



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:01 pm GMT

PDB ID : 2C5X  
Title : DIFFERENTIAL BINDING OF INHIBITORS TO ACTIVE AND INACTIVE CDK2 PROVIDES INSIGHTS FOR DRUG DESIGN  
Authors : Kontopidis, G.; Mcinnes, C.; Pandalaneni, S.R.; Mcnae, I.; Gibson, D.; Mezna, M.; Thomas, M.; Wood, G.; Wang, S.; Walkinshaw, M.D.; Fischer, P.M.  
Deposited on : 2005-11-03  
Resolution : 2.90 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

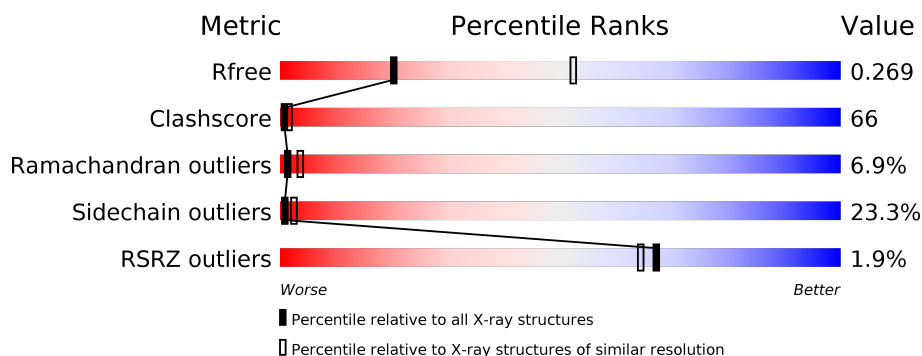
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)

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	298	<div> <div>2%</div> <div>26% 50% 20% . .</div> </div>
1	C	298	<div> <div>3%</div> <div>22% 46% 26% 6% .</div> </div>
2	B	259	<div> <div>2%</div> <div>19% 52% 25% .</div> </div>
2	D	259	<div> <div>%</div> <div>27% 50% 19% .</div> </div>

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MTW	C	1297	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9085 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.

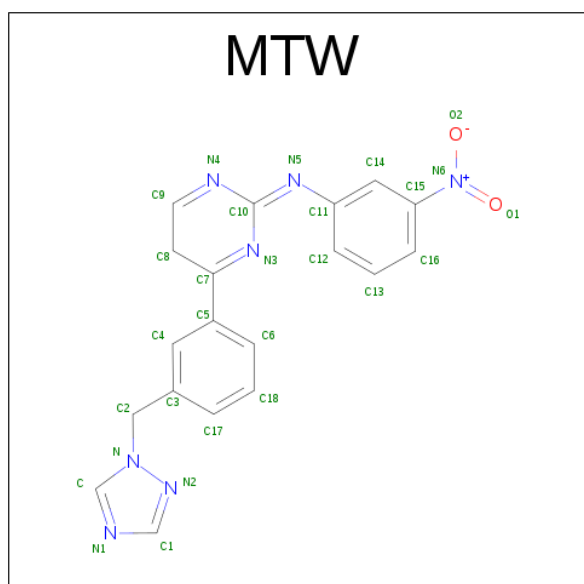
- Molecule 1 is a protein called CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2378	1547	403	420	8			
1	C	296	Total	C	N	O	S	0	1	0
			2388	1553	406	421	8			

- Molecule 2 is a protein called CYCLIN A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S	0	0	0
			2083	1350	339	383	11			
2	D	258	Total	C	N	O	S	0	1	0
			2092	1354	340	387	11			

- Molecule 3 is HYDROXY(OXO)(3-{[(2Z)-4-[3-(1H-1,2,4-TRIAZOL-1-YLMETHYL)PHE NYL]PYRIMIDIN-2(5H)-YLIDENE]AMINO}PHENYL)AMMONIUM (three-letter code: MTW) (formula: C<sub>19</sub>H<sub>15</sub>N<sub>7</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			28	19	7	2		
3	C	1	Total	C	N	O	0	0
			28	19	7	2		

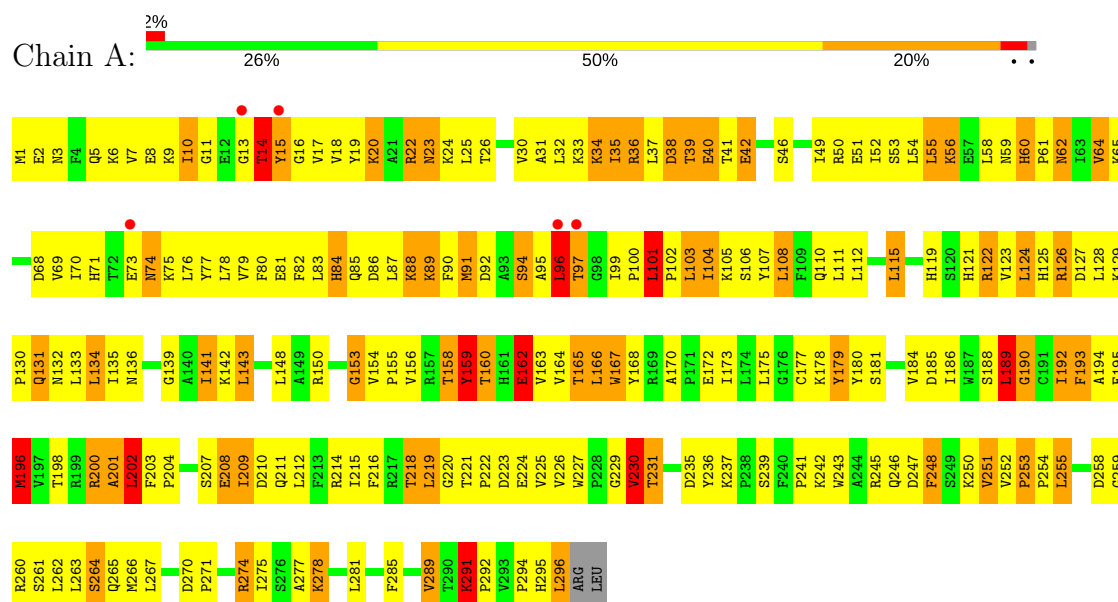
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	26	Total	O	0	0
			26	26		
4	B	17	Total	O	0	0
			17	17		
4	C	28	Total	O	0	0
			28	28		
4	D	17	Total	O	0	0
			17	17		

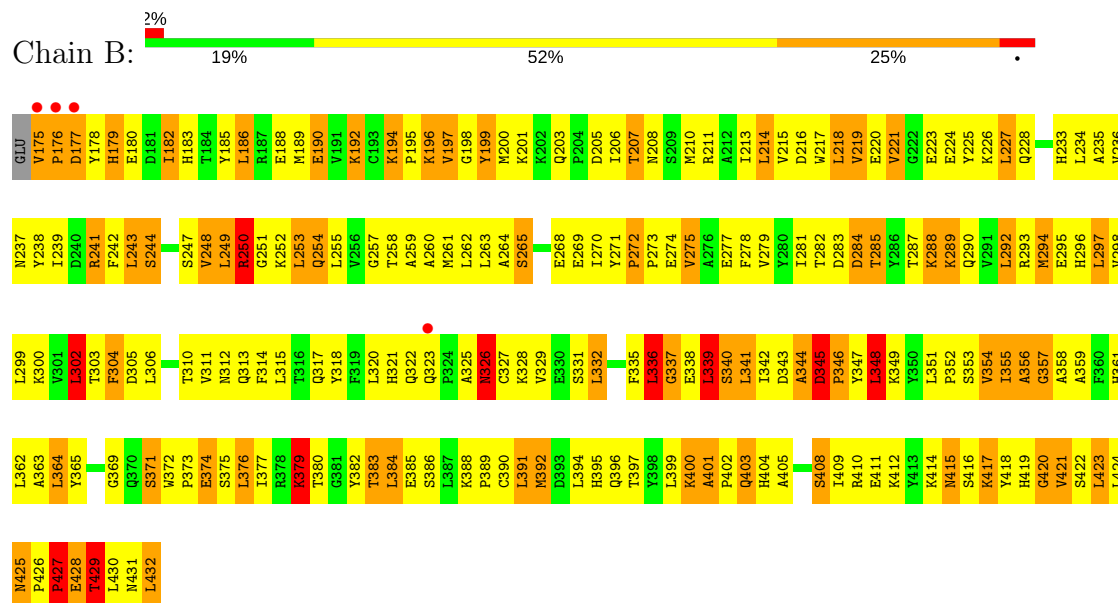
### 3 Residue-property plots

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

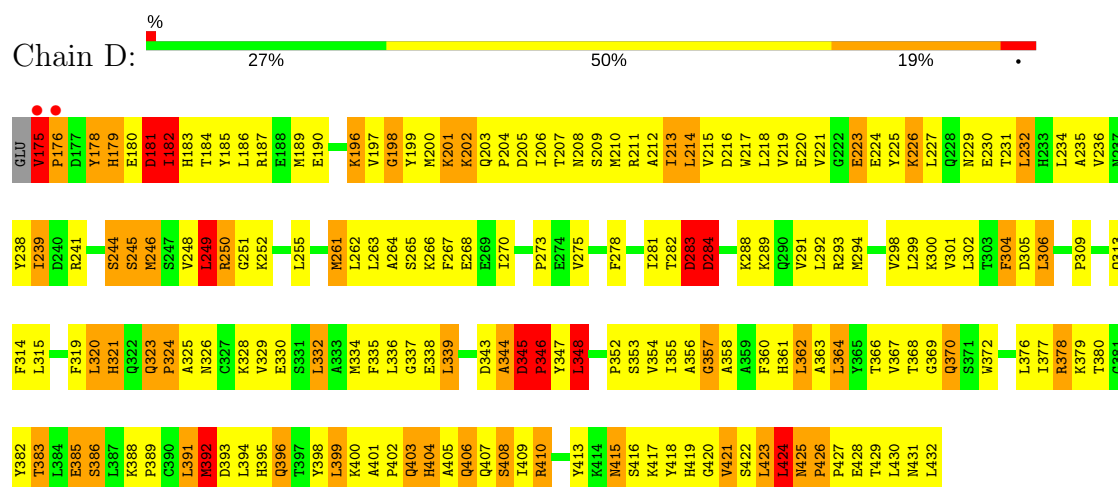
#### • Molecule 1: CELL DIVISION PROTEIN KINASE 2



• Molecule 2: CYCLIN A2



• Molecule 2: CYCLIN A2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	74.33Å 112.35Å 154.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 19.97 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-2.90) 99.1 (19.97-2.90)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.200 , 0.264 0.201 , 0.269	Depositor DCC
$R_{free}$ test set	1197 reflections (4.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.8	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 63.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9085	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

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

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	0.71	0/2440	1.44	23/3313 (0.7%)
1	C	0.75	1/2451 (0.0%)	1.44	28/3328 (0.8%)
2	B	0.69	0/2133	1.38	22/2897 (0.8%)
2	D	0.73	0/2142	1.45	21/2908 (0.7%)
All	All	0.72	1/9166 (0.0%)	1.43	94/12446 (0.8%)

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	8
1	C	0	10
2	B	0	9
2	D	0	8
All	All	0	35

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	177	CYS	CB-SG	-5.16	1.73	1.81

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	LEU	CB-CG-CD1	-10.06	93.90	111.00
2	D	250	ARG	NE-CZ-NH1	-9.99	115.31	120.30
2	D	175	VAL	C-N-CD	9.22	147.76	128.40
2	D	232	LEU	CB-CG-CD1	-9.01	95.68	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	LEU	CB-CG-CD1	-8.88	95.89	111.00
1	A	124	LEU	CB-CG-CD1	-8.44	96.65	111.00
2	D	227	LEU	CB-CG-CD1	-8.33	96.84	111.00
1	A	14	THR	N-CA-C	-8.29	88.61	111.00
1	C	25	LEU	CB-CG-CD2	-8.06	97.29	111.00
2	B	302	LEU	CB-CG-CD1	-7.89	97.58	111.00
2	B	186	LEU	CA-CB-CG	-7.51	98.03	115.30
1	A	255	LEU	CB-CG-CD1	-7.40	98.42	111.00
2	B	339	LEU	CB-CG-CD2	-7.38	98.46	111.00
1	C	64	VAL	CB-CA-C	-7.21	97.69	111.40
1	A	274	ARG	NE-CZ-NH2	-7.21	116.70	120.30
2	D	320	LEU	CA-CB-CG	-7.11	98.94	115.30
2	B	332	LEU	CB-CG-CD1	-6.99	99.11	111.00
2	D	246	MET	CG-SD-CE	6.83	111.13	100.20
1	C	133	LEU	CB-CG-CD2	-6.69	99.62	111.00
1	C	25	LEU	CA-CB-CG	-6.68	99.93	115.30
1	C	124	LEU	CB-CA-C	-6.60	97.67	110.20
2	D	362	LEU	CB-CG-CD2	-6.60	99.78	111.00
1	C	18	VAL	CB-CA-C	-6.58	98.89	111.40
2	B	376	LEU	CB-CG-CD2	6.50	122.06	111.00
1	C	124	LEU	CB-CG-CD1	-6.50	99.95	111.00
1	C	270	ASP	CB-CG-OD2	6.49	124.14	118.30
2	D	181[A]	ASP	CB-CG-OD1	6.47	124.13	118.30
2	D	181[B]	ASP	CB-CG-OD1	6.47	124.13	118.30
1	C	177	CYS	CA-CB-SG	-6.42	102.44	114.00
1	C	124	LEU	CA-CB-CG	6.41	130.04	115.30
1	C	274	ARG	NE-CZ-NH2	-6.37	117.11	120.30
2	D	393	ASP	CB-CG-OD2	6.36	124.03	118.30
1	C	270	ASP	N-CA-CB	6.28	121.89	110.60
1	C	189	LEU	CB-CG-CD1	-6.25	100.38	111.00
1	A	281	LEU	CB-CG-CD2	-6.21	100.44	111.00
1	A	133	LEU	CB-CG-CD1	-6.20	100.46	111.00
1	A	124	LEU	CB-CA-C	-6.20	98.42	110.20
2	D	175	VAL	C-N-CA	-6.14	96.19	122.00
2	B	186	LEU	CB-CG-CD1	6.14	121.44	111.00
2	B	248	VAL	CB-CA-C	-6.06	99.88	111.40
1	A	30	VAL	CG1-CB-CG2	-6.06	101.21	110.90
1	C	206	ASP	CB-CG-OD2	-6.06	112.85	118.30
1	C	167	TRP	CA-CB-CG	-5.95	102.40	113.70
2	D	362	LEU	CB-CG-CD1	-5.94	100.90	111.00
1	C	26	THR	CA-CB-CG2	-5.91	104.12	112.40
1	C	58	LEU	CA-CB-CG	-5.90	101.73	115.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	214	LEU	CB-CG-CD2	-5.88	101.01	111.00
1	A	159	TYR	C-N-CA	-5.86	107.05	121.70
1	A	267	LEU	CB-CG-CD1	-5.86	101.04	111.00
2	B	243	LEU	CB-CG-CD2	5.85	120.95	111.00
1	A	160	THR	N-CA-CB	5.85	121.41	110.30
1	C	99	ILE	CB-CA-C	-5.78	100.05	111.60
2	D	410	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	A	101	LEU	CB-CG-CD1	-5.74	101.24	111.00
2	B	332	LEU	CA-CB-CG	-5.71	102.16	115.30
2	D	306	LEU	CA-CB-CG	-5.70	102.19	115.30
1	A	134	LEU	CB-CG-CD1	-5.68	101.34	111.00
2	D	214	LEU	CA-CB-CG	-5.64	102.34	115.30
2	D	348	LEU	CB-CG-CD1	5.61	120.54	111.00
1	C	165	THR	N-CA-CB	5.59	120.92	110.30
2	B	339	LEU	CA-CB-CG	-5.58	102.47	115.30
1	C	166	LEU	N-CA-C	-5.56	95.99	111.00
2	B	320	LEU	CA-CB-CG	-5.56	102.52	115.30
2	B	219	VAL	CB-CA-C	-5.55	100.85	111.40
2	B	348	LEU	CB-CG-CD1	-5.54	101.58	111.00
2	B	253	LEU	CB-CG-CD2	-5.50	101.66	111.00
1	C	189	LEU	CA-CB-CG	-5.45	102.77	115.30
2	B	218	LEU	CA-CB-CG	-5.43	102.81	115.30
2	B	379	LYS	CD-CE-NZ	5.41	124.15	111.70
1	C	17	VAL	N-CA-C	5.41	125.60	111.00
1	A	22	ARG	NE-CZ-NH2	-5.38	117.61	120.30
2	D	425	ASN	CB-CA-C	-5.38	99.65	110.40
2	D	399	LEU	CA-CB-CG	-5.37	102.95	115.30
2	B	221	VAL	CB-CA-C	-5.32	101.30	111.40
2	D	249	LEU	CA-CB-CG	-5.28	103.16	115.30
1	C	76	LEU	CB-CG-CD2	-5.28	102.03	111.00
2	B	384	LEU	CA-CB-CG	-5.23	103.27	115.30
1	C	281	LEU	CB-CG-CD1	5.23	119.89	111.00
1	A	40	GLU	CB-CA-C	5.21	120.82	110.40
1	A	189	LEU	CA-CB-CG	-5.21	103.33	115.30
1	C	145	ASP	CB-CG-OD2	-5.17	113.65	118.30
2	D	182	ILE	CG1-CB-CG2	-5.16	100.05	111.40
1	A	219	LEU	CA-CB-CG	-5.15	103.46	115.30
2	B	417	LYS	CD-CE-NZ	5.13	123.51	111.70
2	B	253	LEU	CB-CG-CD1	-5.10	102.33	111.00
1	A	22	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	A	143	LEU	CB-CG-CD2	-5.07	102.37	111.00
2	D	339	LEU	CA-CB-CG	-5.07	103.63	115.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	237	LYS	C-N-CD	5.06	139.03	128.40
1	A	202	LEU	CB-CG-CD2	-5.06	102.40	111.00
1	C	233	MET	O-C-N	-5.05	111.50	121.10
1	A	24	LYS	CD-CE-NZ	5.05	123.32	111.70
2	B	275	VAL	CB-CA-C	-5.04	101.82	111.40
1	C	66	LEU	CB-CG-CD2	-5.02	102.47	111.00

There are no chirality outliers.

