Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 07:39 PM GMT

PDB ID	:	4UYM
Title	:	Crystal structure of sterol 14-alpha demethylase (CYP51B) from a pathogenic filamentous fungus Aspergillus fumigatus in complex with voriconazole
Authors	:	Hargrove, T.Y.; Wawrzak, Z.; Lepesheva, G.I.
Deposited on	:	2014-09-02
Resolution	:	2.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

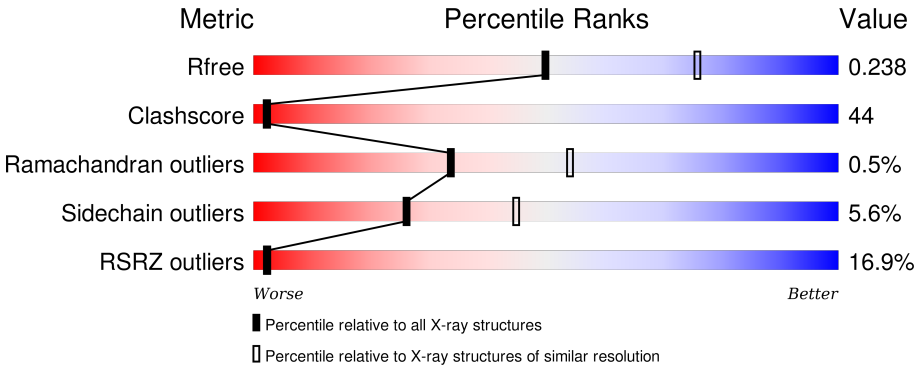
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

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 2.55 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}	91344	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	470	14% 53% 42% 6%
1	B	470	20% 53% 43% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7803 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.

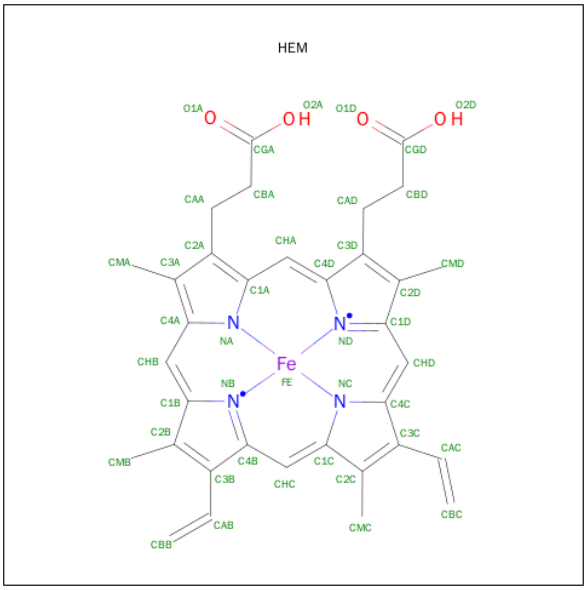
- Molecule 1 is a protein called 14-ALPHA STEROL DEMETHYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	0	0
			3752	2411	639	685	17			
1	B	470	Total	C	N	O	S	0	0	0
			3752	2411	639	685	17			

There are 6 discrepancies between the modelled and reference sequences:

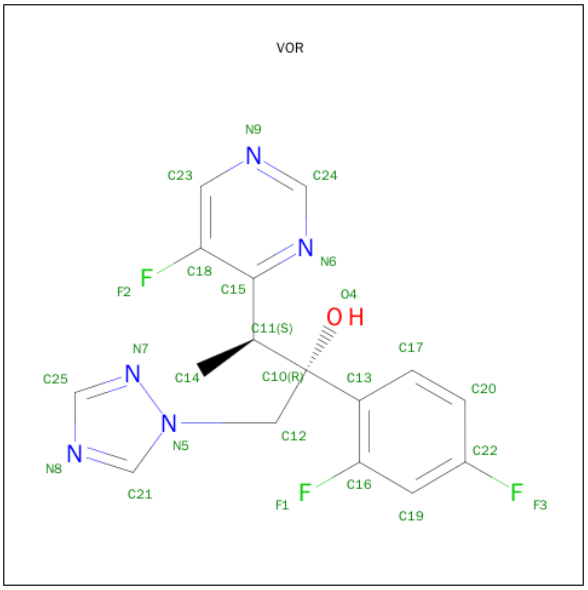
Chain	Residue	Modelled	Actual	Comment	Reference
A	50	LYS	HIS	ENGINEERED MUTATION	UNP Q96W81
A	51	THR	GLU	ENGINEERED MUTATION	UNP Q96W81
A	519	HIS	-	EXPRESSION TAG	UNP Q96W81
B	50	LYS	HIS	ENGINEERED MUTATION	UNP Q96W81
B	51	THR	GLU	ENGINEERED MUTATION	UNP Q96W81
B	519	HIS	-	EXPRESSION TAG	UNP Q96W81

- 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		

- Molecule 3 is VORICONAZOLE (three-letter code: VOR) (formula: $C_{16}H_{14}F_3N_5O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			25	16	3	5	1		
3	B	1	Total	C	F	N	O	0	0
			25	16	3	5	1		

- Molecule 4 is water.

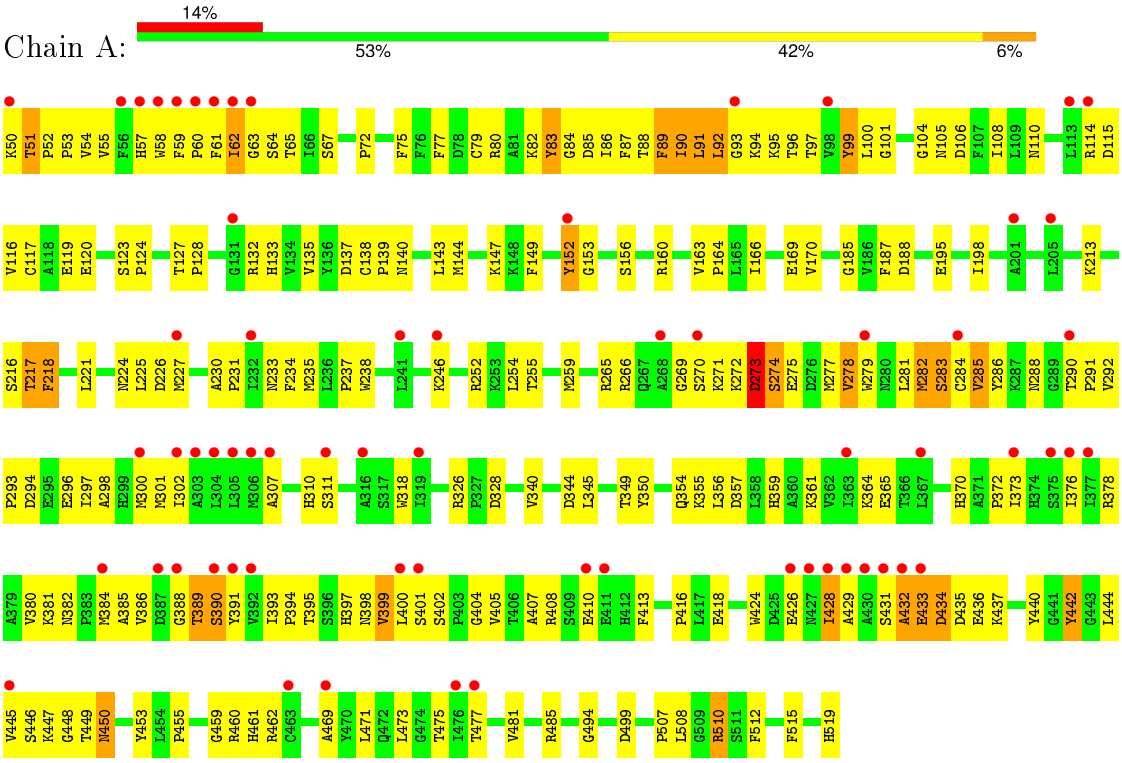
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	87	Total	O	0	0
			87	87		
4	B	76	Total	O	0	0
			76	76		

3 Residue-property plots (i)

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

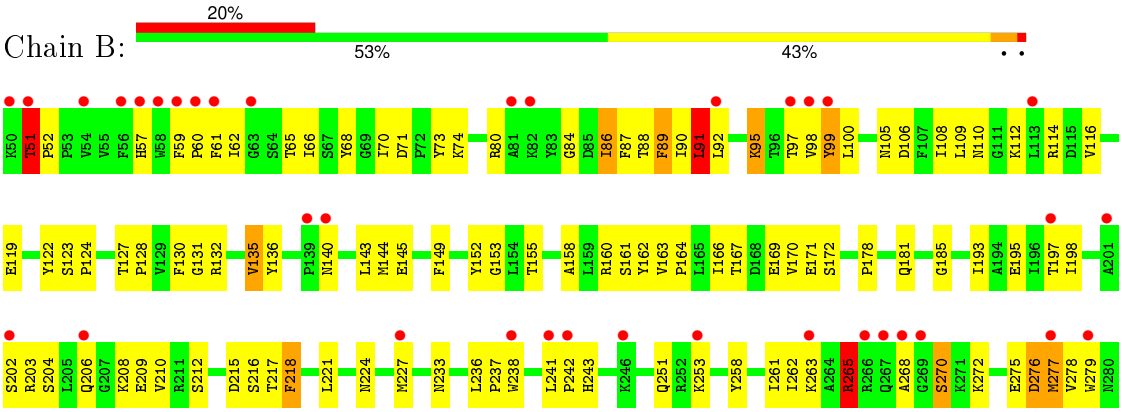
- Molecule 1: 14-ALPHA STEROL DEMETHYLASE

