	A	439	ASN
1	A	442	GLN
1	A	471	GLN
1	A	475	GLN
1	A	486	HIS
1	A	492	HIS
1	B	13	GLN
1	B	18	GLN
1	B	22	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	40	ASN
1	B	102	HIS
1	B	194	HIS
1	B	226	ASN
1	B	240	GLN
1	B	287	ASN
1	B	319	ASN
1	B	321	ASN
1	B	331	GLN
1	B	338	ASN
1	B	403	ASN
1	B	421	HIS
1	B	433	ASN
1	B	436	ASN
1	B	439	ASN
1	B	442	GLN
1	B	475	GLN
1	B	486	HIS
1	C	13	GLN
1	C	18	GLN
1	C	40	ASN
1	C	53	GLN
1	C	194	HIS
1	C	287	ASN
1	C	319	ASN
1	C	321	ASN
1	C	338	ASN
1	C	421	HIS
1	C	439	ASN
1	C	442	GLN
1	C	471	GLN
1	C	475	GLN
1	C	486	HIS
1	C	492	HIS
1	D	13	GLN
1	D	14	HIS
1	D	18	GLN
1	D	33	ASN
1	D	40	ASN
1	D	53	GLN
1	D	148	ASN
1	D	194	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	305	HIS
1	D	319	ASN
1	D	321	ASN
1	D	338	ASN
1	D	403	ASN
1	D	421	HIS
1	D	433	ASN
1	D	439	ASN
1	D	442	GLN
1	D	471	GLN
1	D	475	GLN
1	D	481	ASN
1	D	486	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

4 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	600	1	30,50,50	2.70	10 (33%)	24,82,82	1.99	6 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	HEM	B	600	1	30,50,50	2.82	10 (33%)	24,82,82	2.01	6 (25%)
2	HEM	C	600	1	30,50,50	2.59	9 (30%)	24,82,82	2.05	6 (25%)
2	HEM	D	600	1	30,50,50	2.81	10 (33%)	24,82,82	2.05	7 (29%)

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	600	1	-	0/10/54/54	0/0/8/8
2	HEM	B	600	1	-	0/10/54/54	0/0/8/8
2	HEM	C	600	1	-	0/10/54/54	0/0/8/8
2	HEM	D	600	1	-	0/10/54/54	0/0/8/8

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	HEM	C3B-C4B	-7.11	1.45	1.51
2	B	600	HEM	C2D-C3D	-6.65	1.34	1.54
2	C	600	HEM	C2D-C3D	-6.39	1.35	1.54
2	B	600	HEM	C3C-CAC	-6.08	1.39	1.51
2	A	600	HEM	C2D-C3D	-6.07	1.36	1.54
2	D	600	HEM	C2D-C3D	-6.04	1.36	1.54
2	C	600	HEM	C3B-CAB	-5.87	1.40	1.51
2	B	600	HEM	C3B-CAB	-5.86	1.40	1.51
2	A	600	HEM	C3C-CAC	-5.86	1.40	1.51
2	B	600	HEM	C3B-C4B	-5.80	1.46	1.51
2	C	600	HEM	C3C-CAC	-5.77	1.40	1.51
2	D	600	HEM	C3B-CAB	-5.75	1.40	1.51
2	A	600	HEM	C3B-CAB	-5.45	1.41	1.51
2	A	600	HEM	C3B-C4B	-5.25	1.47	1.51
2	D	600	HEM	C3C-CAC	-5.13	1.41	1.51
2	C	600	HEM	C3B-C4B	-4.81	1.47	1.51
2	B	600	HEM	C3D-C4D	-4.64	1.45	1.51
2	D	600	HEM	C2C-C1C	-4.47	1.44	1.52
2	A	600	HEM	C3D-C4D	-4.44	1.45	1.51
2	B	600	HEM	C2C-C1C	-4.25	1.44	1.52
2	C	600	HEM	C2C-C1C	-4.07	1.44	1.52
2	D	600	HEM	C3D-C4D	-4.05	1.46	1.51
2	A	600	HEM	C2C-C1C	-4.04	1.44	1.52
2	C	600	HEM	C3D-C4D	-3.80	1.46	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	600	HEM	C4C-NC	2.63	1.39	1.36
2	B	600	HEM	CBB-CAB	2.74	1.45	1.29
2	C	600	HEM	CBB-CAB	2.86	1.45	1.29
2	A	600	HEM	CBC-CAC	2.91	1.46	1.29
2	B	600	HEM	CBC-CAC	2.92	1.46	1.29
2	D	600	HEM	C1C-NC	2.99	1.39	1.36
2	B	600	HEM	C1C-NC	3.00	1.39	1.36
2	D	600	HEM	CBB-CAB	3.11	1.47	1.29
2	A	600	HEM	CBB-CAB	3.14	1.47	1.29
2	C	600	HEM	CBC-CAC	3.15	1.47	1.29
2	D	600	HEM	CBC-CAC	3.26	1.48	1.29
2	A	600	HEM	C1C-NC	3.27	1.40	1.36
2	D	600	HEM	C4C-NC	3.30	1.40	1.36
2	A	600	HEM	C4C-NC	3.48	1.40	1.36
2	B	600	HEM	C4C-NC	3.59	1.40	1.36