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	GLY	Peptide
1	A	13	GLY	Peptide
1	A	166	LEU	Peptide
1	A	19	TYR	Peptide
1	A	295	HIS	Peptide
1	A	59	ASN	Peptide
1	A	62	ASN	Peptide
1	A	91	MET	Peptide
2	B	270	ILE	Peptide
2	B	272	PRO	Peptide
2	B	336	LEU	Peptide
2	B	340	SER	Peptide
2	B	344	ALA	Peptide
2	B	345	ASP	Peptide
2	B	423	LEU	Peptide
2	B	427	PRO	Peptide
2	B	429	THR	Peptide
1	C	11	GLY	Peptide
1	C	15	TYR	Peptide
1	C	161	HIS	Peptide
1	C	164	VAL	Peptide
1	C	165	THR	Peptide
1	C	206	ASP	Peptide
1	C	233	MET	Mainchain
1	C	64	VAL	Mainchain
1	C	70	ILE	Peptide
1	C	8	GLU	Peptide
2	D	198	GLY	Peptide
2	D	283	ASP	Peptide
2	D	324	PRO	Peptide
2	D	344	ALA	Peptide

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
2	D	345	ASP	Peptide
2	D	346	PRO	Peptide
2	D	369	GLY	Peptide
2	D	423	LEU	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2378	0	2426	312	0
1	C	2388	0	2432	370	1
2	B	2083	0	2107	285	1
2	D	2092	0	2110	246	0
3	A	28	0	15	6	0
3	C	28	0	15	13	0
4	A	26	0	0	10	0
4	B	17	0	0	8	0
4	C	28	0	0	17	0
4	D	17	0	0	7	0
All	All	9085	0	9105	1193	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 66.

All (1193) 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:60:HIS:CD2	1:A:61:PRO:HD2	1.21	1.61
1:A:60:HIS:CD2	1:A:61:PRO:CD	1.91	1.50
1:C:164:VAL:HB	4:C:2013:HOH:O	1.27	1.33
1:C:83:LEU:O	3:C:1297:MTW:H12	1.26	1.33
1:A:121:HIS:O	1:A:122:ARG:HG3	1.25	1.33
2:B:206:ILE:HA	2:B:210:MET:CE	1.61	1.31
2:B:282:THR:O	2:B:285:THR:HG22	1.27	1.31
2:B:175:VAL:O	2:B:177:ASP:N	1.64	1.27
2:B:206:ILE:CA	2:B:210:MET:HE1	1.70	1.21

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:ALA:O	1:C:96:LEU:HG	1.41	1.20
2:B:239:ILE:HD11	2:B:257:GLY:HA2	1.25	1.19
1:C:122:ARG:HH21	1:C:122:ARG:CG	1.56	1.19
2:B:327:CYS:HB3	4:B:2011:HOH:O	1.42	1.19
2:B:430:LEU:HB3	2:B:432:LEU:HD22	1.26	1.17
1:A:294:PRO:HB2	1:A:296:LEU:CD1	1.72	1.17
2:B:282:THR:O	2:B:285:THR:CG2	1.94	1.16
1:C:248:PHE:CE2	1:C:263:LEU:HD23	1.80	1.15
1:A:56:LYS:NZ	1:A:56:LYS:O	1.80	1.14
1:A:294:PRO:HB2	1:A:296:LEU:HD13	1.30	1.14
1:C:162:GLU:OE1	1:C:164:VAL:HG13	1.46	1.13
2:B:207:THR:HG22	2:B:210:MET:HE2	1.14	1.13
3:C:1297:MTW:H	3:C:1297:MTW:O1	1.49	1.12
1:A:71:HIS:CD2	2:B:296:HIS:CE1	2.38	1.11
1:A:178:LYS:HG2	1:A:179:TYR:CE2	1.86	1.10
2:D:345:ASP:OD2	2:D:346:PRO:HD3	1.48	1.10
1:A:163:VAL:O	1:A:163:VAL:HG13	1.44	1.08
1:A:42:GLU:OE2	1:A:42:GLU:HA	1.47	1.07
2:D:345:ASP:OD2	2:D:346:PRO:CD	2.03	1.06
2:B:223:GLU:OE2	2:B:412:LYS:HG3	1.52	1.06
2:D:323:GLN:HG2	2:D:323:GLN:O	1.53	1.06
1:A:71:HIS:NE2	2:B:296:HIS:ND1	2.04	1.05
1:A:164:VAL:O	1:A:165:THR:HG22	1.57	1.05
1:C:230:VAL:O	1:C:232:SER:N	1.90	1.05
1:A:60:HIS:HD2	1:A:61:PRO:N	1.56	1.04
1:C:162:GLU:OE2	1:C:163:VAL:N	1.90	1.04
1:C:60:HIS:CD2	1:C:62:ASN:H	1.75	1.04
1:A:166:LEU:HB3	1:A:167:TRP:HD1	1.19	1.03
1:A:34:LYS:HG3	1:A:77:TYR:HE2	1.24	1.02
1:A:34:LYS:HG3	1:A:77:TYR:CE2	1.93	1.02
1:C:12:GLU:HB3	1:C:17:VAL:HG12	1.40	1.01
1:C:60:HIS:HD2	1:C:62:ASN:H	1.06	1.01
2:B:395:HIS:CE1	2:B:399:LEU:HD11	1.94	1.01
2:D:196:LYS:HG3	4:D:2003:HOH:O	1.61	1.01
2:B:207:THR:HG22	2:B:210:MET:CE	1.92	1.00
1:C:60:HIS:CG	1:C:61:PRO:HD2	1.95	1.00
1:A:294:PRO:CB	1:A:296:LEU:CD1	2.41	0.99
1:A:60:HIS:CD2	1:A:61:PRO:N	2.31	0.99
2:D:404:HIS:CD2	2:D:406:GLN:H	1.79	0.98
2:B:207:THR:H	2:B:210:MET:HE3	1.28	0.98
2:B:425:ASN:HB2	4:B:2017:HOH:O	1.64	0.98

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:LEU:CD2	1:C:79:VAL:HG22	1.95	0.97
2:D:401:ALA:HB1	2:D:410:ARG:HD2	1.46	0.97
1:A:241:PRO:HG2	1:A:243:TRP:CZ3	2.00	0.97
1:A:164:VAL:O	1:A:165:THR:CG2	2.13	0.96
2:B:373:PRO:HG2	2:B:376:LEU:HD12	1.48	0.96
1:A:164:VAL:O	1:A:165:THR:CB	2.13	0.96
1:C:40:GLU:O	2:D:288:LYS:NZ	1.96	0.96
2:B:263:LEU:HD21	2:B:295:GLU:HG3	1.48	0.96
1:A:121:HIS:C	1:A:122:ARG:HG3	1.83	0.95
1:C:122:ARG:HH21	1:C:122:ARG:HG3	1.28	0.95
1:A:60:HIS:NE2	1:A:61:PRO:HD2	1.81	0.95
1:A:294:PRO:CB	1:A:296:LEU:HD13	1.98	0.94
1:A:178:LYS:CG	1:A:179:TYR:CE2	2.49	0.94
1:C:101:LEU:H	1:C:101:LEU:CD2	1.80	0.94
1:A:241:PRO:HG2	1:A:243:TRP:CH2	2.03	0.94
2:D:385:GLU:HA	2:D:385:GLU:OE1	1.65	0.94
1:A:95:ALA:O	1:A:96:LEU:HB3	1.67	0.93
1:C:200:ARG:CG	1:C:200:ARG:HH11	1.81	0.93
1:C:75:LYS:HB3	4:C:2003:HOH:O	1.67	0.93
1:A:52:ILE:HD11	1:A:78:LEU:HD21	1.48	0.93
1:C:15:TYR:N	1:C:15:TYR:CD1	2.37	0.93
1:C:122:ARG:HG2	1:C:122:ARG:HH21	1.31	0.93
1:A:139:GLY:HA2	4:A:2014:HOH:O	1.67	0.93
2:B:199:TYR:CD1	2:B:200:MET:N	2.38	0.92
1:C:200:ARG:HH11	1:C:200:ARG:HG2	1.34	0.92
1:A:14:THR:O	1:A:16:GLY:N	2.01	0.92
1:A:60:HIS:CG	1:A:61:PRO:CD	2.52	0.91
2:D:336:LEU:HD13	2:D:362:LEU:HD23	1.51	0.91
1:C:39:THR:O	1:C:39:THR:CG2	2.18	0.91
1:A:163:VAL:O	1:A:163:VAL:CG1	2.19	0.91
1:A:97:THR:HB	4:A:2011:HOH:O	1.69	0.90
1:C:14:THR:HB	1:C:15:TYR:CE1	2.06	0.90
2:B:199:TYR:CD1	2:B:199:TYR:C	2.45	0.90
1:C:160:THR:C	1:C:161:HIS:CD2	2.45	0.90
1:C:101:LEU:N	1:C:101:LEU:CD2	2.33	0.89
2:D:335:PHE:HB2	2:D:413:TYR:CD2	2.07	0.89
2:B:395:HIS:CG	2:B:430:LEU:HD21	2.08	0.89
1:A:170:ALA:HB3	1:A:173:ILE:HD12	1.55	0.88
1:A:96:LEU:HB3	4:A:2009:HOH:O	1.73	0.88
1:C:122:ARG:HG2	1:C:122:ARG:NH2	1.87	0.88
1:C:39:THR:HG23	1:C:39:THR:O	1.71	0.88

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:LEU:N	1:C:101:LEU:HD22	1.87	0.88
1:C:32:LEU:HD23	1:C:79:VAL:HG22	1.52	0.88
1:A:294:PRO:HB2	1:A:296:LEU:HD12	1.55	0.88
3:A:1297:MTW:N3	3:A:1297:MTW:H14	1.88	0.87
2:D:214:LEU:HD12	2:D:214:LEU:O	1.74	0.87
2:B:217:TRP:HZ2	2:B:281:ILE:HD12	1.39	0.87
1:C:85:GLN:HG3	1:C:86:ASP:N	1.88	0.86
1:A:166:LEU:HB3	1:A:167:TRP:CD1	2.09	0.86
2:B:206:ILE:CA	2:B:210:MET:CE	2.40	0.86
1:C:125:HIS:CG	1:C:128:LEU:HD21	2.10	0.86
2:B:430:LEU:HB3	2:B:432:LEU:CD2	2.06	0.85
3:C:1297:MTW:C	3:C:1297:MTW:O1	2.24	0.85
2:D:262:LEU:HD11	2:D:266:LYS:HE3	1.58	0.84
2:D:379:LYS:HG3	4:D:2002:HOH:O	1.76	0.84
1:C:101:LEU:H	1:C:101:LEU:HD23	1.41	0.84
1:C:115:LEU:HD12	1:C:189:LEU:CD2	2.08	0.84
2:B:415:ASN:OD1	2:B:417:LYS:N	2.10	0.84
1:C:135:ILE:CG2	1:C:141:ILE:HD12	2.08	0.84
1:A:38:ASP:OD2	1:A:41:THR:HB	1.78	0.83
1:C:159:TYR:CD2	1:C:162:GLU:HG2	2.13	0.83
2:D:415:ASN:OD1	2:D:417:LYS:N	2.11	0.83
2:B:239:ILE:CD1	2:B:257:GLY:HA2	2.09	0.83
2:D:214:LEU:HD12	2:D:214:LEU:C	1.98	0.83
1:C:70:ILE:N	1:C:77:TYR:O	2.11	0.83
1:A:236:TYR:CD1	1:A:237:LYS:N	2.47	0.83
2:B:223:GLU:OE1	2:B:223:GLU:HA	1.77	0.82
2:B:190:GLU:OE1	2:B:352:PRO:HD2	1.80	0.81
2:B:194:LYS:HG2	2:B:195:PRO:HD2	1.61	0.81
1:C:159:TYR:O	1:C:161:HIS:N	2.14	0.81
2:B:233:HIS:CD2	4:B:2010:HOH:O	2.34	0.81
2:D:223:GLU:OE1	2:D:223:GLU:HA	1.79	0.81
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.63	0.81
2:B:419:HIS:O	2:B:421:VAL:N	2.14	0.80
1:A:60:HIS:HD2	1:A:61:PRO:CD	1.66	0.80
1:A:159:TYR:HD1	1:A:159:TYR:N	1.76	0.80
2:D:217:TRP:CH2	2:D:281:ILE:HD12	2.16	0.80
2:D:218:LEU:HD22	2:D:261:MET:CE	2.12	0.80
1:C:248:PHE:CZ	1:C:263:LEU:HD23	2.16	0.80
2:B:353:SER:O	2:B:356:ALA:HB3	1.82	0.80
1:C:115:LEU:HD12	1:C:189:LEU:HD22	1.64	0.80
2:B:252:LYS:HG3	1:C:25:LEU:O	1.82	0.79