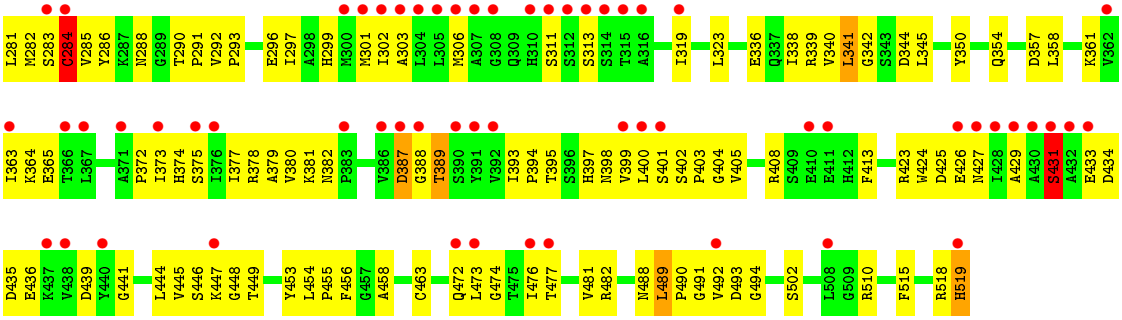
Chain A:



- Molecule 1: 14-ALPHA STEROL DEMETHYLASE

Chain B:




L281 M282 S283 C284 V285 Y286 K287 N288 G289 T290 P291 V292 P293 E296 I297 A298 H299 M300 M301 I302 A303 L304 L305 M306 A307 G308 Q309 H310 S311 S312 S313 S314 T315 A316 I319 L323 E336 Q337 I338 R339 V340 L341 G342 S343 D344 L345 Y350 Q354 D357 L358 K361 V362
I363 K364 E365 T366 L367 A371 P372 I373 H374 S375 I376 I377 R378 A379 V380 K381 N382 P383 V386 D387 G388 T389 S390 Y391 V392 I393 P394 T395 S396 H397 N398 V399 L400 S401 S402 P403 G404 V405 R408 S409 E410 E411 H412 F413 R423 W424 D425 E426 N427 I428 A429 A430 S431 A432 E433 D434
D435 E436 K437 V438 D439 Y440 G441 L444 V445 S446 K447 G448 T449 Y453 L454 P455 F456 G457 A458 C463 Q472 L473 G474 T475 I476 T477 V481 R482 N488 L489 P490 G491 V492 D493 G494 S502 L508 G509 R510 F515 R518 H519

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	109.19Å 109.19Å 90.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.55 28.01 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.00-2.55) 99.4 (28.01-2.55)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.210 , 0.239 0.217 , 0.238	Depositor DCC
R_{free} test set	1905 reflections (5.16%)	DCC
Wilson B-factor (Å^2)	68.3	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 76.1	EDS
Estimated twinning fraction	0.013 for -h,-k,l 0.035 for h,-h-k,-l 0.016 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 38824 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7803	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.44	0/3854	0.62	5/5229 (0.1%)
1	B	0.35	0/3854	0.62	7/5229 (0.1%)
All	All	0.40	0/7708	0.62	12/10458 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	2
All	All	0	7

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	265	ARG	NE-CZ-NH2	-15.10	112.75	120.30
1	B	265	ARG	NE-CZ-NH1	13.17	126.89	120.30
1	A	217	THR	CB-CA-C	-6.00	95.41	111.60
1	A	89	PHE	N-CA-C	-5.84	95.23	111.00
1	B	89	PHE	N-CA-C	-5.47	96.24	111.00
1	B	95	LYS	N-CA-C	-5.47	96.24	111.00
1	B	284	CYS	N-CA-C	-5.44	96.32	111.00
1	B	90	ILE	CB-CA-C	-5.27	101.07	111.60
1	B	91	LEU	N-CA-C	-5.27	96.78	111.00
1	A	442	TYR	N-CA-C	-5.24	96.86	111.00
1	A	285	VAL	N-CA-C	5.17	124.97	111.00
1	A	273	ASP	C-N-CA	5.03	134.27	121.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	273	ASP	Peptide
1	A	388	GLY	Peptide
1	A	432	ALA	Peptide
1	A	485	ARG	Sidechain
1	A	93	GLY	Peptide
1	B	270	SER	Peptide
1	B	431	SER	Peptide

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	3752	0	3719	357	0
1	B	3752	0	3719	290	0
2	A	43	0	30	5	0
2	B	43	0	30	8	0
3	A	25	0	14	4	0
3	B	25	0	14	6	0
4	A	87	0	0	11	0
4	B	76	0	0	12	0
All	All	7803	0	7526	660	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 44.

All (660) 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:265:ARG:NH1	1:A:277:MET:HG3	1.33	1.43
1:B:152:TYR:HB3	1:B:279:TRP:CZ2	1.69	1.25
1:B:262:ILE:HG12	1:B:277:MET:CE	1.74	1.17
1:B:224:ASN:HA	1:B:227:MET:HE2	1.18	1.15
1:A:86:ILE:HD11	1:A:99:TYR:CD1	1.81	1.15
1:B:262:ILE:HG12	1:B:277:MET:HE1	1.25	1.14