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	600	HEM	CAA-C2A-C1A	2.25	129.45	127.01
2	B	600	HEM	CMD-C2D-C3D	2.31	124.57	114.35
2	A	600	HEM	CMD-C2D-C3D	2.55	125.61	114.35
2	D	600	HEM	CMD-C2D-C3D	2.57	125.72	114.35
2	D	600	HEM	C2D-C3D-C4D	2.61	105.92	101.50
2	A	600	HEM	C2D-C3D-C4D	2.74	106.14	101.50
2	C	600	HEM	CMD-C2D-C3D	2.80	126.73	114.35
2	C	600	HEM	C2D-C3D-C4D	3.00	106.58	101.50
2	B	600	HEM	C2D-C3D-C4D	3.01	106.60	101.50
2	C	600	HEM	CMB-C2B-C3B	3.24	124.63	116.53
2	D	600	HEM	CMB-C2B-C3B	3.74	125.87	116.53
2	B	600	HEM	CMC-C2C-C3C	3.78	125.97	116.53
2	A	600	HEM	CMC-C2C-C3C	3.85	126.15	116.53
2	A	600	HEM	CMB-C2B-C3B	3.90	126.26	116.53
2	B	600	HEM	CMB-C2B-C3B	3.93	126.34	116.53
2	D	600	HEM	CMC-C2C-C3C	3.96	126.43	116.53
2	B	600	HEM	CAD-C3D-C4D	4.09	126.91	112.47
2	C	600	HEM	CAD-C3D-C4D	4.25	127.47	112.47
2	A	600	HEM	CAD-C3D-C4D	4.32	127.72	112.47
2	D	600	HEM	CAD-C3D-C4D	4.35	127.82	112.47
2	C	600	HEM	CAD-C3D-C2D	4.39	125.85	113.22
2	A	600	HEM	CAD-C3D-C2D	4.42	125.92	113.22
2	C	600	HEM	CMC-C2C-C3C	4.49	127.75	116.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	D	600	HEM	CAD-C3D-C2D	4.53	126.24	113.22
2	B	600	HEM	CAD-C3D-C2D	4.61	126.47	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	HEM	2	0
2	B	600	HEM	3	0
2	C	600	HEM	2	0
2	D	600	HEM	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	499/527 (94%)	0.29	2 (0%) 93 92	10, 13, 14, 15	0
1	B	500/527 (94%)	0.28	2 (0%) 93 92	10, 12, 14, 15	0
1	C	499/527 (94%)	0.34	4 (0%) 87 83	10, 13, 14, 16	0
1	D	499/527 (94%)	0.32	3 (0%) 90 88	11, 13, 14, 16	0
All	All	1997/2108 (94%)	0.30	11 (0%) 90 88	10, 13, 14, 16	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	21	ALA	7.5
1	B	21	ALA	4.5
1	D	20	ALA	4.4
1	C	21	ALA	3.4
1	C	451	LEU	2.9
1	C	102	HIS	2.9
1	A	21	ALA	2.8
1	B	447	TYR	2.2
1	A	111	VAL	2.1
1	C	485	VAL	2.1
1	D	52	VAL	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

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	HEM	A	600	43/43	0.90	0.23	1.58	10,13,14,15	0
2	HEM	C	600	43/43	0.91	0.23	0.88	11,12,13,14	0
2	HEM	B	600	43/43	0.89	0.22	0.84	12,13,15,15	0
2	HEM	D	600	43/43	0.90	0.21	0.41	12,13,14,15	0

## 6.5 Other polymers

There are no such residues in this entry.