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:207:THR:N	2:B:210:MET:HE3	1.97	0.79
1:A:154:VAL:HG13	1:A:155:PRO:HD2	1.62	0.79
1:A:23:ASN:C	1:A:23:ASN:OD1	2.20	0.79
2:B:401:ALA:HB3	2:B:402:PRO:HD3	1.61	0.79
1:C:111:LEU:HD23	1:C:143:LEU:HD23	1.64	0.79
1:C:206:ASP:HB2	1:C:210:ASP:OD2	1.82	0.79
2:B:211:ARG:O	2:B:215:VAL:HG23	1.83	0.79
1:C:128:LEU:HD23	1:C:128:LEU:N	1.97	0.79
1:A:139:GLY:CA	4:A:2014:HOH:O	2.25	0.79
1:A:115:LEU:HD13	1:A:119:HIS:CE1	2.18	0.79
2:B:217:TRP:CZ2	2:B:281:ILE:HD12	2.17	0.79
2:B:331:SER:HB2	2:B:421:VAL:HG11	1.64	0.79
1:C:156:VAL:HG12	1:C:156:VAL:O	1.81	0.79
2:D:431:ASN:O	2:D:432:LEU:HD23	1.83	0.79
1:A:83:LEU:HD21	1:A:142:LYS:HD2	1.63	0.79
1:C:122:ARG:NH2	1:C:122:ARG:CG	2.27	0.79
2:B:273:PRO:HB2	2:B:278:PHE:CE2	2.18	0.79
2:D:404:HIS:CD2	2:D:406:GLN:N	2.50	0.78
1:A:81:GLU:O	3:A:1297:MTW:H9	1.84	0.78
1:A:42:GLU:OE2	1:A:42:GLU:CA	2.28	0.78
1:A:60:HIS:CG	1:A:61:PRO:HD2	2.08	0.78
1:C:95:ALA:O	1:C:96:LEU:CG	2.29	0.78
1:C:115:LEU:CD1	1:C:189:LEU:HD22	2.12	0.78
1:C:83:LEU:O	3:C:1297:MTW:C12	2.22	0.78
1:A:159:TYR:CD1	1:A:159:TYR:N	2.49	0.78
1:A:62:ASN:ND2	1:A:110:GLN:HB3	1.99	0.78
2:D:389:PRO:O	2:D:392:MET:HB2	1.82	0.78
1:C:91:MET:HE2	1:C:195:GLU:HG2	1.66	0.78
2:D:207:THR:HG23	2:D:210:MET:H	1.48	0.78
1:A:178:LYS:HG2	1:A:179:TYR:HE2	1.48	0.77
2:D:323:GLN:CG	2:D:323:GLN:O	2.32	0.77
1:A:164:VAL:O	1:A:165:THR:HB	1.83	0.77
1:A:178:LYS:HG2	1:A:179:TYR:CD2	2.20	0.77
1:C:233:MET:O	1:C:234:PRO:C	2.23	0.77
1:C:60:HIS:C	1:C:60:HIS:CD2	2.59	0.77
1:C:74:ASN:OD1	1:C:75:LYS:HD3	1.85	0.77
2:B:207:THR:N	2:B:210:MET:CE	2.47	0.76
1:A:121:HIS:O	1:A:123:VAL:HG23	1.85	0.76
1:C:12:GLU:HB3	1:C:17:VAL:CG1	2.15	0.76
1:C:226:VAL:O	1:C:226:VAL:HG13	1.86	0.76
2:B:321:HIS:CE1	2:B:379:LYS:HE2	2.21	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:430:LEU:CB	2:B:432:LEU:HD22	2.13	0.75
1:C:165:THR:O	4:C:2012:HOH:O	2.04	0.75
2:B:282:THR:HB	2:B:285:THR:HG23	1.68	0.75
1:C:29:VAL:HG12	1:C:30:VAL:N	2.01	0.75
2:B:345:ASP:CB	2:B:346:PRO:CD	2.64	0.75
1:C:88:LYS:HD2	1:C:92:ASP:OD2	1.86	0.75
2:B:205:ASP:OD2	2:B:250:ARG:HG2	1.87	0.75
2:B:219:VAL:HG21	2:B:409:ILE:HG13	1.68	0.75
1:C:122:ARG:O	1:C:122:ARG:HG3	1.85	0.75
1:C:10:ILE:HD13	1:C:20:LYS:HB3	1.68	0.74
1:C:166:LEU:O	1:C:168:TYR:N	2.20	0.74
2:D:345:ASP:OD2	2:D:346:PRO:HD2	1.83	0.74
1:C:162:GLU:OE2	1:C:163:VAL:C	2.25	0.74
1:C:111:LEU:HD23	1:C:143:LEU:CD2	2.18	0.74
1:C:159:TYR:HD2	1:C:162:GLU:CB	2.00	0.74
2:D:361:HIS:CD2	2:D:391:LEU:HD21	2.21	0.74
2:D:419:HIS:O	4:D:2015:HOH:O	2.04	0.74
2:B:268:GLU:HA	2:B:268:GLU:OE1	1.88	0.74
1:C:200:ARG:HH11	1:C:200:ARG:CB	2.00	0.74
1:C:51:GLU:O	1:C:55:LEU:HB2	1.87	0.74
1:A:71:HIS:NE2	2:B:296:HIS:CE1	2.49	0.74
1:C:137:THR:HG23	4:C:2010:HOH:O	1.86	0.74
2:D:319:PHE:CE2	2:D:330:GLU:HG2	2.22	0.74
2:B:199:TYR:C	2:B:199:TYR:HD1	1.89	0.74
1:C:31:ALA:HB3	1:C:80:PHE:HB2	1.70	0.74
2:D:238:TYR:OH	2:D:306:LEU:HB3	1.88	0.74
1:A:38:ASP:O	1:A:38:ASP:OD1	2.06	0.74
2:B:342:ILE:HD11	2:B:409:ILE:HD12	1.69	0.74
2:B:388:LYS:N	2:B:389:PRO:HD2	2.02	0.74
1:C:86:ASP:C	1:C:86:ASP:OD1	2.25	0.74
2:B:293:ARG:HB3	1:C:25:LEU:HD11	1.70	0.74
1:C:159:TYR:C	1:C:161:HIS:H	1.91	0.74
1:A:87:LEU:O	1:A:91:MET:HG3	1.87	0.73
2:B:384:LEU:HD12	2:B:384:LEU:O	1.88	0.73
1:C:159:TYR:HD2	1:C:162:GLU:HB3	1.53	0.73
1:A:170:ALA:HB3	1:A:173:ILE:CD1	2.18	0.73
1:A:181:SER:HB3	4:A:2016:HOH:O	1.89	0.73
2:D:236:VAL:HA	2:D:239:ILE:HG13	1.70	0.73
1:C:159:TYR:HD2	1:C:162:GLU:HG2	1.51	0.73
1:A:60:HIS:CD2	1:A:62:ASN:H	2.07	0.73
2:D:305:ASP:C	2:D:306:LEU:HD23	2.09	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:VAL:HG12	1:A:180:TYR:HD1	1.53	0.73
1:A:222:PRO:HA	4:A:2018:HOH:O	1.88	0.72
1:A:227:TRP:O	1:A:230:VAL:HG22	1.88	0.72
2:D:407:GLN:O	2:D:409:ILE:N	2.21	0.72
1:A:227:TRP:CD2	1:A:230:VAL:HG13	2.23	0.72
2:B:255:LEU:HG	2:B:294:MET:HG3	1.72	0.72
2:B:331:SER:CB	2:B:421:VAL:HG11	2.20	0.72
1:C:162:GLU:CD	1:C:163:VAL:C	2.48	0.72
2:D:321:HIS:CD2	2:D:321:HIS:N	2.56	0.72
1:A:105:LYS:HE3	1:A:285:PHE:CZ	2.25	0.72
2:D:336:LEU:HD13	2:D:362:LEU:CD2	2.18	0.72
1:A:154:VAL:HG13	1:A:155:PRO:CD	2.20	0.72
1:A:115:LEU:HD11	1:A:185:ASP:HB3	1.71	0.72
1:A:38:ASP:C	1:A:38:ASP:OD1	2.26	0.72
2:B:233:HIS:HD2	4:B:2010:HOH:O	1.68	0.72
2:D:335:PHE:HD1	2:D:413:TYR:CG	2.08	0.72
1:A:224:GLU:OE2	1:A:231:THR:OG1	2.07	0.71
3:C:1297:MTW:N3	3:C:1297:MTW:H14	2.05	0.71
1:A:96:LEU:CD2	4:A:2009:HOH:O	2.38	0.71
1:C:127:ASP:OD2	1:C:129:LYS:HE2	1.89	0.71
1:A:69:VAL:HG13	1:A:78:LEU:HD23	1.72	0.71
1:C:48:ALA:O	1:C:52:ILE:HD12	1.90	0.71
2:D:218:LEU:HD22	2:D:261:MET:HE1	1.72	0.71
2:B:182:ILE:HG22	2:B:183:HIS:N	2.05	0.70
1:C:1:MET:HE2	1:C:70:ILE:HD13	1.73	0.70
1:C:212:LEU:HD22	1:C:216:PHE:CZ	2.26	0.70
1:A:156:VAL:HG12	1:A:180:TYR:CD1	2.26	0.70
2:D:343:ASP:HB3	2:D:345:ASP:OD2	1.90	0.70
2:D:344:ALA:HB1	2:D:348:LEU:HD22	1.72	0.70
1:C:200:ARG:NH1	1:C:200:ARG:CB	2.55	0.70
1:C:60:HIS:HD2	1:C:62:ASN:N	1.86	0.70
2:D:315:LEU:HD23	2:D:356:ALA:HB1	1.73	0.70
2:B:178:TYR:O	2:B:179:HIS:C	2.27	0.69
1:C:127:ASP:OD2	1:C:129:LYS:CE	2.40	0.69
1:C:12:GLU:CB	1:C:17:VAL:HG12	2.20	0.69
1:C:60:HIS:CG	1:C:61:PRO:CD	2.74	0.69
1:C:260:ARG:O	1:C:264:SER:OG	2.09	0.69
1:A:202:LEU:HD13	1:A:203:PHE:CE2	2.27	0.69
1:A:247:ASP:O	1:A:250:LYS:HB2	1.93	0.69
1:C:200:ARG:CG	1:C:200:ARG:NH1	2.52	0.69
1:C:245:ARG:HG3	1:C:245:ARG:NH1	2.07	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:PRO:CA	4:A:2018:HOH:O	2.40	0.69
1:C:91:MET:CE	1:C:195:GLU:HG2	2.22	0.69
2:B:338:GLU:O	2:B:341:LEU:HB2	1.92	0.69
2:B:207:THR:H	2:B:210:MET:CE	2.02	0.69
2:B:206:ILE:HA	2:B:210:MET:HE1	0.77	0.69
1:C:159:TYR:C	1:C:161:HIS:N	2.46	0.69
2:B:225:TYR:HE1	2:B:281:ILE:HG21	1.57	0.69
1:C:60:HIS:CD2	1:C:61:PRO:HD2	2.28	0.69
2:D:378:ARG:HB3	2:D:378:ARG:HH11	1.57	0.69
1:A:121:HIS:C	1:A:122:ARG:CG	2.60	0.69
1:C:160:THR:O	1:C:161:HIS:CB	2.39	0.69
1:A:227:TRP:CE3	1:A:230:VAL:HG13	2.28	0.69
1:C:70:ILE:CG2	1:C:71:HIS:N	2.56	0.69
2:D:306:LEU:HD23	2:D:306:LEU:N	2.06	0.69
1:A:38:ASP:OD1	1:A:41:THR:N	2.21	0.69
2:B:271:TYR:HB2	2:B:272:PRO:HD2	1.75	0.68
2:B:345:ASP:HB3	2:B:346:PRO:HD3	1.74	0.68
1:C:259:GLY:HA2	1:C:285:PHE:CD1	2.28	0.68
2:D:319:PHE:CD2	2:D:330:GLU:HG2	2.28	0.68
1:A:34:LYS:CG	1:A:77:TYR:CE2	2.75	0.68
2:B:208:ASN:HB3	2:B:345:ASP:OD1	1.93	0.68
1:A:95:ALA:O	1:A:96:LEU:CB	2.39	0.68
1:C:166:LEU:O	1:C:169:ARG:N	2.26	0.68
1:C:159:TYR:CD2	1:C:162:GLU:HB3	2.29	0.68
2:B:395:HIS:CD2	2:B:430:LEU:HD21	2.28	0.68
1:C:159:TYR:HD2	1:C:162:GLU:CG	2.06	0.68
1:C:72:THR:OG1	1:C:75:LYS:HG2	1.93	0.68
1:A:14:THR:O	1:A:15:TYR:C	2.31	0.68
1:C:94:SER:O	1:C:97:THR:HG23	1.93	0.68
2:B:336:LEU:O	2:B:339:LEU:HB2	1.94	0.68
1:C:162:GLU:CD	1:C:163:VAL:N	2.47	0.68
2:D:214:LEU:O	2:D:217:TRP:HB3	1.94	0.68
2:D:335:PHE:CD1	2:D:413:TYR:CG	2.82	0.68
2:B:354:VAL:O	2:B:355:ILE:C	2.30	0.68
1:C:85:GLN:HA	3:C:1297:MTW:H13	1.76	0.68
1:A:227:TRP:CE3	1:A:230:VAL:CG1	2.76	0.67
1:C:60:HIS:CD2	1:C:61:PRO:N	2.62	0.67
1:C:165:THR:C	4:C:2012:HOH:O	2.32	0.67
2:D:362:LEU:HG	2:D:362:LEU:O	1.95	0.67
1:A:209:ILE:O	1:A:209:ILE:HG13	1.95	0.67
1:A:70:ILE:HB	1:A:77:TYR:HB2	1.76	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:415:ASN:OD1	2:B:415:ASN:C	2.32	0.67
1:C:60:HIS:CD2	1:C:61:PRO:CD	2.78	0.67
2:B:345:ASP:HB2	2:B:346:PRO:HD2	1.75	0.67
1:C:12:GLU:N	1:C:12:GLU:OE2	2.24	0.67
1:A:1:MET:HE2	1:A:70:ILE:HD12	1.75	0.66
1:A:294:PRO:CG	1:A:296:LEU:HD13	2.24	0.66
2:D:282:THR:O	2:D:283:ASP:HB2	1.93	0.66
2:D:415:ASN:C	2:D:415:ASN:OD1	2.34	0.66
2:B:203:GLN:HB3	2:B:206:ILE:HG12	1.76	0.66
2:B:415:ASN:OD1	2:B:416:SER:N	2.28	0.66
1:C:101:LEU:HB2	1:C:102:PRO:HD3	1.76	0.66
2:B:297:LEU:O	2:B:297:LEU:HD12	1.95	0.66
1:C:162:GLU:OE2	1:C:163:VAL:CA	2.44	0.66
2:D:329:VAL:HG23	2:D:367:VAL:HB	1.75	0.66
1:C:162:GLU:OE2	1:C:163:VAL:O	2.14	0.66
1:C:165:THR:O	4:C:2013:HOH:O	2.13	0.66
2:D:229:ASN:HD22	2:D:334:MET:CE	2.09	0.66
2:B:189:MET:O	2:B:192:LYS:N	2.28	0.66
2:B:197:VAL:HG23	2:B:198:GLY:N	2.10	0.66
2:B:364:LEU:O	2:B:365:TYR:C	2.34	0.66
1:A:89:LYS:O	1:A:90:PHE:C	2.33	0.66
1:A:166:LEU:CB	1:A:167:TRP:HD1	2.01	0.66
1:A:175:LEU:HA	1:A:235:ASP:HB2	1.77	0.66
1:A:277:ALA:O	1:A:278:LYS:C	2.33	0.66
1:C:160:THR:O	1:C:161:HIS:HB2	1.96	0.66
1:A:101:LEU:CB	1:A:102:PRO:HD3	2.26	0.65
1:A:170:ALA:HB1	1:A:172:GLU:OE2	1.95	0.65
1:A:129:LYS:HD2	1:A:131:GLN:HG3	1.77	0.65
2:B:314:PHE:CE2	2:B:353:SER:HB3	2.32	0.65
1:C:101:LEU:N	1:C:102:PRO:HD2	2.10	0.65
1:C:61:PRO:O	1:C:142:LYS:HE2	1.97	0.65
1:C:6:LYS:HE3	4:C:2001:HOH:O	1.97	0.65
1:A:96:LEU:HD22	4:A:2009:HOH:O	1.94	0.65
2:D:338:GLU:O	2:D:339:LEU:C	2.35	0.65
1:C:85:GLN:NE2	1:C:89:LYS:HB3	2.11	0.65
2:B:400:LYS:O	2:B:401:ALA:C	2.33	0.65
2:D:215:VAL:O	2:D:219:VAL:HG23	1.95	0.65
1:A:1:MET:HG2	1:A:70:ILE:CD1	2.27	0.65
1:C:131:GLN:NE2	1:C:131:GLN:N	2.44	0.65
1:C:70:ILE:O	1:C:76:LEU:HD12	1.97	0.65
2:B:344:ALA:CB	2:B:348:LEU:HD22	2.25	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:335:PHE:CD1	2:D:413:TYR:CB	2.80	0.65
1:A:50:ARG:O	1:A:51:GLU:C	2.33	0.64
1:C:64:VAL:HG22	1:C:143:LEU:O	1.97	0.64
1:C:121:HIS:O	1:C:122:ARG:CG	2.45	0.64
1:A:99:ILE:HD12	1:A:196:MET:HG2	1.80	0.64
1:C:85:GLN:HA	3:C:1297:MTW:C13	2.28	0.64
1:A:115:LEU:HD13	1:A:119:HIS:HE1	1.60	0.64
2:B:395:HIS:ND1	2:B:430:LEU:HD21	2.12	0.64
1:C:158:THR:HB	1:C:178:LYS:O	1.98	0.64
1:C:130:PRO:HB2	1:C:131:GLN:NE2	2.11	0.64
1:C:293:VAL:CG2	1:C:293:VAL:O	2.45	0.64
2:B:418:TYR:O	2:B:421:VAL:HG22	1.98	0.64
2:B:400:LYS:O	2:B:402:PRO:N	2.30	0.64
2:D:217:TRP:HH2	2:D:281:ILE:HD12	1.62	0.64
1:C:119:HIS:O	1:C:122:ARG:N	2.27	0.63
1:A:202:LEU:HD22	1:A:202:LEU:O	1.97	0.63
2:B:343:ASP:HB3	2:B:345:ASP:HB2	1.80	0.63
2:D:413:TYR:HB3	2:D:422:SER:HB3	1.79	0.63
2:B:332:LEU:HD23	2:B:363:ALA:HA	1.80	0.63
2:D:404:HIS:HD2	2:D:406:GLN:N	1.96	0.63
2:B:315:LEU:O	2:B:318:TYR:HB2	1.99	0.63
1:C:70:ILE:CG2	1:C:71:HIS:H	2.11	0.63
1:A:166:LEU:O	1:A:168:TYR:N	2.32	0.63
1:A:56:LYS:HZ3	1:A:56:LYS:HA	1.63	0.63
2:B:241:ARG:O	2:B:244:SER:HB2	1.99	0.63
2:D:357:GLY:O	2:D:358:ALA:C	2.37	0.63
2:D:417:LYS:HD2	2:D:418:TYR:CE2	2.33	0.63
1:C:11:GLY:O	1:C:17:VAL:HB	1.99	0.62
2:B:315:LEU:O	2:B:318:TYR:N	2.32	0.62
2:B:182:ILE:O	2:B:183:HIS:C	2.36	0.62
1:C:170:ALA:HB3	1:C:173:ILE:HD13	1.82	0.62
1:A:294:PRO:HG2	1:A:296:LEU:HD13	1.82	0.62
1:C:268[B]:HIS:O	1:C:269:TYR:O	2.17	0.62
2:B:214:LEU:HD22	2:B:253:LEU:HG	1.79	0.62
1:C:17:VAL:CG2	1:C:17:VAL:O	2.47	0.62
1:C:200:ARG:NH1	1:C:200:ARG:HB3	2.15	0.62
2:D:336:LEU:CD1	2:D:362:LEU:HD23	2.26	0.62
1:A:135:ILE:HD12	1:A:296:LEU:HD11	1.82	0.62
2:B:395:HIS:CE1	2:B:430:LEU:CD2	2.83	0.62
1:C:159:TYR:HB3	1:C:162:GLU:H	1.65	0.62
2:D:202:LYS:HB3	2:D:202:LYS:NZ	2.15	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:CE	1:A:70:ILE:HD12	2.30	0.62
2:B:419:HIS:C	2:B:421:VAL:H	2.04	0.62
1:C:152:PHE:C	1:C:154:VAL:N	2.51	0.62
1:C:176:GLY:HA2	4:C:2014:HOH:O	1.99	0.62
1:C:159:TYR:CD1	2:D:270:ILE:HD12	2.35	0.62
1:C:268[B]:HIS:C	1:C:269:TYR:O	2.26	0.62
2:D:282:THR:O	2:D:283:ASP:CB	2.48	0.62
2:D:415:ASN:OD1	2:D:417:LYS:HG2	1.99	0.62
1:A:108:LEU:O	1:A:112:LEU:HD12	1.99	0.61
1:A:203:PHE:CE1	1:A:215:ILE:HA	2.34	0.61
1:C:145:ASP:OD2	1:C:145:ASP:C	2.36	0.61
1:C:83:LEU:HD21	1:C:142:LYS:HD2	1.81	0.61
2:B:395:HIS:CE1	2:B:430:LEU:HD21	2.35	0.61
1:A:172:GLU:HG2	1:A:173:ILE:N	2.15	0.61
2:B:365:TYR:HE2	2:B:430:LEU:HA	1.65	0.61
1:A:10:ILE:HD13	1:A:20:LYS:N	2.15	0.61
2:B:254:GLN:OE1	2:B:282:THR:HG22	2.00	0.61
2:B:345:ASP:HB2	2:B:346:PRO:CD	2.29	0.61
2:D:418:TYR:O	2:D:420:GLY:N	2.33	0.61
1:C:245:ARG:HG2	1:C:246:GLN:N	2.12	0.61
1:C:236:TYR:CG	1:C:237:LYS:N	2.69	0.61
1:A:170:ALA:HB1	1:A:172:GLU:CD	2.21	0.61
1:A:178:LYS:HG3	1:A:179:TYR:CE2	2.36	0.61
1:C:245:ARG:CG	1:C:245:ARG:HH11	2.14	0.61
2:D:400:LYS:O	2:D:401:ALA:C	2.38	0.61
1:A:202:LEU:CD2	1:A:202:LEU:O	2.49	0.60
2:B:277:GLU:OE1	2:B:277:GLU:HA	2.01	0.60
1:C:70:ILE:HG22	1:C:71:HIS:N	2.15	0.60
1:A:108:LEU:HG	1:A:112:LEU:HD12	1.84	0.60
1:A:150:ARG:NH1	2:B:268:GLU:O	2.35	0.60
2:B:278:PHE:O	2:B:281:ILE:HG13	2.01	0.60
1:C:29:VAL:CG1	1:C:30:VAL:N	2.65	0.60
2:D:392:MET:HA	2:D:392:MET:CE	2.30	0.60
3:C:1297:MTW:N1	3:C:1297:MTW:O2	2.34	0.60
2:D:175:VAL:O	2:D:175:VAL:CG1	2.49	0.60
2:D:248:VAL:HG12	2:D:249:LEU:O	2.01	0.60
2:D:335:PHE:CE2	2:D:339:LEU:HD11	2.36	0.60
2:D:421:VAL:HA	2:D:424:LEU:HD22	1.84	0.60
1:A:100:PRO:C	1:A:102:PRO:HD2	2.22	0.60
2:B:225:TYR:CE1	2:B:281:ILE:HG21	2.36	0.60
2:D:405:ALA:HB1	2:D:406:GLN:HE22	1.66	0.60