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:THR:OG1	1:A:52:PRO:HD3	1.48	1.13
1:B:519:HIS:HA	4:B:2076:HOH:O	1.46	1.12
1:A:94:LYS:HE3	1:A:398:ASN:ND2	1.65	1.11
1:A:65:THR:HG22	1:A:91:LEU:HA	1.19	1.10
1:A:55:VAL:HG13	1:A:88:THR:O	1.51	1.09
1:B:106:ASP:HB2	1:B:449:THR:HG21	1.29	1.09
1:B:51:THR:HB	1:B:52:PRO:CD	1.85	1.07
1:A:284:CYS:O	1:A:292:VAL:HG23	1.56	1.06
1:A:275:GLU:HG3	1:A:277:MET:HB3	1.36	1.05
1:A:59:PHE:CD1	1:A:60:PRO:HD2	1.91	1.04
1:B:284:CYS:O	1:B:292:VAL:HG23	1.57	1.04
1:B:152:TYR:HB3	1:B:279:TRP:CE2	1.92	1.04
1:A:90:ILE:HD12	1:A:90:ILE:H	1.20	1.02
1:A:265:ARG:HH12	1:A:277:MET:HG3	1.23	1.02
1:B:493:ASP:OD1	1:B:494:GLY:N	1.92	1.02
1:A:50:LYS:O	1:A:51:THR:HG22	1.58	1.01
1:B:152:TYR:HB3	1:B:279:TRP:HZ2	1.26	1.01
1:A:90:ILE:HG22	1:A:95:LYS:HA	1.38	1.01
1:A:110:ASN:OD1	1:A:447:LYS:HB2	1.61	1.01
1:A:51:THR:OG1	1:A:52:PRO:CD	2.07	1.01
1:A:152:TYR:HB3	1:A:279:TRP:CZ2	1.97	1.00
1:A:217:THR:O	1:A:217:THR:HG22	1.62	0.99
1:A:59:PHE:CD2	1:A:62:ILE:HG12	1.98	0.99
1:A:265:ARG:NH1	1:A:277:MET:CG	2.24	0.98
1:B:106:ASP:CB	1:B:449:THR:HG21	1.93	0.98
1:A:53:PRO:HD3	1:A:391:TYR:CE1	1.98	0.98
1:B:209:GLU:OE1	1:B:209:GLU:N	1.97	0.97
1:A:55:VAL:HG21	1:A:89:PHE:CB	1.96	0.96
1:B:473:LEU:O	1:B:477:THR:HG23	1.64	0.96
1:A:65:THR:HG21	1:A:92:LEU:H	1.31	0.96
1:B:106:ASP:HB2	1:B:449:THR:CG2	1.96	0.94
1:B:95:LYS:HD3	1:B:397:HIS:NE2	1.83	0.94
1:B:65:THR:OG1	1:B:92:LEU:HD21	1.67	0.94
1:A:90:ILE:CG2	1:A:95:LYS:HA	1.98	0.94
1:B:51:THR:HB	1:B:52:PRO:HD2	1.48	0.93
1:A:51:THR:O	1:A:391:TYR:HD1	1.52	0.93
1:A:119:GLU:OE1	1:A:119:GLU:N	2.03	0.92
1:A:216:SER:O	1:A:217:THR:HB	1.69	0.92
1:B:224:ASN:CA	1:B:227:MET:HE2	1.99	0.91
1:A:114:ARG:NE	1:A:115:ASP:OD1	2.03	0.91
1:A:59:PHE:CG	1:A:60:PRO:HD2	2.05	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:TYR:CB	1:B:279:TRP:HE1	1.84	0.90
1:A:361:LYS:NZ	1:A:428:ILE:HG22	1.86	0.90
1:B:224:ASN:HA	1:B:227:MET:CE	2.01	0.89
1:A:124:PRO:O	1:A:128:PRO:CD	2.21	0.89
1:A:55:VAL:CG2	1:A:89:PHE:HA	2.03	0.88
1:B:153:GLY:N	1:B:279:TRP:NE1	2.21	0.88
1:A:55:VAL:HG22	1:A:88:THR:O	1.72	0.88
1:B:265:ARG:CZ	1:B:275:GLU:OE2	2.22	0.87
1:A:413:PHE:O	1:A:416:PRO:HG3	1.73	0.87
1:A:152:TYR:HB3	1:A:279:TRP:HZ2	1.38	0.86
1:B:152:TYR:CB	1:B:279:TRP:CZ2	2.58	0.86
1:A:51:THR:O	1:A:391:TYR:CD1	2.28	0.86
1:A:55:VAL:CG1	1:A:88:THR:O	2.23	0.86
1:A:188:ASP:OD2	1:A:510:ARG:HD3	1.74	0.86
1:A:62:ILE:O	1:A:65:THR:HG23	1.75	0.86
1:A:59:PHE:CE2	1:A:62:ILE:HG23	2.11	0.85
1:A:59:PHE:HD2	1:A:62:ILE:HG12	1.37	0.85
1:A:65:THR:HG22	1:A:91:LEU:CA	2.06	0.85
1:B:95:LYS:CD	1:B:397:HIS:NE2	2.39	0.85
1:A:115:ASP:HB3	1:A:384:MET:CE	2.06	0.84
1:B:149:PHE:O	1:B:152:TYR:HB2	1.76	0.84
1:A:433:GLU:HG2	1:A:434:ASP:H	1.41	0.84
1:B:152:TYR:HB2	1:B:279:TRP:HE1	1.40	0.84
1:A:124:PRO:O	1:A:128:PRO:HD3	1.77	0.84
1:A:53:PRO:HD3	1:A:391:TYR:HE1	1.42	0.84
1:A:90:ILE:HG22	1:A:95:LYS:CA	2.07	0.84
1:A:224:ASN:HA	1:A:227:MET:HE2	1.60	0.83
1:A:92:LEU:HD12	1:A:235:MET:HE2	1.60	0.83
1:B:262:ILE:CG1	1:B:277:MET:HE1	2.08	0.83
1:B:158:ALA:O	1:B:161:SER:HB3	1.79	0.82
1:B:106:ASP:CA	1:B:449:THR:HG21	2.09	0.82
1:B:95:LYS:HD2	1:B:397:HIS:CD2	2.15	0.81
1:A:217:THR:O	1:A:217:THR:CG2	2.28	0.81
1:A:51:THR:HG23	1:A:52:PRO:N	1.96	0.81
1:A:94:LYS:HE3	1:A:398:ASN:HD21	1.44	0.81
1:A:85:ASP:O	1:A:86:ILE:HD13	1.79	0.81
1:A:361:LYS:HZ3	1:A:428:ILE:HG22	1.45	0.81
1:B:152:TYR:CB	1:B:279:TRP:NE1	2.44	0.80
1:B:210:VAL:HG13	1:B:218:PHE:CE2	2.16	0.80
1:B:262:ILE:HG12	1:B:277:MET:HE2	1.61	0.80
1:A:284:CYS:HB2	1:A:291:PRO:HB3	1.64	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:LYS:HB2	1:A:83:TYR:CD1	2.18	0.79
1:A:97:THR:HG1	1:A:397:HIS:HD1	1.29	0.79
1:A:50:LYS:O	1:A:51:THR:CG2	2.30	0.79
1:B:51:THR:CB	1:B:52:PRO:CD	2.61	0.78
1:A:216:SER:O	1:A:217:THR:CB	2.32	0.78
1:B:65:THR:CB	1:B:92:LEU:HD21	2.14	0.77
1:B:66:ILE:O	1:B:70:ILE:HG12	1.85	0.77
1:A:82:LYS:HB2	1:A:83:TYR:CE1	2.20	0.77
1:B:152:TYR:HB3	1:B:279:TRP:NE1	2.00	0.76
1:A:195:GLU:O	1:A:198:ILE:HG22	1.85	0.76
1:A:59:PHE:CE1	1:A:60:PRO:HD2	2.20	0.76
1:A:65:THR:CG2	1:A:91:LEU:HA	2.08	0.76
1:A:91:LEU:O	1:A:91:LEU:HD12	1.85	0.76
1:A:326:ARG:NH2	1:A:328:ASP:OD2	2.19	0.76
1:A:275:GLU:CG	1:A:277:MET:HB3	2.16	0.75
1:B:210:VAL:HG13	1:B:218:PHE:HE2	1.51	0.75
1:A:447:LYS:HA	1:A:459:GLY:H	1.51	0.74
1:B:209:GLU:OE2	1:B:265:ARG:NH2	2.20	0.74
1:A:404:GLY:O	1:A:407:ALA:HB3	1.88	0.74
1:A:97:THR:OG1	1:A:397:HIS:ND1	2.18	0.74
1:B:444:LEU:O	1:B:445:VAL:HG13	1.87	0.74
1:A:79:CYS:HB3	1:A:87:PHE:CZ	2.22	0.74
1:A:55:VAL:HG21	1:A:89:PHE:CA	2.17	0.74
1:B:195:GLU:O	1:B:198:ILE:HG22	1.88	0.74
1:A:59:PHE:CD2	1:A:62:ILE:HG23	2.23	0.73
1:B:152:TYR:C	1:B:279:TRP:CE2	2.62	0.73
1:A:86:ILE:CD1	1:A:99:TYR:CD1	2.67	0.73
1:B:106:ASP:OD1	1:B:110:ASN:ND2	2.21	0.73
1:B:388:GLY:O	1:B:389:THR:HG23	1.87	0.73
1:A:429:ALA:HB1	1:A:431:SER:O	1.89	0.73
1:B:152:TYR:CB	1:B:279:TRP:HZ2	1.96	0.73
1:A:55:VAL:CG2	1:A:88:THR:O	2.37	0.73
1:A:266:ARG:NH2	1:A:294:ASP:OD2	2.21	0.73
1:A:432:ALA:HB1	1:A:433:GLU:HB2	1.69	0.73
1:A:86:ILE:HD11	1:A:99:TYR:CG	2.24	0.72
1:A:55:VAL:HG21	1:A:89:PHE:HB3	1.68	0.72
1:A:357:ASP:OD2	1:A:361:LYS:HE2	1.88	0.72
1:B:381:LYS:O	1:B:382:ASN:OD1	2.08	0.72
1:B:152:TYR:O	1:B:279:TRP:CZ2	2.42	0.72
1:A:90:ILE:N	1:A:90:ILE:HD12	1.99	0.72
1:B:65:THR:HB	1:B:92:LEU:CD2	2.19	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:GLU:O	1:A:300:MET:HG3	1.90	0.71
1:B:98:VAL:CG1	1:B:100:LEU:HD21	2.20	0.71
1:A:361:LYS:NZ	1:A:428:ILE:CG2	2.52	0.71
1:A:435:ASP:HB2	1:A:448:GLY:HA3	1.71	0.71
1:A:55:VAL:HG21	1:A:89:PHE:HA	1.71	0.71
1:A:51:THR:CB	1:A:52:PRO:CD	2.69	0.71
1:A:365:GLU:OE1	1:A:365:GLU:HA	1.90	0.71
1:B:275:GLU:HG3	1:B:277:MET:HB3	1.71	0.71
1:A:277:MET:HA	1:A:277:MET:CE	2.21	0.70
3:B:590:VOR:C21	3:B:590:VOR:C17	2.69	0.70
1:A:86:ILE:CD1	1:A:99:TYR:HA	2.21	0.70
1:B:444:LEU:O	1:B:445:VAL:CG1	2.39	0.70
1:B:288:ASN:ND2	1:B:290:THR:OG1	2.25	0.70
1:A:255:THR:O	1:A:259:MET:HG3	1.92	0.70
1:A:277:MET:HE2	1:A:277:MET:HA	1.73	0.70
1:A:90:ILE:HG22	1:A:94:LYS:O	1.91	0.70
1:A:55:VAL:HG22	1:A:89:PHE:HA	1.73	0.70
1:B:268:ALA:HB1	4:B:2039:HOH:O	1.92	0.69
1:A:51:THR:HG23	1:A:52:PRO:CD	2.23	0.69
1:A:435:ASP:CB	1:A:448:GLY:HA3	2.22	0.69
1:B:65:THR:CB	1:B:92:LEU:CD2	2.70	0.69
1:B:463:CYS:HB2	2:B:580:HEM:NA	2.06	0.69
1:B:209:GLU:HB2	1:B:261:ILE:HD13	1.75	0.69
1:A:442:TYR:CE2	1:A:445:VAL:HG11	2.28	0.69
1:B:400:LEU:HD23	1:B:401:SER:N	2.08	0.69
1:B:265:ARG:NH2	1:B:275:GLU:OE2	2.26	0.69
1:A:114:ARG:HG3	1:A:115:ASP:OD1	1.93	0.68
1:A:94:LYS:CE	1:A:398:ASN:ND2	2.49	0.68
1:B:436:GLU:OE2	1:B:447:LYS:HE2	1.92	0.68
1:A:275:GLU:HG2	1:A:278:VAL:HG23	1.76	0.68
1:B:185:GLY:HA3	1:B:515:PHE:CE2	2.27	0.68
1:B:364:LYS:NZ	1:B:429:ALA:O	2.22	0.68
1:A:288:ASN:OD1	1:A:290:THR:N	2.26	0.68
1:B:463:CYS:HB2	2:B:580:HEM:C1A	2.29	0.67
1:B:71:ASP:OD2	1:B:74:LYS:HD3	1.94	0.67
1:A:428:ILE:HD12	1:A:428:ILE:C	2.15	0.67
1:B:132:ARG:H	1:B:299:HIS:CE1	2.11	0.67
1:B:373:ILE:HD12	1:B:373:ILE:N	2.09	0.67
1:B:152:TYR:C	1:B:279:TRP:NE1	2.48	0.67
3:A:590:VOR:C17	3:A:590:VOR:H21	2.23	0.67
1:A:285:VAL:HG12	1:A:286:TYR:O	1.95	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:CYS:O	1:A:292:VAL:N	2.28	0.67
1:A:58:TRP:CG	1:A:58:TRP:O	2.48	0.67
1:A:90:ILE:HG22	1:A:94:LYS:C	2.16	0.66
1:A:282:MET:C	1:A:284:CYS:H	1.98	0.66
1:A:404:GLY:O	1:A:408:ARG:HG2	1.96	0.66
1:A:288:ASN:OD1	1:A:290:THR:HG22	1.96	0.66
1:A:378:ARG:HB2	1:A:399:VAL:HG23	1.78	0.66
1:B:65:THR:HB	1:B:92:LEU:HD23	1.77	0.66
1:A:266:ARG:HH22	1:A:294:ASP:CG	1.99	0.66
1:A:94:LYS:CE	1:A:398:ASN:HD21	2.09	0.66
1:A:402:SER:OG	1:A:405:VAL:HG23	1.94	0.66
1:B:152:TYR:C	1:B:279:TRP:CZ2	2.70	0.65
1:A:394:PRO:O	1:A:397:HIS:HB2	1.97	0.65
1:A:510:ARG:HE	1:A:510:ARG:HA	1.61	0.65
1:B:152:TYR:CB	1:B:279:TRP:CE2	2.75	0.65
1:B:380:VAL:HG23	1:B:397:HIS:O	1.97	0.65
1:A:386:VAL:HG22	1:A:391:TYR:O	1.96	0.65
1:A:79:CYS:HB3	1:A:87:PHE:CE2	2.31	0.65
1:A:217:THR:O	1:A:221:LEU:HG	1.96	0.65
1:B:463:CYS:HA	2:B:580:HEM:C4D	2.32	0.65
3:A:590:VOR:C17	3:A:590:VOR:C21	2.74	0.65
1:B:433:GLU:OE1	1:B:446:SER:OG	2.15	0.65
1:B:404:GLY:O	1:B:408:ARG:HG2	1.96	0.64
1:B:340:VAL:HG23	1:B:341:LEU:HD23	1.79	0.64
1:A:400:LEU:HD23	1:A:401:SER:N	2.12	0.64
1:A:55:VAL:CG2	1:A:89:PHE:CA	2.73	0.64
1:B:286:TYR:OH	1:B:296:GLU:OE1	2.15	0.64
1:B:342:GLY:HA3	1:B:344:ASP:OD1	1.98	0.64
1:A:143:LEU:O	1:A:147:LYS:HG3	1.98	0.64
1:A:440:TYR:HE1	1:A:445:VAL:HG23	1.62	0.64
1:B:435:ASP:HB2	1:B:448:GLY:HA3	1.79	0.63
1:A:283:SER:OG	1:A:283:SER:O	2.16	0.63
1:A:266:ARG:NH1	4:A:2050:HOH:O	2.23	0.63
1:B:153:GLY:CA	1:B:279:TRP:CD1	2.82	0.63
1:B:365:GLU:OE1	1:B:365:GLU:HA	1.98	0.63
1:B:98:VAL:HG12	1:B:100:LEU:CD2	2.29	0.63
1:A:265:ARG:HH22	1:A:275:GLU:CD	2.02	0.63
1:A:59:PHE:HE2	1:A:62:ILE:HG23	1.62	0.62
1:A:265:ARG:HH11	1:A:277:MET:HG3	1.52	0.62
1:B:282:MET:O	1:B:284:CYS:N	2.32	0.62
1:A:79:CYS:HB3	1:A:87:PHE:CE1	2.33	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:ASN:O	1:A:227:MET:HE2	2.00	0.62
1:B:288:ASN:HD21	1:B:290:THR:CB	2.11	0.62
1:B:262:ILE:HG23	1:B:281:LEU:HD21	1.81	0.62
1:B:275:GLU:HG2	1:B:278:VAL:HG22	1.80	0.62
1:A:284:CYS:SG	1:A:285:VAL:HG23	2.38	0.62
1:A:284:CYS:CB	1:A:291:PRO:HB3	2.30	0.62
1:A:224:ASN:CA	1:A:227:MET:HE2	2.30	0.62
1:A:65:THR:CG2	1:A:92:LEU:H	2.09	0.62
1:B:288:ASN:HD21	1:B:290:THR:HB	1.65	0.62
1:B:340:VAL:HG23	1:B:341:LEU:CD2	2.30	0.62
1:A:437:LYS:HE3	1:A:446:SER:HB2	1.80	0.62
1:B:216:SER:OG	1:B:217:THR:N	2.33	0.62
1:A:152:TYR:CD2	1:A:279:TRP:HZ2	2.18	0.62
1:B:265:ARG:NH1	1:B:275:GLU:OE2	2.33	0.62
1:A:132:ARG:O	1:A:133:HIS:HB2	1.99	0.62
1:A:115:ASP:HB3	1:A:384:MET:HE2	1.81	0.62
1:A:400:LEU:C	1:A:400:LEU:HD23	2.19	0.62
1:B:86:ILE:HB	1:B:99:TYR:CD1	2.35	0.61
1:B:449:THR:O	1:B:449:THR:HG22	2.00	0.61
1:B:340:VAL:O	1:B:341:LEU:HD23	2.00	0.61
1:A:272:LYS:HE3	4:A:2039:HOH:O	2.00	0.61
1:A:381:LYS:O	1:A:382:ASN:OD1	2.18	0.61
1:A:59:PHE:CG	1:A:60:PRO:CD	2.81	0.61
1:B:493:ASP:HB3	4:B:2072:HOH:O	2.00	0.61
1:A:110:ASN:OD1	1:A:447:LYS:CB	2.45	0.61
1:A:95:LYS:HD2	1:A:397:HIS:CD2	2.35	0.61
1:A:59:PHE:CE2	1:A:62:ILE:CG2	2.84	0.61
1:B:285:VAL:HG12	1:B:286:TYR:O	2.01	0.61
2:A:580:HEM:HHA	2:A:580:HEM:HBD2	1.83	0.61
1:B:209:GLU:OE2	1:B:265:ARG:CZ	2.50	0.60
1:A:284:CYS:HB2	1:A:291:PRO:CB	2.30	0.60
1:A:361:LYS:HZ1	1:A:428:ILE:CG2	2.12	0.60
1:A:51:THR:HG23	1:A:52:PRO:HD2	1.83	0.60
1:A:55:VAL:O	1:A:57:HIS:HD2	1.83	0.60
1:B:380:VAL:CG2	1:B:397:HIS:O	2.50	0.60
1:B:57:HIS:ND1	1:B:59:PHE:O	2.34	0.60
1:B:258:TYR:O	1:B:262:ILE:HG13	2.02	0.60
1:B:61:PHE:CE1	1:B:92:LEU:O	2.54	0.60
1:A:82:LYS:CB	1:A:83:TYR:CD1	2.85	0.60
1:A:277:MET:O	1:A:281:LEU:HG	2.01	0.60
1:B:51:THR:HG22	1:B:52:PRO:HD3	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:CYS:CB	1:A:87:PHE:CE2	2.85	0.60
1:B:233:ASN:OD1	1:B:243:HIS:NE2	2.31	0.60
1:A:357:ASP:O	1:A:361:LYS:HG3	2.03	0.59
1:B:233:ASN:O	1:B:237:PRO:HD3	2.01	0.59
1:B:236:LEU:HD23	1:B:238:TRP:CZ2	2.37	0.59
1:A:59:PHE:CD2	1:A:60:PRO:HD2	2.38	0.59
1:A:389:THR:HG22	1:A:390:SER:H	1.65	0.59
1:A:51:THR:CG2	1:A:52:PRO:CD	2.80	0.59
1:B:394:PRO:O	1:B:397:HIS:HB2	2.02	0.59
1:A:51:THR:HG1	1:A:52:PRO:HD3	1.63	0.59
1:A:82:LYS:CB	1:A:83:TYR:CE1	2.85	0.59
1:B:212:SER:O	1:B:215:ASP:HB2	2.02	0.59
1:B:400:LEU:C	1:B:400:LEU:HD23	2.23	0.59
1:A:435:ASP:CB	1:A:448:GLY:CA	2.80	0.58
1:A:123:SER:N	1:A:124:PRO:HD2	2.18	0.58
1:A:246:LYS:NZ	4:A:2042:HOH:O	2.36	0.58
1:B:381:LYS:C	1:B:382:ASN:OD1	2.41	0.58
1:A:344:ASP:OD1	1:A:344:ASP:N	2.35	0.58
1:B:95:LYS:CD	1:B:397:HIS:CD2	2.84	0.58
1:A:79:CYS:CB	1:A:87:PHE:CZ	2.85	0.58
1:B:87:PHE:CE1	1:B:98:VAL:HB	2.39	0.58
1:B:402:SER:OG	1:B:405:VAL:HG23	2.04	0.58
3:B:590:VOR:C17	3:B:590:VOR:H21	2.32	0.58
1:B:340:VAL:C	1:B:341:LEU:HD23	2.23	0.58
1:A:51:THR:OG1	1:A:52:PRO:HD2	2.02	0.58
1:A:378:ARG:HH21	1:A:461:HIS:HD2	1.52	0.58
1:A:152:TYR:CB	1:A:279:TRP:HZ2	2.14	0.58
1:A:60:PRO:O	1:A:61:PHE:HB3	2.03	0.58
1:A:92:LEU:HD12	1:A:235:MET:CE	2.31	0.58
4:A:2085:HOH:O	1:B:510:ARG:NE	2.37	0.58
1:B:153:GLY:HA2	1:B:279:TRP:CD1	2.39	0.58
1:A:83:TYR:N	1:A:83:TYR:CD1	2.71	0.58
1:A:364:LYS:HE3	1:A:429:ALA:H	1.68	0.57
1:A:357:ASP:OD1	1:A:428:ILE:HG21	2.04	0.57
1:B:80:ARG:O	1:B:84:GLY:N	2.37	0.57
1:A:80:ARG:N	1:A:87:PHE:CZ	2.72	0.57
1:A:378:ARG:NH2	1:A:461:HIS:CD2	2.73	0.57
1:A:86:ILE:HD13	1:A:99:TYR:HA	1.87	0.57
1:A:51:THR:CG2	1:A:52:PRO:HD2	2.34	0.57
1:B:456:PHE:HB3	1:B:463:CYS:HB3	1.87	0.57
1:B:429:ALA:C	1:B:431:SER:H	2.08	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:CYS:CA	1:B:292:VAL:H	2.17	0.57
1:B:209:GLU:CB	1:B:261:ILE:HD13	2.35	0.57
1:B:89:PHE:CE2	1:B:91:LEU:HG	2.40	0.57
1:A:59:PHE:CD2	1:A:62:ILE:CG2	2.88	0.56
1:A:97:THR:N	1:A:398:ASN:O	2.26	0.56
1:B:453:TYR:CE1	1:B:455:PRO:HG3	2.41	0.56
1:B:433:GLU:OE1	1:B:448:GLY:HA3	2.05	0.56
1:B:387:ASP:OD1	1:B:387:ASP:N	2.39	0.56
1:A:106:ASP:OD1	1:A:110:ASN:ND2	2.36	0.56
1:B:444:LEU:C	1:B:445:VAL:HG13	2.25	0.56
1:A:477:THR:O	1:A:481:VAL:HG23	2.05	0.56
1:A:133:HIS:H	1:A:137:ASP:HB3	1.69	0.56
1:B:112:LYS:HD3	1:B:114:ARG:NE	2.20	0.56
1:B:277:MET:O	1:B:281:LEU:HG	2.05	0.56
1:B:98:VAL:HG11	1:B:100:LEU:HD21	1.86	0.56
1:A:282:MET:C	1:A:284:CYS:N	2.58	0.56
2:A:580:HEM:HBC2	2:A:580:HEM:CMC	2.35	0.56
1:A:224:ASN:HA	1:A:227:MET:CE	2.33	0.56
1:B:435:ASP:HB2	1:B:448:GLY:CA	2.36	0.56
1:A:357:ASP:CG	1:A:361:LYS:HE2	2.26	0.55
1:A:361:LYS:HZ1	1:A:428:ILE:HG22	1.64	0.55
1:A:99:TYR:CG	1:A:104:GLY:HA2	2.41	0.55
1:B:127:THR:HB	1:B:128:PRO:HD3	1.88	0.55
1:A:90:ILE:HG22	1:A:95:LYS:N	2.21	0.55
1:A:440:TYR:HE1	1:A:445:VAL:CG2	2.18	0.55
1:A:284:CYS:SG	1:A:291:PRO:HB3	2.46	0.55
1:A:117:CYS:SG	1:A:119:GLU:CD	2.85	0.55
1:B:89:PHE:HE2	1:B:91:LEU:HG	1.72	0.55
1:A:265:ARG:NH2	1:A:275:GLU:OE2	2.37	0.55
3:B:590:VOR:C21	3:B:590:VOR:C13	2.83	0.55
1:B:372:PRO:HD3	4:B:2045:HOH:O	2.05	0.55
1:B:153:GLY:N	1:B:279:TRP:HE1	2.04	0.54
1:A:231:PRO:O	1:A:234:PHE:HB2	2.07	0.54
1:A:440:TYR:CE1	1:A:445:VAL:CG2	2.90	0.54
1:B:123:SER:N	1:B:124:PRO:HD2	2.22	0.54
1:A:265:ARG:HH12	1:A:277:MET:CG	2.07	0.54
1:B:60:PRO:O	1:B:61:PHE:HB3	2.08	0.54
1:B:208:LYS:NZ	1:B:272:LYS:HD3	2.23	0.54
1:B:319:ILE:O	1:B:323:LEU:HG	2.08	0.54
1:A:53:PRO:CD	1:A:391:TYR:CE1	2.82	0.54
1:A:447:LYS:O	1:A:448:GLY:C	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:TYR:HB2	1:B:288:ASN:OD1	2.07	0.54