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:404:HIS:HD2	2:B:405:ALA:N	1.99	0.60
1:C:1:MET:CE	1:C:70:ILE:HD13	2.31	0.60
2:D:332:LEU:O	2:D:332:LEU:HD12	2.02	0.60
1:A:203:PHE:HE1	1:A:218:THR:HG1	1.50	0.60
2:D:248:VAL:HG12	2:D:249:LEU:N	2.17	0.60
2:D:420:GLY:O	2:D:422:SER:N	2.35	0.60
1:A:23:ASN:OD1	1:A:25:LEU:N	2.34	0.60
2:B:219:VAL:HG12	2:B:220:GLU:N	2.11	0.60
2:D:372:TRP:NE1	2:D:382:TYR:O	2.26	0.60
1:A:1:MET:HG2	1:A:70:ILE:HD13	1.83	0.60
2:B:252:LYS:HD3	2:B:252:LYS:N	2.17	0.60
1:C:166:LEU:CD2	1:C:169:ARG:CZ	2.79	0.60
1:A:122:ARG:HB3	2:B:182:ILE:HG12	1.84	0.59
1:C:101:LEU:O	1:C:104:ILE:N	2.35	0.59
1:C:34:LYS:O	1:C:34:LYS:CG	2.48	0.59
1:A:100:PRO:C	1:A:102:PRO:CD	2.71	0.59
2:D:235:ALA:O	2:D:239:ILE:HG12	2.02	0.59
2:D:377:ILE:HG13	2:D:382:TYR:O	2.01	0.59
2:B:216:ASP:OD1	2:B:408:SER:HB2	2.03	0.59
2:B:259:ALA:HB2	2:B:294:MET:HB3	1.83	0.59
2:B:268:GLU:OE1	2:B:268:GLU:CA	2.47	0.59
1:C:204:PRO:O	1:C:214:ARG:HD3	2.03	0.59
1:C:70:ILE:HG23	1:C:71:HIS:H	1.68	0.59
1:A:108:LEU:HG	1:A:112:LEU:CD1	2.33	0.59
2:B:211:ARG:HG2	2:B:211:ARG:HH11	1.67	0.59
2:B:332:LEU:HB3	2:B:363:ALA:HB1	1.85	0.59
1:C:252:VAL:N	1:C:253:PRO:CD	2.66	0.59
1:A:86:ASP:OD1	1:A:89:LYS:N	2.36	0.59
2:B:233:HIS:HB3	4:B:2010:HOH:O	2.01	0.59
1:C:206:ASP:CB	1:C:210:ASP:OD2	2.50	0.59
1:A:178:LYS:C	1:A:179:TYR:CD2	2.76	0.58
1:A:252:VAL:O	1:A:253:PRO:C	2.41	0.58
1:A:60:HIS:HD2	1:A:62:ASN:H	1.50	0.58
2:B:249:LEU:C	2:B:251:GLY:N	2.54	0.58
2:B:371:SER:O	2:B:373:PRO:HD3	2.04	0.58
1:C:126:ARG:NH1	1:C:159:TYR:CZ	2.71	0.58
1:C:166:LEU:O	1:C:167:TRP:C	2.39	0.58
2:B:218:LEU:HD22	2:B:261:MET:SD	2.43	0.58
2:B:216:ASP:CG	2:B:408:SER:HB2	2.24	0.58
1:C:30:VAL:HG23	1:C:31:ALA:N	2.19	0.58
2:B:326:ASN:C	2:B:326:ASN:OD1	2.40	0.58

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:ALA:O	1:C:145:ASP:HB3	2.03	0.58
1:C:160:THR:C	1:C:161:HIS:HD2	2.00	0.58
3:A:1297:MTW:C14	3:A:1297:MTW:N3	2.58	0.58
1:C:34:LYS:HG3	1:C:34:LYS:O	2.02	0.58
2:D:415:ASN:OD1	2:D:417:LYS:CG	2.51	0.58
1:A:253:PRO:HB2	1:A:254:PRO:HD3	1.86	0.58
1:C:125:HIS:ND1	1:C:128:LEU:CD2	2.67	0.58
1:C:200:ARG:HB3	1:C:200:ARG:HH11	1.67	0.58
2:D:230:GLU:O	2:D:231:THR:C	2.40	0.58
1:A:15:TYR:O	1:A:35:ILE:HG23	2.04	0.58
2:D:241:ARG:HA	2:D:244:SER:HB2	1.86	0.58
1:C:245:ARG:HG3	1:C:245:ARG:HH11	1.67	0.58
2:D:321:HIS:HD2	2:D:321:HIS:N	2.01	0.58
1:A:88:LYS:HG3	1:A:89:LYS:N	2.17	0.57
1:C:54:LEU:HD13	1:C:123:VAL:HG13	1.86	0.57
1:C:214:ARG:HH11	1:C:214:ARG:HG2	1.69	0.57
2:B:249:LEU:O	2:B:251:GLY:N	2.37	0.57
2:D:294:MET:O	2:D:298:VAL:HG23	2.04	0.57
1:C:12:GLU:HA	1:C:17:VAL:CA	2.34	0.57
1:C:202:LEU:O	1:C:203:PHE:CD1	2.58	0.57
1:C:84:HIS:HD2	1:C:296:LEU:HG	1.69	0.57
1:A:23:ASN:OD1	1:A:23:ASN:O	2.22	0.57
2:B:247:SER:OG	1:C:28:GLU:OE2	2.22	0.57
2:B:410:ARG:O	2:B:411:GLU:C	2.40	0.57
1:A:107:TYR:CD1	1:A:141:ILE:HG21	2.40	0.57
2:B:346:PRO:O	2:B:349:LYS:HB2	2.03	0.57
1:C:214:ARG:CG	1:C:214:ARG:HH11	2.17	0.57
1:C:167:TRP:N	1:C:167:TRP:CD1	2.71	0.57
1:C:23:ASN:O	1:C:27:GLY:N	2.38	0.57
1:C:184:VAL:CG2	1:C:185:ASP:N	2.68	0.56
2:D:418:TYR:O	2:D:419:HIS:C	2.41	0.56
1:A:200:ARG:O	1:A:201:ALA:C	2.43	0.56
1:C:108:LEU:HD22	1:C:193:PHE:CG	2.39	0.56
1:A:105:LYS:CE	1:A:285:PHE:CZ	2.88	0.56
1:A:31:ALA:HB3	3:A:1297:MTW:C9	2.36	0.56
1:A:216:PHE:CE1	1:A:222:PRO:HD3	2.40	0.56
1:C:173:ILE:CD1	1:C:173:ILE:N	2.68	0.56
1:C:173:ILE:HD12	1:C:173:ILE:N	2.19	0.56
1:C:178:LYS:HD3	1:C:179:TYR:CE2	2.40	0.56
1:C:5:GLN:O	1:C:5:GLN:HG3	2.05	0.56
2:D:178:TYR:C	2:D:178:TYR:CD2	2.79	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:235:ALA:O	2:D:239:ILE:CG1	2.53	0.56
1:A:56:LYS:C	1:A:56:LYS:HZ2	1.96	0.56
2:B:361:HIS:CD2	2:B:361:HIS:C	2.79	0.56
1:C:157:ARG:HG2	1:C:157:ARG:HH11	1.69	0.56
2:B:420:GLY:O	2:B:421:VAL:C	2.43	0.56
1:A:266:MET:O	1:A:274:ARG:HD3	2.05	0.56
1:C:214:ARG:NH1	1:C:214:ARG:CG	2.69	0.56
2:D:268:GLU:O	2:D:268:GLU:HG3	2.06	0.56
2:D:299:LEU:HD22	2:D:304:PHE:CE1	2.41	0.56
2:D:345:ASP:CG	2:D:346:PRO:HD3	2.22	0.56
1:A:100:PRO:O	1:A:101:LEU:C	2.41	0.56
1:A:104:ILE:HG22	1:A:105:LYS:N	2.21	0.56
1:A:128:LEU:HB2	1:A:188:SER:CB	2.36	0.56
1:C:200:ARG:NH1	1:C:200:ARG:HG2	2.12	0.56
2:D:383:THR:OG1	2:D:385:GLU:HB3	2.06	0.56
1:C:29:VAL:C	1:C:30:VAL:HG13	2.25	0.56
1:C:115:LEU:CD1	1:C:189:LEU:CD2	2.79	0.56
1:C:160:THR:O	1:C:161:HIS:CD2	2.59	0.56
2:D:223:GLU:OE1	2:D:223:GLU:CA	2.53	0.56
2:D:415:ASN:CG	2:D:417:LYS:HG2	2.26	0.56
1:A:60:HIS:CG	1:A:61:PRO:HD3	2.41	0.55
1:C:29:VAL:C	1:C:30:VAL:CG1	2.75	0.55
2:D:372:TRP:CD1	2:D:377:ILE:HD11	2.40	0.55
1:A:129:LYS:O	1:A:131:GLN:N	2.40	0.55
1:A:128:LEU:HB2	1:A:188:SER:HB2	1.87	0.55
2:B:282:THR:HB	2:B:285:THR:CG2	2.35	0.55
2:B:357:GLY:O	2:B:358:ALA:C	2.45	0.55
1:C:215:ILE:O	1:C:218:THR:N	2.30	0.55
1:C:227:TRP:O	1:C:228:PRO:C	2.44	0.55
1:C:84:HIS:O	3:C:1297:MTW:H13	2.06	0.55
2:D:415:ASN:ND2	2:D:417:LYS:HG2	2.21	0.55
2:D:395:HIS:CE1	2:D:430:LEU:HG	2.41	0.55
1:A:153:GLY:HA3	2:B:313:GLN:HG2	1.88	0.55
1:A:103:LEU:HA	1:A:292:PRO:HG2	1.88	0.55
2:D:178:TYR:HA	2:D:181[B]:ASP:OD2	2.05	0.55
1:A:154:VAL:CG1	1:A:155:PRO:N	2.68	0.55
1:C:256:ASP:O	1:C:260:ARG:HG3	2.06	0.55
1:A:129:LYS:HA	1:A:192:ILE:HD11	1.87	0.55
2:B:389:PRO:HG2	2:B:390:CYS:H	1.70	0.55
1:A:159:TYR:O	1:A:160:THR:C	2.43	0.55
1:C:113:GLN:HA	1:C:281:LEU:HD11	1.88	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:ILE:O	1:C:64:VAL:C	2.45	0.55
1:A:71:HIS:CE1	2:B:296:HIS:HD1	2.25	0.55
1:C:17:VAL:HG23	1:C:17:VAL:O	2.07	0.55
1:C:121:HIS:O	1:C:122:ARG:HG2	2.05	0.55
1:C:129:LYS:HE2	4:C:2009:HOH:O	2.07	0.55
1:C:14:THR:HB	1:C:15:TYR:CD1	2.41	0.55
2:D:216:ASP:CG	2:D:406:GLN:HB3	2.28	0.55
2:D:217:TRP:CZ2	2:D:281:ILE:HD12	2.42	0.55
2:D:338:GLU:OE1	2:D:413:TYR:HE1	1.90	0.55
1:C:110:GLN:O	1:C:111:LEU:C	2.45	0.54
1:C:129:LYS:O	1:C:130:PRO:C	2.45	0.54
1:C:105:LYS:HB2	1:C:285:PHE:CE2	2.42	0.54
2:D:347:TYR:OH	2:D:394:LEU:HA	2.07	0.54
2:D:207:THR:HG22	2:D:210:MET:SD	2.47	0.54
1:A:62:ASN:HD22	1:A:110:GLN:HB3	1.71	0.54
1:A:68:ASP:O	1:A:79:VAL:HG23	2.07	0.54
1:A:83:LEU:HD23	1:A:136:ASN:HB3	1.88	0.54
1:A:39:THR:O	2:B:289:LYS:HE2	2.08	0.54
2:D:211:ARG:O	2:D:212:ALA:C	2.44	0.54
2:D:404:HIS:HD2	2:D:406:GLN:O	1.90	0.54
1:A:223:ASP:OD1	1:A:225:VAL:HB	2.07	0.54
1:C:246:GLN:O	1:C:247:ASP:C	2.45	0.54
2:D:383:THR:HG23	2:D:386:SER:OG	2.07	0.54
1:A:101:LEU:N	1:A:102:PRO:CD	2.71	0.54
1:A:248:PHE:CE2	1:A:264:SER:CB	2.91	0.54
1:C:252:VAL:O	1:C:252:VAL:HG23	2.07	0.54
1:C:289:VAL:C	1:C:290:THR:HG23	2.28	0.54
1:C:32:LEU:HD22	1:C:79:VAL:HG22	1.86	0.54
2:D:354:VAL:O	2:D:355:ILE:C	2.45	0.54
1:A:158:THR:OG1	1:A:178:LYS:HA	2.08	0.54
2:B:384:LEU:CD1	2:B:384:LEU:O	2.54	0.54
1:C:282:ALA:HB1	4:C:2028:HOH:O	2.08	0.54
1:C:84:HIS:CD2	1:C:296:LEU:HG	2.42	0.54
1:C:40:GLU:O	1:C:41:THR:O	2.26	0.54
2:B:322:GLN:OE1	2:B:325:ALA:HA	2.07	0.54
1:A:56:LYS:HZ3	1:A:56:LYS:CA	2.21	0.54
1:A:84:HIS:CD2	1:A:84:HIS:N	2.76	0.54
2:B:317:GLN:O	2:B:318:TYR:C	2.44	0.54
1:C:122:ARG:NH2	1:C:122:ARG:HG3	2.08	0.54
1:C:125:HIS:ND1	1:C:128:LEU:HD23	2.23	0.54
1:C:152:PHE:O	1:C:153:GLY:C	2.46	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:TYR:CD1	1:C:237:LYS:N	2.76	0.54
2:D:321:HIS:CE1	2:D:379:LYS:HD3	2.43	0.54
1:A:103:LEU:O	1:A:106:SER:HB3	2.07	0.54
2:B:409:ILE:O	2:B:412:LYS:HB3	2.08	0.53
2:D:335:PHE:CZ	2:D:339:LEU:HD11	2.44	0.53
2:D:368:THR:OG1	2:D:370:GLN:HG3	2.09	0.53
1:A:195:GLU:O	1:A:196:MET:C	2.45	0.53
2:B:197:VAL:CG2	2:B:198:GLY:N	2.70	0.53
1:C:162:GLU:OE1	1:C:164:VAL:N	2.41	0.53
2:D:335:PHE:HB2	2:D:413:TYR:CE2	2.44	0.53
1:A:294:PRO:CB	1:A:296:LEU:HD12	2.23	0.53
2:B:258:THR:O	2:B:259:ALA:C	2.45	0.53
2:B:321:HIS:CE1	2:B:379:LYS:CE	2.91	0.53
2:B:347:TYR:HH	2:B:397:THR:HG1	1.56	0.53
1:A:2:GLU:HG3	1:C:73:GLU:OE1	2.08	0.53
2:D:209:SER:O	2:D:212:ALA:HB3	2.08	0.53
2:D:249:LEU:CD1	2:D:249:LEU:N	2.69	0.53
1:C:12:GLU:HA	1:C:17:VAL:HA	1.89	0.53
2:D:220:GLU:HG3	2:D:408:SER:OG	2.08	0.53
2:B:216:ASP:OD1	2:B:408:SER:CB	2.56	0.53
2:D:190:GLU:N	2:D:309:PRO:HG3	2.24	0.53
2:D:198:GLY:HA3	4:D:2003:HOH:O	2.08	0.53
1:A:164:VAL:C	1:A:165:THR:HG22	2.27	0.53
1:A:84:HIS:H	1:A:84:HIS:CD2	2.27	0.53
2:B:188:GLU:HB2	4:B:2003:HOH:O	2.08	0.53
1:C:224:GLU:OE2	1:C:231:THR:OG1	2.26	0.53
1:C:96:LEU:C	1:C:96:LEU:HD12	2.29	0.53
2:D:284:ASP:N	2:D:284:ASP:OD1	2.42	0.53
1:A:139:GLY:C	4:A:2014:HOH:O	2.42	0.53
1:C:131:GLN:NE2	1:C:131:GLN:H	2.06	0.53
1:C:178:LYS:HG2	1:C:179:TYR:CD2	2.44	0.53
1:C:11:GLY:O	1:C:17:VAL:HA	2.09	0.53
1:C:29:VAL:O	1:C:30:VAL:CG1	2.57	0.53
1:A:23:ASN:OD1	1:A:26:THR:N	2.35	0.53
1:A:248:PHE:HA	1:A:251:VAL:HG23	1.90	0.53
1:C:212:LEU:HD22	1:C:216:PHE:CE1	2.44	0.53
1:C:130:PRO:HB2	1:C:131:GLN:HE21	1.74	0.53
1:C:245:ARG:NH1	1:C:245:ARG:CG	2.70	0.53
1:C:87:LEU:HD22	1:C:87:LEU:O	2.09	0.53
1:A:7:VAL:O	1:A:8:GLU:HB3	2.09	0.52
2:B:400:LYS:C	2:B:402:PRO:CD	2.78	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:VAL:HG23	4:C:2012:HOH:O	2.09	0.52
1:A:241:PRO:CG	1:A:243:TRP:CH2	2.88	0.52
1:C:125:HIS:CE1	1:C:128:LEU:HD23	2.44	0.52
1:C:230:VAL:C	1:C:232:SER:H	2.12	0.52
1:C:189:LEU:HB3	1:C:266:MET:CE	2.39	0.52
2:D:198:GLY:O	2:D:201:LYS:HG2	2.09	0.52
2:D:335:PHE:CD1	2:D:413:TYR:HB2	2.44	0.52
2:D:383:THR:HG1	2:D:386:SER:H	1.56	0.52
1:A:236:TYR:CD1	1:A:236:TYR:C	2.81	0.52
2:B:337:GLY:O	2:B:338:GLU:C	2.46	0.52
1:C:245:ARG:CG	1:C:246:GLN:N	2.69	0.52
2:D:407:GLN:O	2:D:410:ARG:N	2.42	0.52
1:A:64:VAL:O	1:A:64:VAL:CG1	2.56	0.52
2:B:249:LEU:C	2:B:251:GLY:H	2.13	0.52
1:A:49:ILE:HG23	2:B:306:LEU:HD12	1.92	0.52
2:B:321:HIS:N	2:B:321:HIS:CD2	2.77	0.52
2:B:404:HIS:CD2	2:B:405:ALA:N	2.77	0.52
1:C:100:PRO:O	1:C:101:LEU:C	2.46	0.52
1:C:9:LYS:N	1:C:19:TYR:CD2	2.78	0.52
2:B:249:LEU:O	2:B:250:ARG:C	2.44	0.52
2:D:250:ARG:O	2:D:251:GLY:C	2.48	0.52
2:D:326:ASN:OD1	2:D:326:ASN:C	2.47	0.52
2:B:194:LYS:HG2	2:B:195:PRO:CD	2.36	0.52
2:B:271:TYR:CB	2:B:272:PRO:HD2	2.39	0.52
2:B:374:GLU:HA	2:B:377:ILE:HD12	1.92	0.52
1:C:177:CYS:HB3	1:C:233:MET:CE	2.40	0.52
1:C:29:VAL:O	1:C:30:VAL:HG12	2.09	0.52
1:A:60:HIS:CD2	1:A:60:HIS:C	2.83	0.51
2:B:321:HIS:HE1	2:B:379:LYS:HE2	1.74	0.51
2:B:410:ARG:O	2:B:412:LYS:N	2.43	0.51
2:D:198:GLY:N	4:D:2003:HOH:O	2.32	0.51
2:D:262:LEU:CD1	2:D:266:LYS:HE3	2.36	0.51
2:D:320:LEU:HB2	2:D:321:HIS:HD2	1.75	0.51
1:A:38:ASP:OD2	1:A:41:THR:CB	2.53	0.51
2:B:410:ARG:C	2:B:412:LYS:N	2.62	0.51
1:C:195:GLU:O	1:C:199:ARG:N	2.44	0.51
2:D:230:GLU:HG3	2:D:234:LEU:HD12	1.91	0.51
2:D:314:PHE:O	2:D:315:LEU:C	2.48	0.51
2:B:346:PRO:HG2	2:B:347:TYR:CD2	2.45	0.51
2:D:358:ALA:HB1	2:D:391:LEU:HD13	1.92	0.51
1:A:214:ARG:O	1:A:215:ILE:C	2.48	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:310:THR:HB	4:B:2010:HOH:O	2.10	0.51
1:C:125:HIS:CG	1:C:128:LEU:CD2	2.90	0.51
2:D:275:VAL:HG21	2:D:292:LEU:HD11	1.93	0.51
1:A:252:VAL:N	1:A:253:PRO:HD3	2.26	0.51
1:C:64:VAL:HG22	1:C:144:ALA:HB2	1.93	0.51
1:C:184:VAL:HG23	1:C:185:ASP:N	2.26	0.51
1:C:259:GLY:CA	1:C:285:PHE:CD1	2.93	0.51
1:A:134:LEU:N	1:A:134:LEU:HD23	2.24	0.51
2:B:328:LYS:O	2:B:329:VAL:C	2.49	0.51
2:B:354:VAL:O	2:B:356:ALA:N	2.44	0.51
1:C:20:LYS:HB2	1:C:82:PHE:CE2	2.46	0.51
2:B:264:ALA:O	2:B:265:SER:C	2.48	0.51
1:C:117:PHE:CE2	1:C:121:HIS:CE1	2.98	0.51
1:C:255:LEU:O	1:C:260:ARG:NH1	2.44	0.51
2:D:407:GLN:O	2:D:408:SER:C	2.48	0.51
1:A:229:GLY:O	1:A:230:VAL:C	2.49	0.51
1:A:56:LYS:C	1:A:56:LYS:NZ	2.58	0.51
1:C:84:HIS:HB2	4:C:2010:HOH:O	2.10	0.51
2:D:229:ASN:ND2	2:D:334:MET:CE	2.74	0.51
1:A:2:GLU:CG	1:C:73:GLU:OE1	2.59	0.51
2:B:386:SER:O	2:B:389:PRO:HD2	2.10	0.51
2:B:396:GLN:O	2:B:397:THR:C	2.49	0.51
1:C:39:THR:HG22	1:C:39:THR:O	2.09	0.51
2:D:378:ARG:CB	2:D:378:ARG:HH11	2.22	0.51
2:D:391:LEU:O	2:D:392:MET:C	2.49	0.51
1:A:101:LEU:N	1:A:102:PRO:HD3	2.25	0.50
2:B:351:LEU:HD22	2:B:352:PRO:CD	2.41	0.50
1:C:7:VAL:HB	1:C:20:LYS:HG3	1.93	0.50
1:C:83:LEU:HD22	1:C:134:LEU:HB2	1.93	0.50
1:C:96:LEU:HG	1:C:97:THR:HG22	1.91	0.50
1:A:105:LYS:CE	1:A:285:PHE:CE2	2.94	0.50
1:A:153:GLY:CA	2:B:313:GLN:HG2	2.41	0.50
1:A:55:LEU:HD23	1:A:80:PHE:HE2	1.76	0.50
2:D:263:LEU:O	2:D:264:ALA:C	2.45	0.50
1:A:91:MET:HE3	1:A:196:MET:HA	1.93	0.50
1:C:289:VAL:HG22	1:C:290:THR:N	2.27	0.50
2:D:262:LEU:HD11	2:D:266:LYS:CE	2.34	0.50
2:B:214:LEU:HD12	2:B:217:TRP:HE3	1.75	0.50
1:C:293:VAL:HG23	1:C:293:VAL:O	2.09	0.50
2:D:406:GLN:N	2:D:406:GLN:CD	2.65	0.50
1:A:216:PHE:O	1:A:220:GLY:HA2	2.10	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:217:TRP:CZ2	2:B:281:ILE:CD1	2.92	0.50
2:B:251:GLY:C	2:B:252:LYS:HD3	2.32	0.50
1:C:216:PHE:N	1:C:216:PHE:CD1	2.77	0.50
2:D:395:HIS:ND1	2:D:430:LEU:HG	2.26	0.50
1:C:38:ASP:O	1:C:40:GLU:N	2.32	0.50
2:D:401:ALA:HB3	2:D:402:PRO:HD3	1.92	0.50
2:B:199:TYR:CD1	2:B:200:MET:CA	2.95	0.50
2:B:332:LEU:O	2:B:335:PHE:HB3	2.11	0.50
2:B:401:ALA:HB3	2:B:402:PRO:CD	2.38	0.50
1:C:23:ASN:O	1:C:27:GLY:HA2	2.12	0.50
2:B:347:TYR:OH	2:B:397:THR:OG1	2.25	0.50
1:C:188:SER:O	1:C:192:ILE:HG13	2.12	0.50
1:C:44:VAL:HG12	1:C:49:ILE:HG12	1.94	0.50
2:D:229:ASN:HD22	2:D:334:MET:HE1	1.77	0.50
2:B:283:ASP:O	2:B:284:ASP:C	2.49	0.50
1:C:283:HIS:CE1	1:C:284:PRO:HD2	2.47	0.50
1:C:85:GLN:HE22	1:C:89:LYS:HB3	1.75	0.50
1:A:25:LEU:O	2:D:252:LYS:HD2	2.12	0.50
1:C:251:VAL:O	1:C:252:VAL:HG13	2.12	0.49
2:D:206:ILE:HA	2:D:210:MET:SD	2.52	0.49
2:D:420:GLY:C	2:D:422:SER:H	2.15	0.49
1:A:105:LYS:HB2	1:A:285:PHE:CE2	2.48	0.49
2:B:221:VAL:HG22	2:B:281:ILE:HD13	1.94	0.49
2:B:388:LYS:N	2:B:389:PRO:CD	2.73	0.49
1:C:11:GLY:O	1:C:17:VAL:CA	2.60	0.49
1:C:217:ARG:HB3	1:C:243:TRP:CZ3	2.46	0.49
1:A:129:LYS:O	1:A:132:ASN:N	2.29	0.49
1:C:38:ASP:C	1:C:40:GLU:H	2.13	0.49
1:A:129:LYS:O	1:A:130:PRO:C	2.50	0.49
1:A:1:MET:HG2	1:A:70:ILE:HD12	1.93	0.49
2:B:419:HIS:C	2:B:421:VAL:N	2.64	0.49
2:D:321:HIS:H	2:D:321:HIS:CD2	2.29	0.49
2:D:383:THR:O	2:D:386:SER:HB2	2.11	0.49
2:B:216:ASP:O	2:B:219:VAL:HB	2.13	0.49
2:B:239:ILE:HG22	2:B:243:LEU:HD12	1.93	0.49
1:C:204:PRO:HD2	1:C:214:ARG:HH11	1.76	0.49
1:C:20:LYS:NZ	1:C:82:PHE:CZ	2.80	0.49
2:D:418:TYR:O	2:D:421:VAL:HG13	2.13	0.49
2:B:186:LEU:O	2:B:190:GLU:HB3	2.13	0.49
2:B:420:GLY:O	2:B:422:SER:N	2.45	0.49
1:A:111:LEU:HD21	1:A:141:ILE:HG12	1.94	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:351:LEU:HD22	2:B:352:PRO:HD3	1.95	0.49
2:B:383:THR:HG1	2:B:386:SER:H	1.60	0.49
1:C:288:ASP:OD1	1:C:288:ASP:N	2.45	0.49
2:D:212:ALA:O	2:D:213:ILE:C	2.49	0.49
2:D:403:GLN:HB2	2:D:403:GLN:HE21	1.38	0.49
2:B:338:GLU:O	2:B:340:SER:N	2.45	0.49
1:C:230:VAL:O	1:C:231:THR:C	2.47	0.49
2:D:190:GLU:HA	2:D:309:PRO:HG3	1.95	0.49
1:C:162:GLU:OE1	1:C:164:VAL:CG1	2.39	0.49
1:C:226:VAL:O	1:C:227:TRP:HB2	2.13	0.49
2:D:175:VAL:O	2:D:176:PRO:C	2.47	0.49
2:D:190:GLU:OE1	2:D:352:PRO:HD2	2.12	0.49
1:A:178:LYS:CG	1:A:179:TYR:HE2	2.12	0.48
1:A:259:GLY:HA2	1:A:285:PHE:CD1	2.47	0.48
2:B:235:ALA:O	2:B:238:TYR:HB2	2.12	0.48
2:B:342:ILE:HD11	2:B:409:ILE:CD1	2.41	0.48
1:C:162:GLU:OE1	1:C:163:VAL:C	2.51	0.48
2:D:198:GLY:CA	4:D:2003:HOH:O	2.61	0.48
2:D:388:LYS:O	2:D:391:LEU:N	2.46	0.48
1:A:33:LYS:NZ	3:A:1297:MTW:H17	2.28	0.48
2:B:185:TYR:O	2:B:186:LEU:C	2.51	0.48
2:B:430:LEU:CB	2:B:432:LEU:CD2	2.82	0.48
1:C:99:ILE:CG2	1:C:104:ILE:HG13	2.43	0.48
1:C:11:GLY:O	1:C:17:VAL:CB	2.61	0.48
1:A:190:GLY:N	1:A:266:MET:CE	2.76	0.48
2:B:220:GLU:O	2:B:221:VAL:C	2.50	0.48
1:C:223:ASP:HB3	4:C:2021:HOH:O	2.12	0.48
2:D:298:VAL:CG1	2:D:302:LEU:HD12	2.44	0.48
2:D:396:GLN:O	2:D:399:LEU:HB2	2.13	0.48
2:D:421:VAL:O	2:D:424:LEU:HB2	2.13	0.48
1:A:291:LYS:H	1:A:292:PRO:HD3	1.78	0.48
2:B:252:LYS:O	2:B:255:LEU:HB3	2.14	0.48
2:B:302:LEU:O	2:B:305:ASP:HB2	2.13	0.48
2:B:391:LEU:O	2:B:392:MET:C	2.49	0.48
2:D:362:LEU:HB2	2:D:391:LEU:HD11	1.94	0.48
2:D:338:GLU:OE1	2:D:413:TYR:CE1	2.67	0.48
1:A:128:LEU:HD23	1:A:128:LEU:HA	1.58	0.48
1:A:178:LYS:O	1:A:179:TYR:CD2	2.67	0.48
2:B:347:TYR:OH	2:B:394:LEU:HA	2.12	0.48
1:A:107:TYR:CD1	1:A:141:ILE:CG2	2.96	0.48
1:A:207:SER:O	1:A:208:GLU:C	2.52	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:GLY:HA3	2:D:313:GLN:HG2	1.96	0.48
2:D:399:LEU:HD23	2:D:399:LEU:HA	1.52	0.48
2:B:175:VAL:O	2:B:176:PRO:C	2.33	0.48
2:B:196:LYS:HA	2:B:196:LYS:HD2	1.43	0.48
2:B:207:THR:CG2	2:B:210:MET:CE	2.81	0.48
1:C:231:THR:HA	1:C:236:TYR:CE1	2.48	0.48
2:D:329:VAL:HG11	2:D:364:LEU:HD13	1.96	0.48
1:A:121:HIS:O	1:A:122:ARG:CG	2.22	0.48
1:A:38:ASP:O	1:A:38:ASP:CG	2.49	0.48
1:A:91:MET:HE1	1:A:196:MET:N	2.29	0.48
1:C:15:TYR:H	1:C:15:TYR:HD1	1.44	0.48
1:A:237:LYS:HB3	1:A:239:SER:HB3	1.96	0.48
2:B:395:HIS:ND1	2:B:430:LEU:CD2	2.76	0.48
2:D:214:LEU:CD1	2:D:214:LEU:C	2.68	0.48
2:D:216:ASP:O	2:D:217:TRP:C	2.52	0.48
2:D:372:TRP:CD1	2:D:377:ILE:CD1	2.97	0.48
2:B:225:TYR:O	2:B:227:LEU:HD23	2.13	0.48
2:B:425:ASN:O	2:B:426:PRO:O	2.31	0.48
1:C:116:ALA:O	1:C:120:SER:HB3	2.14	0.48
1:A:5:GLN:NE2	1:A:6:LYS:O	2.47	0.47
1:C:125:HIS:CE1	1:C:128:LEU:CD2	2.97	0.47
1:C:135:ILE:HG23	1:C:141:ILE:HD12	1.93	0.47
1:C:7:VAL:HG23	1:C:21:ALA:HA	1.96	0.47
2:D:224:GLU:HG3	2:D:224:GLU:O	2.14	0.47
2:D:298:VAL:HG12	2:D:302:LEU:HD12	1.96	0.47
1:A:190:GLY:O	1:A:193:PHE:HB3	2.15	0.47
1:A:193:PHE:CZ	1:A:255:LEU:HD21	2.49	0.47
2:B:186:LEU:HB3	2:B:314:PHE:CZ	2.49	0.47
2:B:206:ILE:C	2:B:210:MET:CE	2.82	0.47
1:C:6:LYS:CE	4:C:2001:HOH:O	2.60	0.47
2:D:210:MET:O	2:D:213:ILE:HB	2.14	0.47
2:D:264:ALA:O	2:D:267:PHE:N	2.46	0.47
1:C:159:TYR:CE1	2:D:270:ILE:HD12	2.49	0.47
1:A:178:LYS:HE3	1:A:179:TYR:OH	2.13	0.47
1:A:219:LEU:HD23	1:A:219:LEU:N	2.22	0.47
1:A:46:SER:O	1:A:50:ARG:HD2	2.14	0.47
2:D:183:HIS:C	2:D:183:HIS:ND1	2.67	0.47
2:D:248:VAL:CG1	2:D:249:LEU:N	2.77	0.47
1:A:52:ILE:O	1:A:56:LYS:HB2	2.15	0.47
2:B:268:GLU:HG3	2:B:268:GLU:O	2.14	0.47