1:B:426:GLU:O	1:B:427:ASN:OD1	2.26	0.53
1:B:98:VAL:HG12	1:B:100:LEU:HD21	1.87	0.53
1:B:178:PRO:HA	1:B:181:GLN:HG2	1.90	0.53
1:B:297:ILE:O	1:B:301:MET:HG2	2.09	0.53
3:A:590:VOR:C13	3:A:590:VOR:C21	2.85	0.53
1:B:124:PRO:O	1:B:128:PRO:CD	2.56	0.53
3:A:590:VOR:H17	3:A:590:VOR:H21	1.89	0.53
1:A:90:ILE:HG23	1:A:95:LYS:HA	1.89	0.53
1:A:92:LEU:CD1	1:A:235:MET:CE	2.87	0.53
1:A:435:ASP:CG	1:A:448:GLY:HA3	2.29	0.53
1:A:166:ILE:O	1:A:170:VAL:HG23	2.09	0.53
1:B:160:ARG:HA	1:B:350:TYR:HB2	1.90	0.53
1:B:221:LEU:HD21	1:B:253:LYS:HD3	1.91	0.53
1:B:433:GLU:CD	1:B:446:SER:OG	2.46	0.53
1:B:80:ARG:HA	1:B:84:GLY:O	2.09	0.53
1:A:277:MET:CA	1:A:277:MET:CE	2.84	0.52
1:A:149:PHE:O	1:A:279:TRP:NE1	2.35	0.52
1:A:450:ASN:N	1:A:450:ASN:HD22	2.07	0.52
1:A:433:GLU:HG2	1:A:434:ASP:N	2.18	0.52
1:A:271:LYS:CG	1:A:272:LYS:N	2.72	0.52
1:B:172:SER:HB3	4:B:2004:HOH:O	2.09	0.52
1:B:338:ILE:O	1:B:341:LEU:O	2.28	0.52
1:B:395:THR:O	1:B:395:THR:HG22	2.10	0.52
1:A:311:SER:HB2	2:A:580:HEM:CAB	2.40	0.52
1:A:435:ASP:O	1:A:437:LYS:NZ	2.40	0.52
1:A:266:ARG:O	1:A:269:GLY:N	2.43	0.52
1:B:135:VAL:HG12	1:B:136:TYR:CG	2.45	0.52
1:B:95:LYS:HB2	1:B:397:HIS:CD2	2.45	0.51
1:A:52:PRO:HA	1:A:391:TYR:CD1	2.44	0.51
1:A:80:ARG:HA	1:A:87:PHE:CZ	2.45	0.51
1:A:62:ILE:HG13	1:A:63:GLY:N	2.24	0.51
1:A:378:ARG:HB2	1:A:399:VAL:CG2	2.39	0.51
1:B:110:ASN:OD1	1:B:447:LYS:HG3	2.10	0.51
1:B:109:LEU:HD13	1:B:458:ALA:HB3	1.92	0.51
1:B:162:TYR:CD1	1:B:204:SER:HB2	2.45	0.51
1:B:282:MET:C	1:B:284:CYS:N	2.63	0.51
1:A:434:ASP:OD1	1:A:434:ASP:C	2.48	0.51
1:A:226:ASP:OD1	1:A:310:HIS:NE2	2.41	0.51
1:A:59:PHE:CD2	1:A:60:PRO:O	2.64	0.51
1:B:357:ASP:OD2	1:B:361:LYS:NZ	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:CYS:HB3	1:B:291:PRO:HB3	1.93	0.51
1:A:90:ILE:CD1	1:A:90:ILE:H	1.98	0.50
3:B:590:VOR:H17	3:B:590:VOR:H21	1.92	0.50
1:B:135:VAL:HG12	1:B:136:TYR:CD2	2.47	0.50
1:B:463:CYS:HA	2:B:580:HEM:CHA	2.40	0.50
1:A:152:TYR:HB3	1:A:279:TRP:CE2	2.45	0.50
1:A:152:TYR:HD2	1:A:279:TRP:HZ2	1.57	0.50
1:A:435:ASP:OD2	1:A:448:GLY:HA3	2.11	0.50
1:B:403:PRO:HB3	1:B:454:LEU:HB2	1.94	0.50
1:B:51:THR:CG2	1:B:52:PRO:HD3	2.40	0.50
1:A:494:GLY:HA2	4:A:2025:HOH:O	2.11	0.50
1:B:277:MET:C	1:B:277:MET:SD	2.89	0.50
1:A:449:THR:C	1:A:450:ASN:HD22	2.15	0.50
1:B:112:LYS:CD	1:B:114:ARG:NE	2.74	0.50
1:A:169:GLU:OE1	4:A:2026:HOH:O	2.20	0.50
1:B:166:ILE:O	1:B:170:VAL:HG23	2.11	0.50
1:A:277:MET:C	1:A:279:TRP:H	2.15	0.50
1:A:79:CYS:C	1:A:87:PHE:CE1	2.85	0.50
1:B:275:GLU:O	1:B:277:MET:N	2.45	0.50
1:A:378:ARG:NH2	1:A:461:HIS:HD2	2.09	0.50
1:A:63:GLY:HA3	1:A:90:ILE:HD13	1.93	0.50
1:A:376:ILE:CG2	1:A:378:ARG:HH12	2.25	0.49
1:B:361:LYS:NZ	1:B:425:ASP:OD1	2.40	0.49
1:B:152:TYR:O	1:B:279:TRP:CE2	2.64	0.49
1:B:132:ARG:N	1:B:299:HIS:CE1	2.80	0.49
1:A:435:ASP:HB2	1:A:448:GLY:CA	2.40	0.49
1:A:108:ILE:HD12	1:A:401:SER:HB3	1.95	0.49
1:A:90:ILE:N	1:A:90:ILE:CD1	2.67	0.49
1:A:293:PRO:HG2	1:A:296:GLU:HG3	1.95	0.49
1:A:298:ALA:O	1:A:302:ILE:HG13	2.12	0.49
1:B:284:CYS:HA	1:B:292:VAL:HB	1.95	0.49
1:A:286:TYR:CE1	1:A:292:VAL:HG22	2.46	0.49
1:A:65:THR:HG21	1:A:92:LEU:N	2.14	0.49
1:B:277:MET:O	1:B:277:MET:SD	2.70	0.49
1:B:292:VAL:HG12	1:B:297:ILE:CG1	2.43	0.49
1:A:446:SER:C	1:A:448:GLY:H	2.12	0.49
1:A:400:LEU:CD2	1:A:400:LEU:C	2.80	0.49
1:A:55:VAL:CB	1:A:88:THR:O	2.61	0.49
1:B:439:ASP:OD1	1:B:441:GLY:N	2.40	0.49
1:A:471:LEU:O	1:A:475:THR:OG1	2.22	0.49
1:A:120:GLU:OE2	1:A:381:LYS:NZ	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:GLU:O	1:B:278:VAL:HG22	2.12	0.48
1:B:276:ASP:O	1:B:279:TRP:HB3	2.13	0.48
1:A:80:ARG:CA	1:A:87:PHE:HZ	2.26	0.48
1:A:97:THR:O	1:A:399:VAL:HA	2.14	0.48
1:B:262:ILE:HG23	1:B:281:LEU:CD2	2.43	0.48
1:B:493:ASP:CG	1:B:494:GLY:H	2.08	0.48
1:B:350:TYR:CE2	1:B:354:GLN:NE2	2.82	0.48
1:B:336:GLU:OE1	1:B:358:LEU:HB3	2.13	0.48
1:A:116:VAL:HB	1:A:378:ARG:HB3	1.95	0.48
1:B:377:ILE:O	1:B:378:ARG:NH1	2.43	0.48
1:B:284:CYS:SG	1:B:291:PRO:HB3	2.54	0.48
1:B:311:SER:HB2	2:B:580:HEM:CAB	2.43	0.48
1:B:519:HIS:O	1:B:519:HIS:CG	2.65	0.48
1:B:395:THR:O	1:B:395:THR:CG2	2.61	0.48
1:B:364:LYS:HG2	1:B:424:TRP:CZ2	2.49	0.48
1:B:202:SER:HA	1:B:206:GLN:HB2	1.96	0.48
1:A:275:GLU:HG3	1:A:277:MET:CB	2.26	0.48
1:A:144:MET:HE2	1:A:144:MET:HA	1.96	0.48
1:A:58:TRP:O	1:A:58:TRP:CD2	2.67	0.47
1:A:230:ALA:O	1:A:233:ASN:HB2	2.14	0.47
1:B:224:ASN:O	1:B:227:MET:CE	2.62	0.47
1:A:80:ARG:CA	1:A:87:PHE:CZ	2.97	0.47
1:B:482:ARG:O	1:B:518:ARG:HD2	2.13	0.47
1:B:169:GLU:OE2	1:B:203:ARG:NH1	2.45	0.47
1:B:281:LEU:HD23	1:B:297:ILE:HD13	1.95	0.47
1:B:379:ALA:HA	1:B:398:ASN:OD1	2.14	0.47
1:A:50:LYS:C	1:A:51:THR:HG22	2.31	0.47
1:A:273:ASP:HB3	1:A:274:SER:HB2	1.96	0.47
1:B:275:GLU:C	1:B:277:MET:N	2.68	0.47
1:A:361:LYS:HZ3	1:A:428:ILE:CG2	2.16	0.47
1:A:79:CYS:C	1:A:87:PHE:CZ	2.88	0.47
1:B:112:LYS:O	1:B:116:VAL:HG22	2.14	0.47
1:B:262:ILE:CG1	1:B:277:MET:CE	2.66	0.47
1:B:224:ASN:CA	1:B:227:MET:CE	2.77	0.47
1:A:437:LYS:CE	1:A:446:SER:HB2	2.44	0.47
1:A:79:CYS:HB3	1:A:87:PHE:CD2	2.49	0.47
1:A:294:ASP:OD1	4:A:2050:HOH:O	2.21	0.47
1:B:86:ILE:HA	1:B:98:VAL:O	2.15	0.47
1:B:136:TYR:OH	2:B:580:HEM:CBD	2.62	0.47
1:B:373:ILE:CD1	1:B:373:ILE:N	2.77	0.47
1:A:372:PRO:HG2	1:A:373:ILE:HD12	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:TYR:OH	1:B:375:SER:OG	2.28	0.47
1:B:153:GLY:N	1:B:279:TRP:CD1	2.83	0.47
1:A:293:PRO:HD2	1:A:296:GLU:OE1	2.15	0.47
1:B:98:VAL:CG1	1:B:100:LEU:CD2	2.87	0.47
1:B:71:ASP:OD1	1:B:73:TYR:N	2.45	0.47
1:A:356:LEU:HB3	1:A:359:HIS:HB2	1.97	0.47
1:A:120:GLU:OE1	1:A:381:LYS:HE2	2.14	0.46
1:A:385:ALA:N	4:A:2071:HOH:O	2.39	0.46
1:A:152:TYR:HD2	1:A:279:TRP:CZ2	2.32	0.46
1:B:153:GLY:HA2	1:B:279:TRP:CG	2.50	0.46
1:A:265:ARG:NH1	1:A:278:VAL:HG22	2.30	0.46
1:A:59:PHE:HB3	1:A:62:ILE:HG12	1.97	0.46
1:A:83:TYR:N	1:A:83:TYR:HD1	2.13	0.46
1:B:132:ARG:N	1:B:299:HIS:ND1	2.63	0.46
1:A:160:ARG:HG2	1:A:350:TYR:CG	2.50	0.46
1:A:86:ILE:HD11	1:A:99:TYR:CE1	2.45	0.46
1:B:453:TYR:CZ	1:B:455:PRO:HG2	2.50	0.46
1:A:77:PHE:HE1	1:A:405:VAL:HG13	1.81	0.46
1:A:381:LYS:HB3	4:A:2006:HOH:O	2.16	0.46
1:B:149:PHE:CD1	1:B:283:SER:OG	2.68	0.46
1:A:79:CYS:HB2	1:A:87:PHE:CE2	2.50	0.46
1:B:275:GLU:O	1:B:276:ASP:C	2.54	0.46
1:B:281:LEU:HD23	1:B:297:ILE:CD1	2.45	0.46
1:A:288:ASN:ND2	4:A:2051:HOH:O	2.49	0.46
1:B:145:GLU:OE1	1:B:286:TYR:HA	2.15	0.46
1:B:140:ASN:O	1:B:144:MET:HG2	2.15	0.46
1:A:59:PHE:CE2	1:A:60:PRO:O	2.69	0.46
1:B:453:TYR:CZ	1:B:455:PRO:CG	2.99	0.46
1:A:156:SER:O	1:A:160:ARG:HG3	2.15	0.46
1:A:277:MET:SD	1:A:281:LEU:HD21	2.56	0.46
1:B:262:ILE:HA	1:B:277:MET:CE	2.47	0.46
1:B:122:TYR:OH	3:B:590:VOR:H24	2.16	0.46
1:B:374:HIS:CE1	1:B:375:SER:HG	2.31	0.46
1:B:119:GLU:O	1:B:123:SER:HB2	2.16	0.45
1:A:114:ARG:HG3	1:A:115:ASP:N	2.31	0.45
1:A:152:TYR:CD2	1:A:279:TRP:CZ2	3.01	0.45
1:A:108:ILE:HD13	1:A:399:VAL:HB	1.98	0.45
1:A:133:HIS:H	1:A:137:ASP:CB	2.30	0.45
1:A:424:TRP:C	1:A:426:GLU:N	2.69	0.45
1:B:131:GLY:HA3	1:B:299:HIS:ND1	2.32	0.45
1:A:59:PHE:CD1	1:A:60:PRO:CD	2.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:SER:HB2	2:B:580:HEM:HAB	1.99	0.45
1:A:376:ILE:HG22	1:A:378:ARG:NH1	2.31	0.45
1:A:436:GLU:C	1:A:437:LYS:HD2	2.37	0.45
1:B:241:LEU:HB3	1:B:242:PRO:HD2	1.99	0.45
1:B:472:GLN:O	1:B:476:ILE:HG13	2.17	0.45
1:A:286:TYR:CD1	1:A:290:THR:HG23	2.52	0.44
1:A:55:VAL:HG21	1:A:89:PHE:HB2	1.93	0.44
1:B:338:ILE:HD13	1:B:345:LEU:HD21	1.98	0.44
2:A:580:HEM:HBC2	2:A:580:HEM:HMC2	1.98	0.44
1:A:277:MET:C	1:A:279:TRP:N	2.71	0.44
1:B:217:THR:HG21	4:B:2038:HOH:O	2.17	0.44
1:A:378:ARG:HH21	1:A:461:HIS:CD2	2.30	0.44
1:A:90:ILE:CD1	1:A:90:ILE:O	2.65	0.44
1:B:208:LYS:N	4:B:2034:HOH:O	2.44	0.44
1:A:384:MET:HG3	1:A:393:ILE:HB	2.00	0.44
1:A:225:LEU:HD22	1:A:254:LEU:CD1	2.48	0.44
1:A:61:PHE:HZ	1:A:235:MET:HE3	1.83	0.44
1:A:80:ARG:HA	1:A:87:PHE:CE1	2.53	0.44
1:B:135:VAL:HA	1:B:143:LEU:CD1	2.48	0.44
1:B:108:ILE:HD12	1:B:401:SER:HB2	1.99	0.44
1:B:374:HIS:CE1	1:B:375:SER:OG	2.70	0.44
1:A:297:ILE:O	1:A:301:MET:HG2	2.17	0.44
1:B:519:HIS:CD2	1:B:519:HIS:C	2.90	0.44
1:A:428:ILE:HD12	1:A:429:ALA:N	2.32	0.44
1:B:210:VAL:HG13	1:B:218:PHE:CD2	2.52	0.44
1:B:424:TRP:HE3	1:B:427:ASN:O	2.01	0.44
1:B:124:PRO:O	1:B:128:PRO:HD2	2.17	0.44
1:A:213:LYS:HB3	1:A:218:PHE:CD1	2.53	0.43
1:A:79:CYS:HB3	1:A:87:PHE:CD1	2.53	0.43
1:B:515:PHE:C	1:B:515:PHE:CD1	2.91	0.43
1:B:106:ASP:HA	1:B:449:THR:HG21	1.95	0.43
1:A:84:GLY:O	1:A:87:PHE:CE1	2.71	0.43
1:A:340:VAL:HG11	1:A:355:LYS:CB	2.48	0.43
1:A:123:SER:O	1:A:127:THR:OG1	2.31	0.43
1:A:124:PRO:O	1:A:128:PRO:CG	2.66	0.43
1:A:424:TRP:C	1:A:426:GLU:H	2.21	0.43
1:A:163:VAL:HB	1:A:164:PRO:CD	2.47	0.43
1:A:72:PRO:O	1:A:75:PHE:HB3	2.18	0.43
1:A:284:CYS:SG	1:A:285:VAL:CG2	3.07	0.43
1:B:153:GLY:CA	1:B:279:TRP:NE1	2.81	0.43
1:B:51:THR:CB	1:B:52:PRO:HD3	2.44	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:493:ASP:N	4:B:2072:HOH:O	2.42	0.43
1:B:400:LEU:C	1:B:400:LEU:CD2	2.87	0.43
1:A:61:PHE:HZ	1:A:235:MET:CE	2.32	0.43
1:B:98:VAL:HG12	1:B:100:LEU:HD23	2.00	0.43
1:A:233:ASN:OD1	1:A:237:PRO:HA	2.19	0.43
1:B:292:VAL:CG1	1:B:297:ILE:HG12	2.49	0.43
1:A:386:VAL:HG23	1:A:389:THR:H	1.84	0.43
1:B:135:VAL:HG12	1:B:136:TYR:N	2.33	0.43
1:B:435:ASP:CB	1:B:448:GLY:HA3	2.46	0.43
1:A:90:ILE:HA	1:A:94:LYS:O	2.19	0.43
1:A:285:VAL:HA	1:A:290:THR:O	2.19	0.43
1:B:363:ILE:HD11	1:B:474:GLY:HA2	2.01	0.43
1:A:418:GLU:OE1	1:A:418:GLU:HA	2.19	0.43
1:B:477:THR:O	1:B:481:VAL:HG23	2.18	0.42
1:B:92:LEU:HD23	1:B:92:LEU:N	2.33	0.42
1:A:357:ASP:OD2	1:A:361:LYS:CE	2.62	0.42
1:B:344:ASP:OD1	1:B:344:ASP:N	2.51	0.42
1:B:215:ASP:OD1	4:B:2031:HOH:O	2.21	0.42
1:A:318:TRP:CE2	1:A:507:PRO:HG3	2.54	0.42
1:B:491:GLY:C	1:B:492:VAL:HG23	2.39	0.42
1:A:140:ASN:HD21	1:A:460:ARG:HH11	1.66	0.42
1:B:502:SER:HB3	4:B:2074:HOH:O	2.20	0.42
1:B:236:LEU:CD2	1:B:238:TRP:CH2	3.03	0.42
1:B:167:THR:O	1:B:171:GLU:HG3	2.19	0.42
1:B:152:TYR:CA	1:B:279:TRP:CZ2	3.03	0.42
1:A:364:LYS:HE3	1:A:429:ALA:N	2.33	0.42
1:A:127:THR:N	1:A:128:PRO:CD	2.82	0.42
2:B:580:HEM:CMB	2:B:580:HEM:HBB2	2.50	0.42
1:B:132:ARG:H	1:B:299:HIS:HE1	1.65	0.42
1:A:275:GLU:OE2	1:A:277:MET:HB3	2.20	0.42
1:A:380:VAL:HG23	1:A:397:HIS:O	2.19	0.42
1:A:90:ILE:CG2	1:A:95:LYS:CA	2.81	0.42
1:B:393:ILE:HA	1:B:394:PRO:HD2	1.93	0.42
1:A:80:ARG:N	1:A:87:PHE:HZ	2.16	0.42
1:A:120:GLU:OE2	1:A:381:LYS:CE	2.67	0.42
1:A:277:MET:SD	1:A:277:MET:C	2.98	0.42
1:A:307:ALA:O	1:A:311:SER:OG	2.28	0.42
1:B:489:LEU:HG	1:B:490:PRO:HD2	2.02	0.42
1:B:339:ARG:NH2	4:B:2052:HOH:O	2.53	0.42
1:B:224:ASN:O	1:B:227:MET:HE3	2.19	0.42
1:A:115:ASP:HB3	1:A:384:MET:HE3	1.98	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:ASN:ND2	1:B:290:THR:CB	2.77	0.42
1:A:344:ASP:O	1:A:345:LEU:HB2	2.20	0.42
1:B:413:PHE:HB3	1:B:423:ARG:NH1	2.35	0.42
1:B:163:VAL:N	1:B:164:PRO:CD	2.82	0.42
1:A:393:ILE:HA	1:A:394:PRO:HD3	1.82	0.42
1:A:82:LYS:HB2	1:A:83:TYR:HD1	1.74	0.42
1:B:122:TYR:OH	3:B:590:VOR:C24	2.68	0.42
1:B:364:LYS:HD3	1:B:424:TRP:CZ3	2.55	0.42
1:B:377:ILE:HG23	1:B:399:VAL:O	2.19	0.42
1:B:284:CYS:C	1:B:292:VAL:H	2.22	0.42
1:A:91:LEU:O	1:A:92:LEU:HB2	2.20	0.42
1:B:288:ASN:OD1	1:B:290:THR:N	2.43	0.42
1:B:373:ILE:H	1:B:373:ILE:HD12	1.83	0.42
1:B:446:SER:C	1:B:448:GLY:H	2.21	0.42
1:A:187:PHE:O	1:A:512:PHE:HA	2.20	0.42
1:B:197:THR:HG21	1:B:313:SER:HA	2.01	0.42
1:B:224:ASN:C	1:B:227:MET:HE2	2.41	0.41
1:A:82:LYS:HB2	1:A:83:TYR:HE1	1.79	0.41
1:A:350:TYR:O	1:A:354:GLN:NE2	2.53	0.41
1:A:59:PHE:CD2	1:A:60:PRO:CD	3.04	0.41
1:A:59:PHE:CZ	1:A:60:PRO:HD2	2.54	0.41
1:A:436:GLU:O	1:A:437:LYS:HD2	2.20	0.41
1:A:340:VAL:HG11	1:A:355:LYS:HB2	2.02	0.41
1:B:284:CYS:SG	1:B:291:PRO:CB	3.08	0.41
1:B:380:VAL:HG12	1:B:395:THR:HA	2.01	0.41
1:A:153:GLY:HA3	1:A:279:TRP:CD1	2.55	0.41
1:A:447:LYS:HA	1:A:459:GLY:N	2.28	0.41
1:B:123:SER:O	1:B:127:THR:OG1	2.26	0.41
1:A:100:LEU:O	1:A:104:GLY:HA3	2.21	0.41
1:A:395:THR:C	1:A:397:HIS:H	2.23	0.41
1:A:286:TYR:HD1	1:A:290:THR:O	2.03	0.41
1:B:493:ASP:CB	4:B:2072:HOH:O	2.66	0.41
2:A:580:HEM:CMB	2:A:580:HEM:HBB2	2.50	0.41
1:B:377:ILE:HG22	1:B:378:ARG:N	2.36	0.41
1:A:349:THR:HG21	4:A:2065:HOH:O	2.19	0.41
1:A:277:MET:HE3	1:A:277:MET:HB2	1.93	0.41
1:B:488:ASN:HD22	1:B:493:ASP:HA	1.85	0.41
1:B:429:ALA:HB1	1:B:431:SER:CB	2.50	0.41
1:B:105:ASN:O	1:B:109:LEU:HG	2.21	0.41
1:A:318:TRP:CD1	1:A:370:HIS:HB3	2.56	0.41
1:B:302:ILE:O	1:B:306:MET:HG2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:THR:HA	1:B:97:THR:HA	2.03	0.41
1:B:130:PHE:CD1	1:B:303:ALA:HA	2.56	0.41
1:B:404:GLY:O	1:B:408:ARG:CG	2.65	0.41
1:A:64:SER:O	1:A:67:SER:HB3	2.20	0.41
1:B:519:HIS:O	1:B:519:HIS:CD2	2.74	0.41
1:A:376:ILE:CG2	1:A:378:ARG:NH1	2.84	0.41
1:A:55:VAL:HG22	1:A:89:PHE:CA	2.46	0.41
1:A:285:VAL:HA	1:A:291:PRO:HA	2.02	0.41
1:A:290:THR:O	1:A:290:THR:HG23	2.21	0.41
1:A:213:LYS:O	1:A:216:SER:N	2.53	0.41
1:A:434:ASP:OD1	1:A:434:ASP:O	2.39	0.41
1:A:79:CYS:O	1:A:87:PHE:CE1	2.74	0.41
1:B:364:LYS:HG3	1:B:453:TYR:OH	2.21	0.41
1:B:112:LYS:HD2	1:B:114:ARG:CZ	2.51	0.41
1:B:208:LYS:HZ2	1:B:272:LYS:HD3	1.86	0.41
1:B:374:HIS:ND1	1:B:375:SER:OG	2.43	0.41
1:A:185:GLY:HA3	1:A:515:PHE:CE2	2.55	0.41
1:A:469:ALA:O	1:A:473:LEU:HG	2.21	0.41
1:A:138:CYS:HB2	1:A:139:PRO:HD2	2.03	0.41
1:A:75:PHE:HZ	1:A:89:PHE:CG	2.39	0.41
1:B:110:ASN:ND2	1:B:449:THR:OG1	2.53	0.41
1:B:292:VAL:HA	1:B:293:PRO:HD2	1.87	0.40
1:B:106:ASP:N	1:B:449:THR:HG21	2.36	0.40
1:A:106:ASP:HB2	1:A:449:THR:HB	2.04	0.40
1:A:101:GLY:O	1:A:105:ASN:N	2.45	0.40
1:A:114:ARG:CG	1:A:115:ASP:OD1	2.66	0.40
1:A:96:THR:HG22	1:A:398:ASN:HB2	2.04	0.40
1:B:62:ILE:O	1:B:65:THR:HG22	2.21	0.40
1:A:123:SER:N	1:A:124:PRO:CD	2.84	0.40
1:B:429:ALA:HB1	1:B:431:SER:HB2	2.03	0.40
1:A:271:LYS:HG3	1:A:272:LYS:H	1.86	0.40
1:B:57:HIS:CE1	1:B:59:PHE:O	2.75	0.40
1:B:128:PRO:O	1:B:251:GLN:HG3	2.20	0.40
1:A:453:TYR:CZ	1:A:455:PRO:HG2	2.57	0.40
1:A:279:TRP:O	1:A:283:SER:HB3	2.21	0.40
1:A:499:ASP:HB2	1:A:508:LEU:HA	2.03	0.40
1:A:52:PRO:O	1:A:53:PRO:C	2.59	0.40
1:B:106:ASP:HB2	1:B:449:THR:CB	2.51	0.40
1:B:193:ILE:HD13	1:B:193:ILE:HA	1.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	468/470 (100%)	447 (96%)	18 (4%)	3 (1%)	30 48
1	B	468/470 (100%)	454 (97%)	12 (3%)	2 (0%)	39 60
All	All	936/940 (100%)	901 (96%)	30 (3%)	5 (0%)	34 54