2:D:176:PRO:HB2	2:D:178:TYR:CE1	2.48	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:398:TYR:O	2:D:399:LEU:C	2.52	0.47
1:A:55:LEU:HD12	1:A:55:LEU:HA	1.61	0.47
2:B:252:LYS:HA	2:B:252:LYS:HD2	1.43	0.47
2:B:345:ASP:CB	2:B:346:PRO:HD3	2.33	0.47
1:C:1:MET:CE	1:C:70:ILE:CD1	2.91	0.47
1:A:105:LYS:HE3	1:A:285:PHE:CE2	2.50	0.47
1:C:99:ILE:HG23	1:C:103:LEU:HD23	1.97	0.47
1:C:166:LEU:C	1:C:168:TYR:N	2.68	0.47
1:C:252:VAL:N	1:C:253:PRO:HD3	2.29	0.47
2:D:339:LEU:HD23	2:D:339:LEU:HA	1.76	0.47
2:D:430:LEU:O	2:D:431:ASN:CB	2.62	0.47
1:A:294:PRO:CG	1:A:296:LEU:CD1	2.87	0.47
2:D:208:ASN:HD22	2:D:344:ALA:HB3	1.79	0.47
2:D:190:GLU:CA	2:D:309:PRO:HG3	2.44	0.47
1:A:122:ARG:HA	2:B:182:ILE:HD11	1.96	0.47
2:B:254:GLN:HB2	2:B:254:GLN:HE21	1.56	0.47
1:A:49:ILE:HG23	2:B:306:LEU:CD1	2.45	0.47
1:C:129:LYS:HA	1:C:192:ILE:HD11	1.96	0.47
1:C:90:PHE:O	1:C:94:SER:HB2	2.15	0.47
2:D:300:LYS:O	2:D:301:VAL:C	2.52	0.47
2:B:214:LEU:O	2:B:217:TRP:HB3	2.15	0.47
2:B:236:VAL:HG21	2:B:341:LEU:HD22	1.97	0.47
2:D:283:ASP:O	2:D:284:ASP:C	2.53	0.47
1:A:178:LYS:O	1:A:179:TYR:CG	2.68	0.47
2:B:218:LEU:O	2:B:219:VAL:C	2.54	0.47
1:C:258:ASP:HB3	1:C:285:PHE:HA	1.95	0.47
1:C:46:SER:O	1:C:47:THR:C	2.53	0.47
1:C:70:ILE:O	1:C:77:TYR:N	2.44	0.47
2:D:235:ALA:O	2:D:238:TYR:HB2	2.15	0.47
2:D:357:GLY:O	2:D:360:PHE:N	2.48	0.47
1:A:211:GLN:O	1:A:215:ILE:HG13	2.14	0.47
1:A:190:GLY:N	1:A:266:MET:HE2	2.30	0.47
2:B:211:ARG:NH1	2:B:211:ARG:HG2	2.30	0.47
2:B:248:VAL:O	2:B:248:VAL:HG12	2.08	0.47
2:B:260:ALA:O	2:B:261:MET:C	2.53	0.47
1:C:129:LYS:O	1:C:132:ASN:N	2.47	0.47
1:C:284:PRO:HB3	1:C:287:GLN:OE1	2.14	0.47
2:D:329:VAL:CG2	2:D:367:VAL:HB	2.44	0.47
1:A:193:PHE:O	1:A:194:ALA:C	2.52	0.46
2:B:425:ASN:C	2:B:426:PRO:O	2.53	0.46
2:D:175:VAL:O	2:D:175:VAL:HG12	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:361:HIS:O	2:B:362:LEU:C	2.49	0.46
1:C:283:HIS:CG	1:C:284:PRO:HD2	2.51	0.46
2:D:178:TYR:C	2:D:178:TYR:HD2	2.16	0.46
2:D:329:VAL:HG12	2:D:330:GLU:N	2.29	0.46
2:B:304:PHE:CD2	2:B:304:PHE:N	2.84	0.46
1:A:56:LYS:NZ	1:A:56:LYS:CA	2.79	0.46
2:D:420:GLY:C	2:D:422:SER:N	2.69	0.46
1:A:166:LEU:C	1:A:168:TYR:H	2.19	0.46
2:B:343:ASP:HB3	2:B:345:ASP:CB	2.43	0.46
1:C:167:TRP:HE1	1:C:205:GLY:H	1.60	0.46
2:D:202:LYS:CB	2:D:202:LYS:NZ	2.78	0.46
1:A:108:LEU:HA	1:A:108:LEU:HD12	1.69	0.46
1:A:20:LYS:HB2	1:A:20:LYS:HE2	1.85	0.46
2:B:257:GLY:O	2:B:260:ALA:N	2.49	0.46
2:B:221:VAL:CG2	2:B:281:ILE:HD13	2.46	0.46
1:C:108:LEU:HG	1:C:286:PHE:HZ	1.81	0.46
2:D:334:MET:O	2:D:338:GLU:HG3	2.16	0.46
2:D:376:LEU:O	2:D:380:THR:HG23	2.16	0.46
1:A:128:LEU:O	1:A:129:LYS:HB3	2.16	0.46
1:A:236:TYR:HD1	1:A:237:LYS:N	2.11	0.46
1:A:71:HIS:CD2	2:B:296:HIS:HE1	2.21	0.46
1:A:88:LYS:NZ	1:A:92:ASP:OD2	2.49	0.46
1:A:99:ILE:O	1:A:104:ILE:HD12	2.15	0.46
1:C:159:TYR:CE1	2:D:270:ILE:CD1	2.98	0.46
1:C:277:ALA:N	4:C:2027:HOH:O	2.33	0.46
1:C:60:HIS:C	1:C:60:HIS:HD2	2.16	0.46
2:D:396:GLN:NE2	2:D:396:GLN:HA	2.30	0.46
1:C:233:MET:O	1:C:235:ASP:N	2.49	0.46
1:C:291:LYS:HG3	4:C:2007:HOH:O	2.14	0.46
2:D:319:PHE:CZ	2:D:330:GLU:HA	2.51	0.46
1:A:54:LEU:N	1:A:54:LEU:HD23	2.29	0.46
1:A:60:HIS:HD2	1:A:62:ASN:N	2.14	0.46
2:B:287:THR:O	2:B:290:GLN:N	2.48	0.46
1:A:1:MET:HE2	1:A:77:TYR:CB	2.46	0.46
2:B:372:TRP:HA	2:B:373:PRO:HD2	1.77	0.46
2:B:395:HIS:ND1	2:B:399:LEU:HD11	2.30	0.46
2:B:414:LYS:HE2	2:B:423:LEU:HD21	1.98	0.46
1:C:289:VAL:C	1:C:290:THR:CG2	2.84	0.46
2:D:405:ALA:HB1	2:D:406:GLN:NE2	2.31	0.46
1:A:270:ASP:O	1:A:271:PRO:C	2.54	0.45
1:A:294:PRO:HG2	1:A:296:LEU:CD1	2.44	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:ARG:O	1:C:51:GLU:C	2.52	0.45
1:A:1:MET:CE	1:A:77:TYR:CG	2.99	0.45
2:B:214:LEU:CD1	2:B:217:TRP:HE3	2.29	0.45
2:B:215:VAL:O	2:B:216:ASP:C	2.54	0.45
1:C:111:LEU:HD22	1:C:133:LEU:HD13	1.98	0.45
1:C:110:GLN:O	1:C:113:GLN:N	2.50	0.45
1:C:177:CYS:HB3	1:C:233:MET:HE1	1.98	0.45
1:A:193:PHE:C	1:A:193:PHE:CD1	2.90	0.45
1:A:92:ASP:C	1:A:94:SER:H	2.20	0.45
2:B:221:VAL:CG1	2:B:221:VAL:O	2.61	0.45
2:B:351:LEU:O	2:B:352:PRO:C	2.53	0.45
1:C:121:HIS:O	1:C:123:VAL:HG23	2.16	0.45
2:D:202:LYS:HB3	2:D:202:LYS:HZ2	1.79	0.45
1:C:178:LYS:CG	1:C:179:TYR:CD2	3.00	0.45
1:A:125:HIS:HE1	1:A:127:ASP:HB3	1.81	0.45
1:C:125:HIS:CD2	1:C:128:LEU:HD21	2.52	0.45
1:C:167:TRP:N	1:C:167:TRP:HD1	2.13	0.45
2:D:234:LEU:O	2:D:235:ALA:C	2.54	0.45
2:D:370:GLN:HA	4:D:2011:HOH:O	2.16	0.45
1:A:105:LYS:HE2	1:A:285:PHE:CE2	2.52	0.45
2:B:234:LEU:O	2:B:237:ASN:HB3	2.16	0.45
1:C:283:HIS:ND1	1:C:284:PRO:HD2	2.32	0.45
2:D:332:LEU:HB3	2:D:363:ALA:HB1	1.98	0.45
2:B:403:GLN:O	2:B:404:HIS:C	2.53	0.45
2:D:430:LEU:O	2:D:431:ASN:HB3	2.17	0.45
1:A:126:ARG:NH2	1:A:148:LEU:HD22	2.32	0.45
2:B:322:GLN:HB3	2:B:325:ALA:HA	1.99	0.45
2:B:331:SER:HB2	2:B:421:VAL:CG1	2.43	0.45
2:D:181[B]:ASP:O	2:D:184:THR:N	2.50	0.45
2:D:362:LEU:CG	2:D:362:LEU:O	2.63	0.45
1:A:219:LEU:HA	1:A:219:LEU:HD23	1.49	0.45
1:A:71:HIS:HE2	2:B:296:HIS:CG	2.34	0.45
2:B:262:LEU:O	2:B:263:LEU:C	2.55	0.45
2:B:361:HIS:HB2	2:B:372:TRP:HB2	1.99	0.45
2:B:216:ASP:OD2	2:B:408:SER:HB2	2.17	0.45
1:C:131:GLN:HE21	1:C:131:GLN:N	2.15	0.45
1:C:136:ASN:ND2	1:C:140:ALA:HB3	2.32	0.45
1:C:23:ASN:O	1:C:27:GLY:CA	2.65	0.45
2:D:335:PHE:HD1	2:D:413:TYR:CD1	2.35	0.45
1:A:154:VAL:CG1	1:A:155:PRO:CD	2.93	0.44
1:A:255:LEU:HA	1:A:255:LEU:HD12	1.47	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:LYS:N	1:A:292:PRO:CD	2.80	0.44
1:C:58:LEU:HD23	1:C:58:LEU:HA	1.37	0.44
2:D:182:ILE:HG21	2:D:182:ILE:HD13	1.71	0.44
1:A:223:ASP:O	1:A:230:VAL:HG21	2.16	0.44
1:A:60:HIS:HA	1:A:61:PRO:HD3	1.62	0.44
1:C:165:THR:N	4:C:2013:HOH:O	2.46	0.44
1:C:166:LEU:CD2	1:C:169:ARG:NH2	2.81	0.44
1:A:2:GLU:HG2	1:C:73:GLU:HG3	2.00	0.44
2:D:187:ARG:HD2	2:D:190:GLU:OE2	2.17	0.44
2:D:425:ASN:O	2:D:426:PRO:C	2.53	0.44
1:A:210:ASP:O	1:A:214:ARG:HG3	2.17	0.44
1:A:291:LYS:N	1:A:292:PRO:HD3	2.32	0.44
1:A:37:LEU:HD12	1:A:37:LEU:HA	1.83	0.44
1:A:73:GLU:HG3	1:C:2:GLU:OE1	2.17	0.44
2:B:302:LEU:O	2:B:303:THR:C	2.55	0.44
2:B:401:ALA:N	2:B:402:PRO:CD	2.80	0.44
1:C:152:PHE:CD1	1:C:152:PHE:N	2.84	0.44
2:D:215:VAL:O	2:D:218:LEU:HB2	2.16	0.44
1:A:189:LEU:HD12	1:A:189:LEU:HA	1.48	0.44
1:A:38:ASP:CG	1:A:41:THR:H	2.13	0.44
2:B:186:LEU:HD23	2:B:186:LEU:HA	1.41	0.44
2:B:361:HIS:CD2	2:B:361:HIS:O	2.70	0.44
2:D:178:TYR:O	2:D:179:HIS:C	2.55	0.44
2:B:206:ILE:CA	2:B:210:MET:HE3	2.42	0.44
2:B:292:LEU:HD12	2:B:292:LEU:HA	1.56	0.44
2:B:402:PRO:HB3	2:B:410:ARG:NH1	2.32	0.44
2:D:203:GLN:HA	2:D:204:PRO:HD3	1.77	0.44
1:A:85:GLN:HG2	1:A:86:ASP:H	1.83	0.44
1:A:90:PHE:CZ	1:A:294:PRO:HB3	2.53	0.44
1:C:84:HIS:C	3:C:1297:MTW:H13	2.38	0.44
2:D:320:LEU:HB2	2:D:321:HIS:CD2	2.52	0.44
2:D:392:MET:CE	2:D:392:MET:CA	2.95	0.44
2:D:415:ASN:OD1	2:D:416:SER:N	2.50	0.44
2:D:417:LYS:HD2	2:D:418:TYR:HE2	1.80	0.44
1:A:252:VAL:N	1:A:253:PRO:CD	2.80	0.44
2:B:182:ILE:O	2:B:185:TYR:N	2.51	0.44
1:C:85:GLN:CA	3:C:1297:MTW:H13	2.44	0.44
1:C:259:GLY:HA2	1:C:285:PHE:CE1	2.53	0.44
1:C:296:LEU:HD12	1:C:296:LEU:C	2.38	0.44
2:D:320:LEU:HD23	2:D:320:LEU:HA	1.36	0.44
1:A:126:ARG:HE	1:A:126:ARG:HB2	1.55	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:TYR:HD1	1:A:141:ILE:HG21	1.82	0.44
1:A:154:VAL:HG12	1:A:155:PRO:N	2.33	0.44
2:B:275:VAL:O	2:B:278:PHE:HB2	2.17	0.44
1:C:167:TRP:NE1	1:C:205:GLY:N	2.61	0.44
1:C:95:ALA:C	1:C:97:THR:H	2.21	0.44
1:A:275:ILE:HG21	1:A:275:ILE:HD13	1.70	0.43
1:A:289:VAL:CG1	1:A:289:VAL:O	2.64	0.43
2:B:196:LYS:O	2:B:197:VAL:C	2.57	0.43
2:B:356:ALA:O	2:B:359:ALA:HB3	2.18	0.43
2:D:366:THR:OG1	2:D:427:PRO:CG	2.66	0.43
1:A:101:LEU:CB	1:A:102:PRO:CD	2.96	0.43
2:B:178:TYR:O	2:B:180:GLU:N	2.51	0.43
2:B:348:LEU:HD12	2:B:348:LEU:HA	1.12	0.43
2:B:351:LEU:HA	2:B:351:LEU:HD23	1.57	0.43
1:C:101:LEU:N	1:C:102:PRO:CD	2.77	0.43
1:C:80:PHE:CB	3:C:1297:MTW:H9	2.48	0.43
1:C:95:ALA:O	1:C:97:THR:N	2.46	0.43
2:B:228:GLN:N	2:B:269:GLU:OE2	2.33	0.43
2:B:298:VAL:O	2:B:299:LEU:C	2.56	0.43
1:C:37:LEU:HD23	1:C:37:LEU:HA	1.80	0.43
2:D:220:GLU:O	2:D:221:VAL:C	2.56	0.43
1:A:192:ILE:O	1:A:195:GLU:N	2.51	0.43
1:A:212:LEU:HD23	1:A:212:LEU:HA	1.19	0.43
1:A:190:GLY:H	1:A:266:MET:HE2	1.83	0.43
2:B:210:MET:O	2:B:213:ILE:HB	2.18	0.43
2:B:391:LEU:HD13	2:B:391:LEU:HA	1.81	0.43
1:C:203:PHE:N	1:C:204:PRO:HD3	2.32	0.43
2:D:385:GLU:CA	2:D:385:GLU:OE1	2.42	0.43
1:C:174:LEU:HA	1:C:174:LEU:HD23	1.89	0.43
2:D:186:LEU:HD22	2:D:309:PRO:HB3	2.00	0.43
2:D:249:LEU:HA	2:D:249:LEU:HD12	1.53	0.43
2:D:394:LEU:HA	2:D:394:LEU:HD12	1.55	0.43
1:A:223:ASP:OD1	1:A:226:VAL:N	2.35	0.43
2:B:242:PHE:C	2:B:244:SER:N	2.70	0.43
2:D:238:TYR:CD1	2:D:238:TYR:N	2.85	0.43
2:B:417:LYS:HG2	2:B:417:LYS:O	2.19	0.43
2:B:420:GLY:O	2:B:423:LEU:HB2	2.19	0.43
1:C:111:LEU:CD2	1:C:133:LEU:HD13	2.48	0.43
1:C:275:ILE:CG1	1:C:276:SER:N	2.82	0.43
1:C:81:GLU:HG3	1:C:83:LEU:HD12	2.01	0.43
2:D:229:ASN:ND2	2:D:334:MET:HE3	2.33	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:343:ASP:CB	2:B:345:ASP:HB2	2.49	0.43
1:C:248:PHE:HE2	1:C:263:LEU:HD23	1.64	0.43
1:C:275:ILE:HG13	1:C:276:SER:H	1.84	0.43
1:A:261:SER:O	1:A:265:GLN:HG3	2.19	0.43
2:B:344:ALA:HB1	2:B:348:LEU:CD2	2.42	0.43
1:C:204:PRO:HD2	1:C:214:ARG:NH1	2.33	0.43
1:C:105:LYS:HE2	1:C:285:PHE:O	2.19	0.43
1:A:101:LEU:HB2	1:A:102:PRO:HD3	1.98	0.42
1:A:248:PHE:O	1:A:251:VAL:HG23	2.19	0.42
2:B:300:LYS:O	2:B:300:LYS:HG2	2.18	0.42
2:B:389:PRO:HG2	2:B:390:CYS:N	2.34	0.42
1:C:115:LEU:HD22	1:C:119:HIS:CE1	2.54	0.42
2:B:425:ASN:O	2:B:426:PRO:C	2.57	0.42
1:C:6:LYS:HA	1:C:21:ALA:CB	2.49	0.42
2:D:186:LEU:HA	2:D:186:LEU:HD23	1.63	0.42
2:D:321:HIS:HE1	2:D:379:LYS:HD3	1.85	0.42
2:D:417:LYS:CD	2:D:418:TYR:CE2	3.02	0.42
1:A:159:TYR:HB2	1:A:162:GLU:HA	2.01	0.42
1:A:91:MET:HE1	1:A:196:MET:H	1.85	0.42
2:B:274:GLU:O	2:B:275:VAL:C	2.57	0.42
2:D:323:GLN:HA	2:D:324:PRO:HA	1.71	0.42
1:A:203:PHE:N	1:A:204:PRO:HD3	2.35	0.42
1:A:3:ASN:OD1	1:A:25:LEU:CD1	2.67	0.42
1:A:1:MET:HG3	1:A:77:TYR:CD1	2.53	0.42
1:C:230:VAL:C	1:C:232:SER:N	2.61	0.42
1:C:269:TYR:O	1:C:270:ASP:C	2.56	0.42
2:D:205:ASP:OD2	2:D:250:ARG:HG2	2.18	0.42
2:D:345:ASP:CB	2:D:346:PRO:HD3	2.50	0.42
1:A:131:GLN:H	1:A:131:GLN:HG2	1.32	0.42
1:A:195:GLU:O	1:A:198:THR:N	2.51	0.42
1:A:248:PHE:C	1:A:250:LYS:N	2.71	0.42
2:B:288:LYS:HE2	2:B:288:LYS:HB3	1.61	0.42
2:B:299:LEU:HD23	2:B:299:LEU:HA	1.71	0.42
1:C:238:PRO:C	1:C:240:PHE:H	2.22	0.42
1:C:294:PRO:CG	1:C:296:LEU:HD22	2.49	0.42
1:C:54:LEU:HD12	1:C:149:ALA:CB	2.49	0.42
2:D:235:ALA:O	2:D:239:ILE:HG13	2.19	0.42
2:D:249:LEU:N	2:D:249:LEU:HD13	2.33	0.42
2:D:372:TRP:CZ3	2:D:376:LEU:HD13	2.54	0.42
1:A:263:LEU:HD12	1:A:263:LEU:HA	1.55	0.42
1:A:289:VAL:HG13	1:A:289:VAL:O	2.18	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:332:LEU:HA	2:B:332:LEU:HD12	1.33	0.42
3:C:1297:MTW:N3	3:C:1297:MTW:C14	2.69	0.42
1:C:161:HIS:N	1:C:161:HIS:CD2	2.77	0.42
2:D:255:LEU:HD23	2:D:294:MET:HE2	2.00	0.42
1:A:253:PRO:N	1:A:254:PRO:CD	2.83	0.42
1:A:33:LYS:HZ1	3:A:1297:MTW:H17	1.85	0.42
2:B:199:TYR:CD1	2:B:200:MET:HA	2.55	0.42
1:C:108:LEU:HD22	1:C:193:PHE:CD2	2.54	0.42
2:D:268:GLU:O	2:D:268:GLU:CG	2.68	0.42
2:B:233:HIS:CB	4:B:2010:HOH:O	2.65	0.42
2:B:310:THR:H	2:B:313:GLN:NE2	2.18	0.42
1:C:163:VAL:CG1	1:C:163:VAL:O	2.67	0.42
2:D:267:PHE:CD2	2:D:267:PHE:C	2.93	0.42
2:D:275:VAL:O	2:D:278:PHE:N	2.52	0.42
2:D:358:ALA:CB	2:D:391:LEU:HD13	2.49	0.42
1:A:105:LYS:HE3	1:A:105:LYS:HB2	1.65	0.42
1:C:101:LEU:HB2	1:C:102:PRO:CD	2.48	0.42
1:C:160:THR:O	1:C:161:HIS:CG	2.73	0.42
1:C:207:SER:OG	1:C:209:ILE:HG22	2.20	0.42
1:A:10:ILE:HD11	1:A:18:VAL:HG12	2.02	0.42
1:A:125:HIS:CE1	1:A:127:ASP:HB3	2.55	0.42
1:A:35:ILE:HD12	1:A:35:ILE:HG21	1.72	0.42
1:A:90:PHE:O	1:A:94:SER:HB2	2.20	0.42
2:B:380:THR:OG1	2:B:382:TYR:N	2.38	0.42
2:B:419:HIS:O	2:B:420:GLY:C	2.57	0.42
1:C:12:GLU:HA	1:C:17:VAL:HG12	2.02	0.42
1:C:55:LEU:HD12	1:C:55:LEU:HA	1.94	0.42
1:C:64:VAL:CG2	1:C:144:ALA:HA	2.50	0.42
1:A:37:LEU:HB3	1:A:74:ASN:O	2.20	0.41
2:B:277:GLU:CA	2:B:277:GLU:OE1	2.68	0.41
2:B:321:HIS:NE2	2:B:379:LYS:HE2	2.33	0.41
1:C:148:LEU:HD23	1:C:148:LEU:HA	1.74	0.41
1:C:198:THR:C	1:C:199:ARG:CG	2.87	0.41
2:D:245:SER:OG	2:D:246:MET:HG2	2.20	0.41
2:B:207:THR:HG23	2:B:210:MET:H	1.84	0.41
1:C:105:LYS:HB2	1:C:285:PHE:HE2	1.85	0.41
1:C:125:HIS:ND1	1:C:125:HIS:O	2.53	0.41
1:C:34:LYS:HE3	1:C:77:TYR:HE2	1.85	0.41
2:D:180:GLU:O	2:D:184:THR:N	2.34	0.41
1:A:143:LEU:HD23	1:A:143:LEU:HA	1.47	0.41
1:A:91:MET:CE	1:A:196:MET:HA	2.51	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:LYS:HB2	1:A:285:PHE:CZ	2.55	0.41
1:A:56:LYS:CE	1:A:56:LYS:O	2.64	0.41
1:A:20:LYS:HD3	1:A:82:PHE:CZ	2.55	0.41
1:A:99:ILE:HA	1:A:100:PRO:HD2	1.62	0.41
2:B:339:LEU:HA	2:B:339:LEU:HD23	1.21	0.41
2:B:385:GLU:O	2:B:386:SER:C	2.58	0.41
1:C:198:THR:C	1:C:199:ARG:HG2	2.39	0.41
1:C:62:ASN:HD21	1:C:110:GLN:HG2	1.86	0.41
2:D:181[A]:ASP:O	2:D:185:TYR:N	2.52	0.41
2:D:401:ALA:CB	2:D:410:ARG:HD2	2.34	0.41
1:A:179:TYR:N	1:A:179:TYR:CD2	2.89	0.41
1:A:1:MET:HE2	1:A:77:TYR:HB3	2.02	0.41
1:A:248:PHE:HB3	1:A:260:ARG:HD2	2.02	0.41
1:A:3:ASN:OD1	1:A:25:LEU:HD11	2.19	0.41
1:A:91:MET:CE	1:A:196:MET:N	2.83	0.41
1:C:101:LEU:CB	1:C:102:PRO:CD	2.98	0.41
1:C:136:ASN:C	1:C:136:ASN:OD1	2.58	0.41
2:B:383:THR:HG1	2:B:385:GLU:HB3	1.86	0.41
1:C:212:LEU:HA	1:C:212:LEU:HD23	1.84	0.41
1:C:281:LEU:HD23	1:C:281:LEU:HA	1.91	0.41
1:C:149:ALA:C	1:C:150:ARG:HG2	2.41	0.41
1:A:168:TYR:OH	1:A:195:GLU:OE1	2.20	0.41
2:B:395:HIS:CE1	2:B:430:LEU:HD23	2.55	0.41
2:B:428:GLU:HG2	2:B:429:THR:HG22	2.02	0.41
1:C:187:TRP:C	1:C:187:TRP:CD1	2.94	0.41
1:C:240:PHE:HA	1:C:240:PHE:HD1	1.76	0.41
1:C:278:LYS:O	1:C:281:LEU:HB2	2.21	0.41
2:B:277:GLU:O	2:B:278:PHE:C	2.57	0.41
2:B:311:VAL:O	2:B:312:ASN:C	2.57	0.41
2:D:335:PHE:CE2	2:D:339:LEU:CD1	3.03	0.41
2:B:242:PHE:C	2:B:244:SER:H	2.23	0.41
2:B:289:LYS:HB2	2:B:289:LYS:HE3	1.67	0.41
2:B:314:PHE:O	2:B:315:LEU:C	2.59	0.41
2:B:371:SER:OG	2:B:372:TRP:N	2.54	0.41
1:C:109:PHE:HB3	1:C:110:GLN:H	1.66	0.41
1:C:125:HIS:ND1	1:C:125:HIS:C	2.74	0.41
1:C:162:GLU:CD	1:C:163:VAL:O	2.58	0.41
1:C:51:GLU:HG3	1:C:55:LEU:HD22	2.03	0.41
2:D:209:SER:O	2:D:210:MET:C	2.58	0.41
2:D:314:PHE:CD2	2:D:353:SER:HA	2.55	0.41
2:D:335:PHE:HE1	2:D:410:ARG:HA	1.85	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:LEU:HD23	1:A:58:LEU:N	2.35	0.41
1:A:92:ASP:O	1:A:94:SER:N	2.53	0.41
1:C:189:LEU:HD12	1:C:189:LEU:HA	0.96	0.41
1:C:194:ALA:HB3	1:C:202:LEU:HD22	2.03	0.41
2:D:225:TYR:O	2:D:226:LYS:HB2	2.20	0.41
1:A:259:GLY:CA	1:A:285:PHE:CD1	3.04	0.40
2:B:226:LYS:HB2	2:B:226:LYS:HE2	1.79	0.40
2:B:332:LEU:HD23	2:B:363:ALA:CA	2.49	0.40
2:B:341:LEU:HA	2:B:341:LEU:HD23	1.78	0.40
1:A:105:LYS:HG2	1:A:289:VAL:HG23	2.04	0.40
1:A:216:PHE:O	1:A:220:GLY:CA	2.69	0.40
1:A:86:ASP:OD2	1:A:89:LYS:HD3	2.21	0.40
2:B:221:VAL:HG12	2:B:221:VAL:O	2.16	0.40
1:C:64:VAL:CG2	1:C:144:ALA:CB	2.99	0.40
1:A:106:SER:O	1:A:110:GLN:HG3	2.20	0.40
1:A:166:LEU:C	1:A:168:TYR:N	2.74	0.40
2:B:273:PRO:HB2	2:B:278:PHE:HE2	1.80	0.40
2:B:331:SER:HB3	2:B:421:VAL:HG11	1.97	0.40
1:C:10:ILE:HD13	1:C:20:LYS:CB	2.44	0.40
2:D:335:PHE:HB2	2:D:413:TYR:CG	2.53	0.40
1:C:229:GLY:O	1:C:230:VAL:O	2.39	0.40
1:C:242:LYS:HA	1:C:242:LYS:HD3	1.87	0.40
2:D:218:LEU:HD23	2:D:218:LEU:HA	1.85	0.40
2:D:291:VAL:O	2:D:291:VAL:HG12	2.20	0.40
2:D:403:GLN:O	2:D:404:HIS:C	2.60	0.40
2:D:415:ASN:HD21	2:D:417:LYS:HG2	1.87	0.40
2:D:388:LYS:HD3	2:D:432:LEU:HB3	2.04	0.40
1:A:141:ILE:O	1:A:141:ILE:HG23	2.22	0.40
1:A:221:THR:CG2	1:A:222:PRO:HD2	2.51	0.40
1:A:262:LEU:O	1:A:263:LEU:C	2.58	0.40
2:B:268:GLU:CG	2:B:268:GLU:O	2.69	0.40
1:C:13:GLY:O	1:C:16:GLY:HA3	2.21	0.40
1:C:248:PHE:HE2	1:C:263:LEU:HB3	1.86	0.40
1:C:88:LYS:HD3	1:C:88:LYS:O	2.22	0.40
2:D:241:ARG:O	2:D:244:SER:HB2	2.22	0.40
2:D:255:LEU:HG	2:D:294:MET:HG2	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:431:ASN:ND2	1:C:210:ASP:OD1[2_664]	1.73	0.47