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	THR
1	A	433	GLU
1	B	51	THR
1	A	135	VAL
1	B	135	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	411/411 (100%)	384 (93%)	27 (7%)	21 36
1	B	411/411 (100%)	392 (95%)	19 (5%)	33 55
All	All	822/822 (100%)	776 (94%)	46 (6%)	26 45

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	62	ILE
1	A	83	TYR
1	A	90	ILE
1	A	91	LEU
1	A	92	LEU
1	A	99	TYR
1	A	152	TYR
1	A	218	PHE
1	A	238	TRP
1	A	252	ARG
1	A	270	SER
1	A	274	SER
1	A	278	VAL
1	A	282	MET
1	A	283	SER
1	A	389	THR
1	A	390	SER
1	A	399	VAL
1	A	410	GLU
1	A	428	ILE
1	A	434	ASP
1	A	444	LEU
1	A	450	ASN
1	A	462	ARG
1	A	510	ARG
1	A	519	HIS
1	B	51	THR
1	B	86	ILE
1	B	91	LEU
1	B	99	TYR
1	B	155	THR
1	B	218	PHE
1	B	263	LYS
1	B	265	ARG
1	B	270	SER
1	B	276	ASP
1	B	277	MET
1	B	284	CYS
1	B	341	LEU
1	B	387	ASP
1	B	389	THR
1	B	431	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	434	ASP
1	B	489	LEU
1	B	519	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	140	ASN
1	A	398	ASN
1	A	450	ASN
1	A	461	HIS
1	B	183	HIS
1	B	519	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	580	1,3	24,50,50	2.08	7 (29%)	16,82,82	1.54	3 (18%)
3	VOR	A	590	2	21,27,27	1.96	4 (19%)	18,39,39	3.34	8 (44%)
2	HEM	B	580	1,3	24,50,50	1.72	3 (12%)	16,82,82	1.60	4 (25%)
3	VOR	B	590	2	21,27,27	1.80	4 (19%)	18,39,39	2.97	8 (44%)