## 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	294/298 (99%)	226 (77%)	51 (17%)	17 (6%)	2	6
1	C	295/298 (99%)	231 (78%)	44 (15%)	20 (7%)	1	4
2	B	256/259 (99%)	188 (73%)	45 (18%)	23 (9%)	1	2
2	D	257/259 (99%)	205 (80%)	35 (14%)	17 (7%)	1	4
All	All	1102/1114 (99%)	850 (77%)	175 (16%)	77 (7%)	1	3

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	TYR
1	A	36	ARG
1	A	165	THR
1	A	230	VAL
2	B	176	PRO
2	B	304	PHE
2	B	345	ASP
2	B	420	GLY
2	B	421	VAL
2	B	424	LEU
1	C	17	VAL
1	C	30	VAL
1	C	39	THR
1	C	41	THR
1	C	110	GLN
1	C	120	SER
1	C	160	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	215	ILE
1	C	230	VAL
1	C	231	THR
1	C	269	TYR
2	D	284	ASP
2	D	304	PHE
2	D	337	GLY
2	D	424	LEU
1	A	153	GLY
1	A	190	GLY
2	B	284	ASP
2	B	337	GLY
2	B	339	LEU
2	B	341	LEU
2	B	346	PRO
2	B	355	ILE
2	B	357	GLY
2	B	369	GLY
1	C	167	TRP
2	D	181[A]	ASP
2	D	181[B]	ASP
2	D	386	SER
2	D	408	SER
2	D	421	VAL
1	A	96	LEU
1	A	196	MET
1	A	201	ALA
1	A	291	LYS
2	B	326	ASN
2	B	356	ALA
1	C	239	SER
2	D	176	PRO
2	D	325	ALA
2	D	385	GLU
2	D	404	HIS
1	A	14	THR
1	A	162	GLU
1	A	278	LYS
2	B	250	ARG
2	B	336	LEU
2	B	354	VAL
1	C	227	TRP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	346	PRO
1	A	101	LEU
1	A	167	TRP
2	B	364	LEU
2	B	401	ALA
1	C	164	VAL
2	D	392	MET
1	A	60	HIS
1	A	88	LYS
2	B	427	PRO
1	C	162	GLU
1	C	234	PRO
2	D	357	GLY
1	C	153	GLY
1	C	270	ASP
2	D	426	PRO
2	B	197	VAL
1	C	184	VAL