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	580	1,3	-	0/6/54/54	0/0/8/8
3	VOR	A	590	2	-	1/21/21/21	0/3/3/3
2	HEM	B	580	1,3	-	0/6/54/54	0/0/8/8
3	VOR	B	590	2	-	0/21/21/21	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	580	HEM	C3B-C2B	-5.33	1.33	1.40
2	A	580	HEM	C3B-C2B	-4.81	1.34	1.40
2	A	580	HEM	C1B-NB	-4.52	1.30	1.36
3	B	590	VOR	C10-C13	-4.35	1.49	1.53
2	A	580	HEM	C4D-ND	-3.58	1.32	1.36
2	B	580	HEM	C1B-NB	-3.31	1.32	1.36
3	A	590	VOR	C10-C13	-3.29	1.50	1.53
2	A	580	HEM	C3C-C2C	-3.28	1.36	1.40
2	B	580	HEM	C3C-C2C	-2.99	1.36	1.40
3	B	590	VOR	C21-N5	-2.98	1.30	1.33
3	B	590	VOR	C15-C11	-2.64	1.48	1.51
2	A	580	HEM	C1C-NC	-2.48	1.33	1.36
3	A	590	VOR	C15-C11	-2.27	1.48	1.51
2	A	580	HEM	C3D-C2D	-2.16	1.31	1.37
2	A	580	HEM	C4C-NC	-2.13	1.33	1.36
3	A	590	VOR	N7-N5	3.42	1.40	1.35
3	B	590	VOR	C13-C16	4.57	1.45	1.38
3	A	590	VOR	C13-C16	6.67	1.49	1.38

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	590	VOR	C19-C16-C13	-7.57	118.79	124.26
3	A	590	VOR	N9-C24-N6	-5.25	122.22	127.74
3	B	590	VOR	C19-C16-C13	-5.01	120.64	124.26
3	B	590	VOR	N9-C24-N6	-4.82	122.68	127.74
2	B	580	HEM	C3B-CAB-CBB	-3.64	119.07	126.40
2	A	580	HEM	C3C-CAC-CBC	-3.27	119.82	126.40
2	A	580	HEM	C3B-CAB-CBB	-2.52	121.33	126.40
2	B	580	HEM	C3C-CAC-CBC	-2.51	121.34	126.40
3	B	590	VOR	C20-C22-C19	-2.42	120.25	123.32
3	A	590	VOR	C23-C18-C15	-2.34	117.61	120.81
2	A	580	HEM	CAA-CBA-CGA	2.08	116.83	112.78
2	B	580	HEM	CBD-CAD-C3D	2.13	116.20	112.47
3	B	590	VOR	O4-C10-C13	2.17	110.63	107.39
3	A	590	VOR	C17-C20-C22	2.63	121.15	118.34
3	B	590	VOR	C17-C20-C22	2.76	121.28	118.34
2	B	580	HEM	CAA-CBA-CGA	2.83	118.29	112.78
3	B	590	VOR	C16-C19-C22	2.93	119.72	116.63
3	A	590	VOR	C17-C13-C16	2.94	118.87	115.92
3	A	590	VOR	C16-C19-C22	3.24	120.04	116.63
3	B	590	VOR	C23-N9-C24	5.51	122.13	115.91
3	A	590	VOR	C23-N9-C24	5.63	122.26	115.91
3	A	590	VOR	C21-N8-C25	6.14	109.63	102.31
3	B	590	VOR	C21-N8-C25	6.65	110.23	102.31