### 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	261/263 (99%)	196 (75%)	65 (25%)	1	2
1	C	262/263 (100%)	188 (72%)	74 (28%)	0	1
2	B	232/233 (100%)	186 (80%)	46 (20%)	1	5
2	D	233/233 (100%)	187 (80%)	46 (20%)	1	5
All	All	988/992 (100%)	757 (77%)	231 (23%)	1	2

All (231) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	10	ILE
1	A	14	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	17	VAL
1	A	20	LYS
1	A	22	ARG
1	A	23	ASN
1	A	34	LYS
1	A	35	ILE
1	A	36	ARG
1	A	38	ASP
1	A	39	THR
1	A	40	GLU
1	A	42	GLU
1	A	53	SER
1	A	55	LEU
1	A	56	LYS
1	A	64	VAL
1	A	65	LYS
1	A	74	ASN
1	A	75	LYS
1	A	76	LEU
1	A	84	HIS
1	A	89	LYS
1	A	94	SER
1	A	96	LEU
1	A	97	THR
1	A	101	LEU
1	A	103	LEU
1	A	104	ILE
1	A	115	LEU
1	A	122	ARG
1	A	124	LEU
1	A	126	ARG
1	A	131	GLN
1	A	141	ILE
1	A	158	THR
1	A	159	TYR
1	A	162	GLU
1	A	177	CYS
1	A	179	TYR
1	A	184	VAL
1	A	186	ILE
1	A	189	LEU
1	A	192	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	193	PHE
1	A	196	MET
1	A	200	ARG
1	A	202	LEU
1	A	208	GLU
1	A	209	ILE
1	A	218	THR
1	A	230	VAL
1	A	231	THR
1	A	242	LYS
1	A	245	ARG
1	A	246	GLN
1	A	248	PHE
1	A	251	VAL
1	A	253	PRO
1	A	258	ASP
1	A	264	SER
1	A	289	VAL
1	A	291	LYS
1	A	296	LEU
2	B	175	VAL
2	B	177	ASP
2	B	179	HIS
2	B	182	ILE
2	B	190	GLU
2	B	192	LYS
2	B	194	LYS
2	B	196	LYS
2	B	199	TYR
2	B	201	LYS
2	B	207	THR
2	B	224	GLU
2	B	227	LEU
2	B	241	ARG
2	B	244	SER
2	B	249	LEU
2	B	250	ARG
2	B	254	GLN
2	B	265	SER
2	B	279	VAL
2	B	285	THR
2	B	288	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	289	LYS
2	B	292	LEU
2	B	294	MET
2	B	297	LEU
2	B	302	LEU
2	B	323	GLN
2	B	326	ASN
2	B	348	LEU
2	B	371	SER
2	B	374	GLU
2	B	375	SER
2	B	379	LYS
2	B	383	THR
2	B	391	LEU
2	B	392	MET
2	B	400	LYS
2	B	403	GLN
2	B	408	SER
2	B	415	ASN
2	B	425	ASN
2	B	427	PRO
2	B	428	GLU
2	B	429	THR
2	B	432	LEU
1	C	2	GLU
1	C	3	ASN
1	C	5	GLN
1	C	6	LYS
1	C	8	GLU
1	C	9	LYS
1	C	10	ILE
1	C	12	GLU
1	C	15	TYR
1	C	20	LYS
1	C	33	LYS
1	C	34	LYS
1	C	37	LEU
1	C	38	ASP
1	C	39	THR
1	C	41	THR
1	C	55	LEU
1	C	60	HIS

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	64	VAL
1	C	71	HIS
1	C	72	THR
1	C	75	LYS
1	C	83	LEU
1	C	85	GLN
1	C	86	ASP
1	C	87	LEU
1	C	88	LYS
1	C	89	LYS
1	C	91	MET
1	C	97	THR
1	C	101	LEU
1	C	105	LYS
1	C	111	LEU
1	C	115	LEU
1	C	120	SER
1	C	122	ARG
1	C	129	LYS
1	C	131	GLN
1	C	138	GLU
1	C	141	ILE
1	C	154	VAL
1	C	157	ARG
1	C	158	THR
1	C	160	THR
1	C	162	GLU
1	C	163	VAL
1	C	165	THR
1	C	173	ILE
1	C	177	CYS
1	C	178	LYS
1	C	184	VAL
1	C	189	LEU
1	C	199	ARG
1	C	200	ARG
1	C	207	SER
1	C	208	GLU
1	C	209	ILE
1	C	214	ARG
1	C	217	ARG
1	C	225	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	226	VAL
1	C	230	VAL
1	C	239	SER
1	C	240	PHE
1	C	242	LYS
1	C	245	ARG
1	C	248	PHE
1	C	264	SER
1	C	268[A]	HIS
1	C	268[B]	HIS
1	C	278	LYS
1	C	291	LYS
1	C	293	VAL
1	C	296	LEU
2	D	175	VAL
2	D	178	TYR
2	D	179	HIS
2	D	182	ILE
2	D	189	MET
2	D	196	LYS
2	D	197	VAL
2	D	199	TYR
2	D	200	MET
2	D	201	LYS
2	D	202	LYS
2	D	213	ILE
2	D	223	GLU
2	D	226	LYS
2	D	232	LEU
2	D	239	ILE
2	D	244	SER
2	D	245	SER
2	D	249	LEU
2	D	261	MET
2	D	265	SER
2	D	273	PRO
2	D	283	ASP
2	D	284	ASP
2	D	289	LYS
2	D	293	ARG
2	D	321	HIS
2	D	323	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	328	LYS
2	D	332	LEU
2	D	345	ASP
2	D	348	LEU
2	D	364	LEU
2	D	370	GLN
2	D	378	ARG
2	D	383	THR
2	D	391	LEU
2	D	392	MET
2	D	396	GLN
2	D	403	GLN
2	D	406	GLN
2	D	415	ASN
2	D	423	LEU
2	D	424	LEU
2	D	428	GLU
2	D	429	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	84	HIS
1	A	113	GLN
2	B	208	ASN
2	B	313	GLN
2	B	404	HIS
2	B	431	ASN
1	C	59	ASN
1	C	60	HIS
1	C	84	HIS
1	C	85	GLN
1	C	131	GLN
1	C	161	HIS
2	D	208	ASN
2	D	229	ASN
2	D	321	HIS
2	D	322	GLN
2	D	370	GLN
2	D	396	GLN
2	D	403	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	404	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	MTW	A	1297	-	26,31,31	3.33	5 (19%)	29,42,42	2.11	6 (20%)
3	MTW	C	1297	-	26,31,31	3.21	6 (23%)	29,42,42	2.27	13 (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
3	MTW	A	1297	-	-	0/14/26/26	0/3/4/4
3	MTW	C	1297	-	-	0/14/26/26	0/3/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1297	MTW	N2-N	-8.08	1.23	1.35
3	C	1297	MTW	N2-N	-7.49	1.24	1.35
3	C	1297	MTW	C15-N6	-6.63	1.32	1.45
3	A	1297	MTW	C15-N6	-5.38	1.35	1.45
3	C	1297	MTW	C11-N5	-5.13	1.34	1.42
3	A	1297	MTW	C11-N5	-4.70	1.34	1.42
3	A	1297	MTW	C5-C7	-4.00	1.39	1.48
3	C	1297	MTW	C5-C7	-2.92	1.41	1.48
3	C	1297	MTW	C2-C3	2.02	1.56	1.51
3	C	1297	MTW	O1-N6	10.91	1.42	1.22
3	A	1297	MTW	O1-N6	12.19	1.45	1.22

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1297	MTW	N1-C-N	-6.13	104.38	112.04
3	C	1297	MTW	C6-C5-C4	-3.99	114.55	119.23
3	C	1297	MTW	N1-C-N	-3.18	108.06	112.04
3	A	1297	MTW	C6-C5-C7	-2.70	117.38	120.84
3	C	1297	MTW	C18-C17-C3	-2.44	116.92	120.64
3	C	1297	MTW	C11-N5-C10	2.00	126.86	121.08
3	C	1297	MTW	C6-C18-C17	2.09	123.18	120.24
3	C	1297	MTW	C4-C5-C7	2.13	125.75	120.87
3	C	1297	MTW	C2-C3-C4	2.36	123.96	120.23
3	C	1297	MTW	C16-C15-C14	2.51	123.32	120.08
3	C	1297	MTW	C5-C4-C3	2.54	124.71	120.86
3	A	1297	MTW	O1-N6-C15	2.76	123.20	118.80
3	C	1297	MTW	C3-C2-N	3.03	116.62	112.17
3	A	1297	MTW	C14-C15-N6	3.46	121.77	118.81
3	A	1297	MTW	C15-C14-C11	3.50	121.30	118.55
3	C	1297	MTW	C9-C8-C7	3.77	121.45	112.22
3	C	1297	MTW	C-N1-C1	4.07	106.25	102.34
3	C	1297	MTW	C5-C7-N3	4.84	124.41	118.08
3	A	1297	MTW	C-N1-C1	5.06	107.20	102.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1297	MTW	6	0
3	C	1297	MTW	13	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	296/298 (99%)	-0.47	5 (1%) 70 68	12, 32, 66, 93	1 (0%)
1	C	296/298 (99%)	-0.41	10 (3%) 46 39	11, 32, 69, 95	0
2	B	258/259 (99%)	-0.52	4 (1%) 72 70	6, 33, 60, 85	0
2	D	258/259 (99%)	-0.50	2 (0%) 86 85	8, 33, 59, 86	0
All	All	1108/1114 (99%)	-0.47	21 (1%) 67 64	6, 32, 63, 95	1 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	39	THR	4.8
1	C	13	GLY	4.6
2	B	176	PRO	3.9
1	C	15	TYR	3.8
1	C	73	GLU	3.7
1	C	40	GLU	3.6
2	B	323	GLN	3.4
1	C	14	THR	3.4
2	D	175	VAL	3.2
1	C	165	THR	3.1
1	A	73	GLU	2.8
1	A	96	LEU	2.7
1	C	163	VAL	2.5
2	D	176	PRO	2.5
1	A	15	TYR	2.4
2	B	175	VAL	2.3
2	B	177	ASP	2.2
1	A	97	THR	2.2
1	C	295	HIS	2.2
1	A	13	GLY	2.1
1	C	164	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 [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<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( $\text{\AA}^2$ )	Q<0.9
3	MTW	C	1297	28/28	0.87	0.26	1.19	40,79,105,116	0
3	MTW	A	1297	28/28	0.93	0.18	0.29	27,65,91,94	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.