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	590	VOR	C10-C12-N5-C21

There are no ring outliers.

4 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	580	HEM	5	0
3	A	590	VOR	4	0
2	B	580	HEM	8	0
3	B	590	VOR	6	0

5.7 Other polymers (i)

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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	470/470 (100%)	0.78	65 (13%)	4 4	44, 70, 124, 189	0
1	B	470/470 (100%)	0.87	94 (20%)	1 1	47, 78, 123, 205	0
All	All	940/940 (100%)	0.83	159 (16%)	2 2	44, 74, 124, 205	0

All (159) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	428	ILE	14.6
1	A	427	ASN	14.3
1	B	429	ALA	11.3
1	A	58	TRP	10.7
1	B	427	ASN	10.5
1	B	432	ALA	10.4
1	A	431	SER	9.7
1	A	432	ALA	7.4
1	A	428	ILE	7.0
1	B	241	LEU	7.0
1	A	59	PHE	6.5
1	A	429	ALA	6.5
1	B	430	ALA	6.4
1	A	56	PHE	6.3
1	B	60	PRO	6.0
1	A	60	PRO	5.8
1	A	284	CYS	5.6
1	B	50	LYS	5.4
1	B	431	SER	5.4
1	B	519	HIS	4.9
1	B	269	GLY	4.9
1	B	447	LYS	4.8
1	B	59	PHE	4.5
1	B	58	TRP	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	61	PHE	4.4
1	A	426	GLU	4.2
1	B	267	GLN	4.1
1	B	508	LEU	4.1
1	A	303	ALA	4.1
1	B	440	TYR	4.0
1	B	433	GLU	4.0
1	A	50	LYS	4.0
1	B	391	TYR	3.9
1	B	438	VAL	3.9
1	B	392	VAL	3.9
1	A	390	SER	3.8
1	B	283	SER	3.8
1	A	57	HIS	3.8
1	A	304	LEU	3.8
1	B	303	ALA	3.7
1	B	426	GLU	3.7
1	A	270	SER	3.7
1	B	56	PHE	3.7
1	A	388	GLY	3.5
1	A	279	TRP	3.5
1	B	284	CYS	3.4
1	A	62	ILE	3.3
1	A	392	VAL	3.3
1	A	307	ALA	3.3
1	B	305	LEU	3.3
1	B	319	ILE	3.3
1	A	391	TYR	3.2
1	A	319	ILE	3.2
1	A	152	TYR	3.2
1	B	387	ASP	3.2
1	B	437	LYS	3.1
1	B	268	ALA	3.1
1	B	311	SER	3.1
1	A	433	GLU	3.1
1	A	400	LEU	3.1
1	A	387	ASP	3.0
1	B	98	VAL	3.0
1	B	246	LYS	3.0
1	B	477	THR	3.0
1	B	304	LEU	3.0
1	B	410	GLU	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	263	LYS	3.0
1	A	98	VAL	3.0
1	A	376	ILE	3.0
1	B	400	LEU	3.0
1	B	401	SER	2.9
1	B	227	MET	2.9
1	B	306	MET	2.9
1	B	399	VAL	2.8
1	B	57	HIS	2.8
1	B	376	ILE	2.8
1	B	81	ALA	2.8
1	A	246	LYS	2.8
1	A	384	MET	2.8
1	B	99	TYR	2.8
1	A	430	ALA	2.8
1	B	312	SER	2.8
1	A	469	ALA	2.7
1	B	476	ILE	2.7
1	A	114	ARG	2.7
1	B	390	SER	2.7
1	A	302	ILE	2.7
1	A	268	ALA	2.7
1	A	205	LEU	2.7
1	B	113	LEU	2.7
1	A	93	GLY	2.7
1	B	313	SER	2.6
1	A	306	MET	2.6
1	B	279	TRP	2.6
1	B	375	SER	2.6
1	B	139	PRO	2.6
1	A	410	GLU	2.6
1	B	308	GLY	2.6
1	B	492	VAL	2.6
1	A	373	ILE	2.6
1	B	473	LEU	2.6
1	A	363	ILE	2.6
1	A	290	THR	2.6
1	B	366	THR	2.6
1	A	411	GLU	2.6
1	B	63	GLY	2.5
1	B	373	ILE	2.5
1	B	383	PRO	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	472	GLN	2.5
1	A	300	MET	2.5
1	A	63	GLY	2.5
1	A	131	GLY	2.5
1	A	477	THR	2.5
1	A	311	SER	2.4
1	B	411	GLU	2.4
1	A	445	VAL	2.4
1	A	113	LEU	2.4
1	B	82	LYS	2.3
1	B	371	ALA	2.3
1	B	238	TRP	2.3
1	B	315	THR	2.3
1	A	61	PHE	2.3
1	B	310	HIS	2.3
1	B	367	LEU	2.3
1	B	386	VAL	2.3
1	A	375	SER	2.3
1	B	51	THR	2.2
1	A	377	ILE	2.2
1	A	401	SER	2.2
1	B	54	VAL	2.2
1	B	302	ILE	2.2
1	B	277	MET	2.2
1	A	201	ALA	2.2
1	A	476	ILE	2.2
1	B	316	ALA	2.2
1	B	202	SER	2.2
1	B	197	THR	2.2
1	B	362	VAL	2.1
1	B	206	GLN	2.1
1	B	314	SER	2.1
1	A	305	LEU	2.1
1	A	227	MET	2.1
1	B	140	ASN	2.1
1	A	316	ALA	2.1
1	A	241	LEU	2.1
1	A	463	CYS	2.1
1	B	388	GLY	2.1
1	B	201	ALA	2.1
1	B	97	THR	2.1
1	B	266	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	232	ILE	2.1
1	B	363	ILE	2.0
1	B	253	LYS	2.0
1	B	307	ALA	2.0
1	B	92	LEU	2.0
1	B	242	PRO	2.0
1	A	367	LEU	2.0
1	B	300	MET	2.0
1	B	301	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	VOR	A	590	25/25	0.93	0.30	0.68	48,62,73,80	0
2	HEM	A	580	43/43	0.98	0.23	-0.18	41,52,75,85	0
2	HEM	B	580	43/43	0.96	0.19	-0.28	49,64,74,77	0
3	VOR	B	590	25/25	0.95	0.19	-0.58	59,69,99,106	0

6.5 Other polymers (i)

There are no such residues in this entry.